Robert Martin · Jean-Pierre Buisson

Aromatic Hydroxyketones: Preparation & Physical Properties

Aromatic Hydroxyketones from Butanone (C4) to Dotriacontanone (C32)

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Dr Martin wrote this book with Dr Buisson further to their cooperation while at Institut Curie, Paris, France, and could complete it a few months before passing away.

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This book is dedicated to Canon Joseph Clerc priest at Montmorot (Jura, France, 1899–1985) who in 1944 gave a home to the Martin brothers, young Parisian refugees.

Robert Martin

Foreword

Two centuries of organic chemistry have already yielded millions of molecules, either synthesized or isolated as natural products created by biosynthesis, but much still remains to be done. Therefore, from time to time, it is probably useful to gather and classify the scattered data concerning this or that class of compounds in order to save time for chemists planning new syntheses or natural products isolations.

In this work, special effort has been made to select material suitable to meet the needs of chemists who do not benefit from unlimited time for specialized research in the field of hydroxyketones.

These compounds are precursors of substituted aromatic derivatives which are often not straightforwardly obtained but have many potential applications in fine and medicinal chemistry.

In this book, *Aromatic Hydroxyketones, Preparation and Physical Properties* the reader will find more than 5,200 hydroxyketones from butanone C_4 to dotriacontanone C_{32}.

This work will primarily be of great value to professional chemists, from physicists to pharmacists, who are often called upon to solve problems about the synthesis of this kind of aromatic compounds.

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Jean-Claude Florent

Preface

Aromatic hydroxyketones are widely used as starting materials in organic synthesis to obtain medicines, dyes, perfumes, etc., and many of them have also specific uses.

This Handbook contains information on aromatic hydroxyketones from C_4 to C_{32}, collecting more than 5,200 ketones of which an indicated preparation as well as their physicochemical and spectrochemical data are presented.

This book is presented in dictionary style, with a logical classification of the ketones, which makes the information easily available for consultation. Ketones are classified methodically. They are easily accessible to the reader from three tables provided at the end of the book:

- The molecular formula index
- The Chemical Abstracts Registry Numbers
- The usual names index

Since hydroxyketones are widely utilized, themselves or as intermediates, in numerous interesting syntheses, among others, pharmaceuticals, dyes, agrochemicals, perfumes and plastic preservatives, this handbook will be of great value for both academic and industrial research chemists. The multiple ways of hydroxybenzophenones syntheses herein described will certainly help chemists, as most of these methods can be applied to prepare analogues in aromatic and even in some heterocyclic series.

This compilation will supply helpful and easy-to-read informations for the organic chemist.

Antony, France — Robert Martin
Sartrouville, France — Jean-Pierre Buisson

Acknowledgements

I wish to express my heartily thanks to Dr. Pierre Demerseman who accepted me in his laboratory at Institut Curie in 1987.

My thanks are also directed to Prof. Claude Monneret, Head of the Chemical Department at Institut Curie, who has always been so benevolent to me, and all his collaborators for their warm welcome at each of my visits.

I thank my son Serge Martin for friendly advice on the English edition of this book. Moreover, Mr. Serge Martin was a constant aid to me as regards data processing.

The author also thanks Prof. Jean Paul Guetté for all his good advices.

Various friends who readily accepted to translate foreign publications are also to be acknowledged here, in particular Dr. Jean Burkhard who has been of invaluable help for translating German papers over the last 30 years. The diverse abbreviations used in ancient reviews – particularly *Chemisches Zentralblatt* – had no secrets for him.

In this connection, thanks are due to Mrs. Feiga Weisbuch for her precious assistance as regards Rumanian and Russian texts, as well as Dr. Daniel Dauzonne. I wish to express my thanks to Mrs. Mireille Guyonneau, Mrs. Elisabeth Matarasso, Mrs. Françoise Rémy and Mrs. Simonne Rissé for their keen contribution to my bibliographic research, as well as the Orsay University Library for their helpful kindness towards me for 30 years now.

I am also grateful to Mrs. Colette Ledoux for judicious advice in the field of scientific edition.

Before closing, I would like to remember my dear departed. My affectionate thoughts are turned towards Prof. Léon Denivelle who transmitted to me his passion for aromatic organic chemistry in 1945, and Prof. Albert Kirrmann who accepted me among his students in 1961 and was always so amiable and well-disposed whenever I went to him. I cannot mention without emotion Prof. Albert Saint-Maixen who largely communicated to me his knowledge on analytical chemistry.

I also have a personal thought towards my friends from the industry who left us too soon. I am particularly thankful to Drs. Henri Barbier, Félix Lepors and Henri

Ruelleux (SPCA, Ltd.) who gave me the practical means to carry about my work on aromatic hydroxyketones. In this firm, I started my research on Fries reaction. I also wish to acknowledge the late Dr. François Krausz who, at that time, made me benefit from his precious advice.

Robert Martin

Contents of Volume I

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Short Biography

Robert Martin graduated as engineer from CNAM, then as doctor-engineer and doctor es-sciences (Ph. D.) from Paris University. He studied with Professors Léon Denivelle and Albert Kirrmann.

After having worked in the pharmaceutical industry, Robert Martin completed his career of organic chemist at a Research Laboratory of the French CNRS, located in the Curie Institute in Paris.

He has been studying Fries reaction since 1956 without interruption. He prepared a considerable number of aromatic hydroxyketones. A large part of these are included in the reference NMR and IR spectra collection of SADTLER (Philadelphia, USA).

His research on aromatic hydroxyketones gave rise to about 40 publications between 1963 and 1992, some of them in collaboration with Mainz University (Germany) and others with Institut Curie (Paris).

In 1992, he published a review on Fries reaction in the *Organic Preparations and Procedures International*. This was followed by the publishing of two books dealing with aromatic hydroxyketones, published by KLUWER in 1997 and 2000.

For his various works concerning aromatic hydroxyketones he received the silver gilt medal from "Société d'Encouragement à l'Industrie Nationale" in 1985.

Jean-Pierre Buissson is also doctor es-science (Ph.D.) from Paris University. The subject of his thesis was "Phenolic ether desalcoylation with pyridinium hydrochloride".

Chemist at the CNRS, he worked all his career in the chemistry lab of the Institut Curie in Paris with, successively, Drs. Royer, Demerseman, Monneret and Florent.

His research concerns the synthesis of heterocyclic compounds in the benzofuran, naphthofuran and oxaphenalene series.

The major product obtained was the R7000, the most mutagenic compound on bacterial strains, which is now an international reference for biologists.

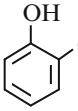
Chapter 1
Butanones: Monoketones

1 Aromatic Hydroxyketones Derived from 1-Butanoic Acid

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-1-butanone

[2887-61-8] $C_{10}H_{12}O_2$ mol. wt. 164.20



Syntheses

-Phenol was energetically mixed with finely divided aluminium chloride (1 mol) and heated to 100° for 30 min (1 mol of hydrochloric acid is evolved); 1 mol of n-butyryl chloride was then added and heated to 125–130° for 1 h (45 %) [2700].

-Also obtained by Fries rearrangement of phenyl butyrate with aluminium chloride,
*without solvent [3382], at 150° [2045], at 160–180° for 2 h (60 %) [726];
*in nitrobenzene at 50° for 18 h (18 %) [776];
*in tetrachloroethane at 95° for 6 h (50 %) [244] or at 70–80° for 7 h [3169];
*in heptane at 80–90° for 6 h (40 %) [244];
*in durene at reflux for 3 h (54 %) [1303].
-Also obtained by Fries rearrangement of phenyl butyrate,
*in the presence of polyphosphoric acid for 10 min at 100° (13 %) [2238];
*in the presence of zirconium halides or hafnium halides in o-dichlorobenzene over 3 h at 120° (85 %) [2096].
-Also obtained by photo-Fries rearrangement of phenyl butyrate in cyclohexane, heptane, benzene or n-amyl alcohol in a sealed tube with an unfiltered Hanovia 450 w medium pressure lamp [2067].
-Also obtained by diazotization of 2-aminobutyrophenone [2147].

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-Also obtained by treatment of 1-(2-hydroxyphenyl)-1-butanol with manganese dioxide in methylene chloride for 7 h at r.t. (46 %) [77].
-Also refer to: [173, 375, 932 (36 %), 970, 1078, 1172–1174, 1572, 1620, 2081, 2120–2124, 2848, 2920, 3028, 3477].

Isolation from natural sources

-Detection of the gel of *Aloe vera* (L.) burm. [1624].

colourless oil [77]; pale yellow, viscous liquid [2147].
$b.p._{\cdot 0.1}$ 64° [932], $b.p._{\cdot 0.01}$ 67–68° [3318], $b.p._{\cdot 5}$ 91–98° [2314], $b.p._{\cdot 9}$ 119° [2700], $b.p._{\cdot 14}$ 124–126° [726], $b.p._{\cdot 18}$ 129° [3169], $b.p._{\cdot 19}$ 130–132° [1762], $b.p._{\cdot 12}$ 135–138° [3477];
m.p. 10.5–10.6° [2700], 10–11° [3318], 8° [726];
^{1}H NMR [77, 2067], ^{13}C NMR [77], IR [77, 1762, 2067], UV [1996, 2067], MS [77, 173, 2067]; ESR [2940];
TLC [1994]; paper chromatography [1183]; GLC [2067]; GC [2067].
$n_D^{20.5} = 1.539$ [3318], $n_D^{20} = 1.5379$ [932].

N.B.: Photodegradation of o-(1-butanoyl)phenol in waste water [1385].

USE: Fungicide [547, 2044, 2045]; Hair dyes and method for highlighting or streaking hair [2785]; Oxidative hair dyes containing diazolium and triazolium compounds in combination with reactive carbonyl compounds [1301].

Oxime [21667-43-6] $C_{10}H_{13}NO_2$ mol. wt. 179.22

-Refer to: [603].

2,4-Dinitrophenylhydrazone $C_{16}H_{16}N_4O_5$ mol. wt. 344.33

m.p. 203° [932, 3169].

Acetate [21550-10-7] $C_{12}H_{14}O_3$ mol. wt. 206.24

-Refer to: [2493]; UV [2493].

Benzoate $C_{17}H_{16}O_3$ mol. wt. 268.31

m.p. 65–66° [3477].

Methyl ether [13404-83-6] $C_{11}H_{14}O_2$ mol. wt. 178.23

-Obtained by reaction of dimethyl sulfate with 2-butyrylphenol in the presence of aqueous sodium hydroxide for 4 h at reflux [2478].
-Also refer to: [1084, 2300 (72 %), 2493].

$b.p._{\cdot 0.8}$ 83° [2478], $b.p._{\cdot 17}$ 146° [2300];
^{1}H NMR [2848], UV [2493], MS [42];
Phosphorescence spectroscopy [2493].

Semicarbazone of the methyl ether $C_{12}H_{17}N_3O_2$ mol. wt. 235.29

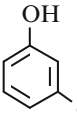
m.p. 146° [2300].

Phenylhydrazone $C_{16}H_{18}N_2O$ mol. wt. 254.33

m.p. 85–87° [726].

1-(3-Hydroxyphenyl)-1-butanone

[103323-29-1] $C_{10}H_{12}O_2$ mol. wt. 164.20



Syntheses

-Synthesis of 3-hydroxybutyrophenone by means of organocadmium derivatives (75 %) [2586].

-Preparation by diazotization of 3-aminobutyrophenone and hydrolysis of the obtained diazonium salt [3002], (97–98 %) [2147].

-Also refer to: [1614, 1618, 1822, 2125].

b.p.$_2$ 155–157° [2586]; m.p. 64.5° [3002], 63° [2147, 2586];
^{1}H NMR [1614, 1618].

p-Nitrophenylhydrazone $C_{16}H_{17}N_3O_3$ mol. wt. 299.33

orange-yellow needles [2147]; m.p. 160° [2147].

Acetate [21999-97-3] $C_{12}H_{14}O_3$ mol. wt. 206.24

b.p.$_1$ 116–118° [2586]; UV [2493].

Methyl ether [21550-06-1] $C_{11}H_{14}O_2$ mol. wt. 178.23

-Obtained by hydrolysis of m-methoxybenzoylethylketene, itself prepared from ethylketene dimethylacetal and m-benzoyl chloride at reflux for 5 h (83 %) [2028].

-Also obtained by reaction of m-benzoyl chloride with dipropylcadmium (78 %) [571].

-Also refer to: [73, 1614, 1618, 2493].

N.B.: Regioselective directed *meta*-acylation of aromatic compounds *via* cycloaddition of nitriles to benzyne-zirconocene complexes [73].

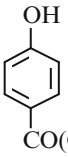
b.p.$_2$ 105–110° [571], b.p.$_{10}$ 121° [3002], b.p$_{11}$ 142–146° [2028],
b.p. 265–270° [1067];
^{1}H NMR [73, 1618], ^{13}C NMR [73], IR [73], UV [2493], MS [73];
Phosphorescence spectroscopy [2493].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{17}H_{18}N_4O_5$ mol. wt. 358.35

m.p. 172–173° [2028].

1-(4-Hydroxyphenyl)-1-butanone

[1009-11-6] $C_{10}H_{12}O_2$ mol. wt. 164.20



Syntheses

-Phenol was energetically mixed with finely divided aluminium chloride (1 mol) and heated to 100° (1 mol of hydrochloric acid is evolved); 1 mol of n-butyryl chloride was then added and heated to 125–130° for 1 h (50 %) [2700].

-Also obtained by reaction of butyryl chloride,
*with phenol in the presence of aluminium chloride in nitrobenzene first at 5–10°, then at r.t. for some hours (76 %) [2970] or at r.t. overnight (67 %) [1769];
*with phenol in the presence of aluminium chloride in methylene chloride for 1 h at 0°, then at r.t. overnight (80 %) [114] or for 14 h at r.t. (43 %) [1910];
*with anisole in the presence of aluminium chloride in nitrobenzene [2923].
-Also obtained by Fries rearrangement of phenyl butyrate with aluminium chloride,
*without solvent [3382], at 150° [2045], for 2 h at 160–180° (19 %) [726];
*in nitrobenzene [2923], [2947] (66 %), for 18 h at 50° (72 %) [776];
*in tetrachloroethane at 95° for 6 h (43 %) [244] or at 70–80° for 7 h [3169];
*in heptane at 80–90° for 6 h (50 %) [244];
*in durene at reflux for 3 h (14 %) [1303].
-Also obtained by Fries rearrangement of phenyl butyrate,
*in the presence of polyphosphoric acid for 10 min at 100° (45 %) [2238];
*in the presence of boron trifluoride for 3 h at 70–75° (65.2 %) [1938].
-Also obtained by photo-Fries rearrangement of phenyl butyrate in cyclohexane, heptane, benzene or n-amyl alcohol in a sealed tube with an unfiltered Hanovia 450 w medium pressure lamp [2067].
-Also obtained by reaction of butyric acid with phenol,
*in the presence of boron trifluoride [511], for 2 h at 70° (81 %) [1685];
*in the presence of polyphosphoric acid for 5 min in a boiling water bath (54 %) [2240] or for 10 min at 100° (76 %) [2238].
-Also obtained by reaction of butyronitrile with phenol in the presence of triflic acid, first 15 days at r.t., then 1 h at reflux (78 %) [425].
-Also obtained by treatment of its methyl ether with boiling pyridinium chloride for 15 min (70 %) [221].
-Also obtained by anaerobic co-metabolic oxidation of 4-butylphenol by *Thauera* sp. strain R5 [2861].
-Also obtained by anaerobic biodegradation of 4-butylphenol in Kamajima paddy soil microcosm supplemented with nitrate [2862].
-Also refer to: [62, 131, 254, 274, 494, 513, 556, 597, 663, 664, 932 (34 %), 1070, 1087, 1510, 1531, 1615, 1616, 1620, 1650, 1651, 1791, 1792, 1805, 1872, 2031, 2032, 2125, 2457, 2711, 2772, 2943, 3418, 3452, 3454, 3471, 3477 (14 %)].

b.p.$_{0.01}$ 144–152° [2970], b.p.$_{1}$ 171° [932], b.p.$_{5.3}$ 171–174° [1769], b.p.$_{9}$ 187–188° [2700], b.p.$_{15}$ 192–200° [2947], b.p.$_{15}$ 200° [726];

white solid [1910];
m.p. 99.6–100° [1910], 93.5° [1685], 92° [2240], 91.5–92.5° [3169], 91–92° [3477], 91–91.5° [2700], 91° [726, 776, 932, 2457], 90.5–92° [425], 90.5–91.5° [1938], 89–90° [2238], 86–89° [1769];
^{1}H NMR [114, 425, 1910, 2067], ^{13}C NMR [114, 1910], IR [425, 1910, 2067], UV [1995, 2067], MS [425, 1910, 2067, 2861, 2862];
X-ray data [3347]; GC/MS [3131]; paper chromatography [1183];
GLC [2067]; GC [2067]; TLC [1910, 1994].

Isolation from natural sources

-From essential oil extracted from fruit of *Zanthoxylum rhetsa* (Roxb.) DC. in Vietnam (6.07 %) [3131].

N.B.: Photodegradation of p-(1-butanoyl)phenol in waste water [1385].

USE: Preparation of 3-phenylpropanoic acids derivatives as antidiabetic agents [3397].

BIOLOGICAL ACTIVITY: Inhibition of 17-β hydroxysteroid dehydrogenase 3 [1910].

-Also refer to: [597, 1510].

Oxime $C_{10}H_{13}NO_2$ mol. wt. 179.22

m.p. 83–84° [3477].

Semicarbazone $C_{11}H_{15}N_3O_2$ mol. wt. 221.26

m.p. 167–169° [3477].

2,4-Dinitrophenylhydrazone $C_{16}H_{16}N_4O_5$ mol. wt. 344.33

m.p. 217° [3169], 215° [932].

O-Ethyloxime [791065-70-8] $C_{12}H_{17}NO_2$ mol. wt. 207.27

-Refer to: [638].

Acetate [13210-98-5] $C_{12}H_{14}O_3$ mol. wt. 206.24

-Refer to: [2493]. UV [2493].

Benzoate $C_{17}H_{16}O_3$ mol. wt. 268.31

m.p. 107–107.5° [2700], 106–107° [726, 3477]; GC [1922] GC/MS [1244].

Sulfate [114] (87 %); ^{1}H NMR [114], ^{13}C NMR [114].

Benzyl ether [26945-71-1] $C_{17}H_{18}O_2$ mol. wt. 254.33

-Preparation by reaction of benzyl chloride with p-hydroxybutyrophenone in the presence of potassium carbonate and potassium iodide in refluxing 90 % ethanol for 5 h (86 %) [556].
-Also refer to: [147, 673, 2480, 2958].

m.p. 67° [556], 63–65° [147, 673], 59–64° [2958].

Methyl ether [4160-51-4] $C_{11}H_{14}O_2$ mol. wt. 178.23

Syntheses

-Preparation by reaction of n-butyryl chloride with anisole,
*in the presence of aluminium chloride in carbon disulfide, first at 0° for 2 h, then between 10 and 25° for 3 h (81 %) [3062];
*in the presence of aluminium chloride in 1,2-dichloroethane [2942], first at 0° for 40 min, then at r.t. for 8–15 h (65 %) [2243];
*in the presence of titanium tetrachloride at 60° for 3 h (89 %) [777];
*in the presence of cobalt (II) acetylacetonate in nitromethane and acetonitrile under mild conditions (excellent yields) [3055];
*in the presence of Si-Fe catalyst at 25° (49 %) [427];
*using moisture insensitive $InCl_3$ impregnated mesoporous Si-MCM-41 catalyst in dichloroethane at 80° for 3 h (87 %) [658];
*over Ga_2O_3 (20 %)/Si-MCM-41 catalyst in dichloroethane at 80° for 3 h (77 %) [657].
-Also obtained by Friedel-Crafts reaction of butyric anhydride with anisole in a chlorobenzene/GALDEN SV 135 mixture at 90° for 1 h,
*in the presence of $Hf[N(SO_2C_8F_{17})_2]_4$ (71–73 %) [1243];
*in the presence of $Hf(OSO_2CF_3)_4$ (44 %) [1243].
-Also obtained by Friedel-Crafts reaction of butyric anhydride with anisole,
*in the presence of large molecular sizes on mesoporous silica catalyst at 453 K for 4 h (82 %) [1466];
*in the presence of $Hf[N(SO_2C_8H_{17})_2]_4$ at 90° for 1 h (88 %) or with $Hf(OSO_2CF_3)_4$ in the same conditions (57 %) [1244];
*in the presence of microcrystalline beta zeolite-II for 3 h at 130° under argon (98 %) [1594].
-Also obtained by acylation of anisole with butyric acid,
*over the HPNbW-WO_3-Nb_2O_5 catalyst at 428 K for 3 h (98 %) [2332];
*on the solid surface of alumina in the presence of trifluoroacetic anhydride for 20 min at r.t. (92 %) [2563];
*over HZSM-5 catalyst for 48 h at 423° K (31 %) [3265];
*in the presence of polyphosphoric acid for 1.5 h at 80° (91 %) [869].
-Also obtained by direct acylation of 4-bromoanisole with butyraldehyde by palladium catalysis (81 %) [2668].
-Also obtained by cross coupling reaction of butyryl chloride with $(4\text{-}CH_3OC_6H_5)_3Bi$ in the presence of Pd(o) as catalyst (65 %) [2565].

-Also obtained by 4-methoxyphenylboronic acid coupling with the benchmark electron-rich olefin n-butyl vinyl ether catalyzed by Pd-dppp (91 %) [2667].
-Also obtained by reaction of butyraldehyde N-tert-butylhydrazone with 4-bromoanisole in the presence of $Pd_2(dba)_3$, DPEphos and NaOtBu in dioxane at 80° for 24 h (94 %) [3042].
-Also obtained in two steps by reaction of p-anisaldehyde with propylmagnesium bromide followed by pyridinium chlorochromate oxydation (46–54 %) [2557].
-Also obtained by oxidation of 1-p-methoxyphenyl-1-butanol with CrO_3 [2924].
-Also obtained by reaction of butyronitrile with anisole in the presence of triflic acid, first 14 days at r.t., then 1 h at reflux (40 %) [425].
-Also obtained by reaction of butyric acid with anisole in the presence of $Cs_{2.5}H_{0.5}PW_{12}O_{40}$ at 110° for 5 h (59 %) [1636].
-Also obtained by irradiation of mixture cyclopropyl 4-methoxyphenyl ketone and trichlorosilane at 23° (87 %) [957].
-Also obtained (low yield) by isomerization of 1-(4-methoxyphenyl)-3-buten-1-ol under the catalysis of $RuCl_2(PPh_3)_3$ in water for 1.5 h at 90–100° [3261].
-Also refer to: [131, 221, 251, 698 (60 %), 864, 895 (68 %), 1009, 1114, 1398, 1489, 1897 (58 %), 2166, 2279, 2292, 2493, 2840, 2901, 3000, 3001, 3015, 3254, 3412, 3472].

Isolation from natural sources

-Of essential oil of in Ocimum basilicum from *Guangxi* [1922].
-In leaf oil of *Persea americana* Mill. var. *drymifolia* CV. Duke (Lauraceae) [2488].

pale yellow oil [2243]; viscous oil [2557];
$b.p._{.3}$ 115° [3254], $b.p._{.2}$ 116–120° [3412], b.p. 123° [3062], $b.p._{.0.8}$ 123–124° [869], $b.p._{.10}$ 135–136° [425], $b.p._{.9}$ 144° [2240], $b.p._{.14.5}$ 155° [2924], $b.p._{.20}$ 160° [777], $b.p._{.14}$ 165–167° [2901], b.p. 285–286° [2924];
m.p. 26° [2240, 2901], 23° [2924], 21–22° [251], 21° [777], 20° [425], 19–21° [895], 16° [869];
^{1}H NMR [425, 698, 1244, 2243, 2557, 2563, 2565, 3261],
^{13}C NMR [698, 1244, 2557, 2565],
IR [425, 698, 2563, 2565], UV [869], MS [425, 698, 1922, 2557, 2565, 3254];
TLC [2557]; GC [1922]; GC/MS [1244, 2488].

Oxime of the methyl ether [423115-90-6] $C_{11}H_{15}NO_2$ mol. wt. 193.25

liquid [2924]; m.p. 58° [452].

Semicarbazone of the methyl ether [91646-56-9] $C_{12}H_{17}N_3O_2$ mol. wt. 235.29

m.p. 183° [251], 181° [2924], 179–181° [895], 173.5° [3178], 172–173° [869].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{17}H_{18}N_4O_5$ mol. wt. 358.35

m.p. 165–166° [869].

Ethyl ether [35031-73-3] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Obtained by reaction of butyric acid with phenetole in the presence of aluminium chloride (76 %) [3477].

b.p.$_{.5}$ 116–120° [3435], b.p. 129° [3477], b.p.$_{.14}$ 162–164° [903], b.p.$_{.23}$ 173–174° [1698].

Oxime of the ethyl ether $C_{12}H_{17}NO_2$ mol. wt. 207.27

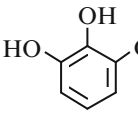
m.p. 103–104° [3477].

Semicarbazone of the ethyl ether [88858-34-8] $C_{13}H_{19}N_3O_2$ mol. wt. 249.31

m.p. 181° [3477].

1-(2,3-Dihydroxyphenyl)-1-butanone

[103324-17-0] $C_{10}H_{12}O_3$ mol. wt. 180.20



Syntheses

-Obtained by treatment of 2,3-dimethoxybutyrophenone with hydriodic acid in refluxing acetic acid (38 %) [199].

-Also obtained by deprotection of its dimethyl ether with boron tribromide in methylene chloride at 0°.
Then, the mixture was stirred overnight at r.t. (91 %) [82].

m.p. 61° [199], 59° [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

USE: Reactant for preparation of lithium gallium/titanium ketone complexes [82].

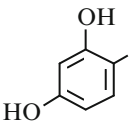
Dimethyl ether [34052-09-0] $C_{12}H_{16}O_3$ mol. wt. 208.26

-Preparation by reaction of propylmagnesium iodide with 2,3-dimethoxybenzaldehyde in ethyl ether, then treated the obtained carbinol with potassium dichromate in dilute sulfuric acid (72 %) [199].
-Also obtained by treatment of 1-(2,3-dimethoxyphenyl)-1-butanol in acetone with potassium dichromate in dilute sulfuric acid (Jones reagent) at r.t. for 3 h (65 %) [82].
-Also prepared from 2,3-dimethoxybenzoyl chloride and di-n-propylcadmium by the general procedure [566], (72 %) [2300].

colourless liquid [199], colourless oil [82];
b.p.$_{0.2}$ 104° [2300], b.p.$_{0.6}$ 112–113° [199];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

1-(2,4-Dihydroxyphenyl)-1-butanone
(Resbutyrophenone)

[4390-92-5] $C_{10}H_{12}O_3$ mol. wt. 180.20



Syntheses
-Obtained by reaction of butyric acid with resorcinol in the presence of,
*fused zinc chloride [2256] at reflux (about 165°) [449, 1128, (76 %) 1527, 2384, (68–78 %) 2501, 2702, 3243];
*boron trifluoride, first at 15°, then at 70° for 2 h (81 %) [643];
*polyphosphoric acid in boiling water bath for 10 min (44 %) [2239];
*cation-exchange resin at 160° for 2–3 h (73.4 %) [2523].
-Also obtained by reaction of butyric anhydride with resorcinol in the presence of cation-exchange resins, sulfonic acid type, Amberlite IR-120 (or Zeokarb) at 160° (82.3 %) [2523].
-Also obtained by reaction of butyronitrile with resorcinol in the presence of,
*trifluoromethanesulfonic acid at r.t. for 14 days (77 %) [425];
*zinc chloride (Hoesch reaction) [1608].
-Also obtained by Fries rearrangement of resorcinol dibutyrate with aluminium chloride (3 mol) at 180–185° for 3 h (20 %) [855].
-Also obtained by reaction of butyryl chloride with resorcinol in the presence of aluminium chloride in nitrobenzene (60 %) [58].
-Also refer to: [22, 385 (57 %), 449, 1024, 1025, 1469, 1508, 2312 (81 %), 2662, 2946].

m.p. 73° [2239], 70° [1608, 2312], 69–70° [1527, 3243], 68–70° [449, 2523], 68° [385, 1469], 65–65.5° [425], 63–65° [1128], 59–60° [58]; ^{1}H NMR [58, 425], ^{13}C NMR [1508], IR [425], MS [425].

BIOLOGICAL ACTIVITY: Bactericide [2662]; Antiseptic and germicidal product [2734]; Anthelmintic [1248]; Toxicity [1248].

Hemihydrate $C_{10}H_{12}O_3$, 0.5 H_2O mol. wt. 189.01

m.p. 51–52° [1608, 3243].

Oxime [22919-59-1] $C_{10}H_{13}NO_3$ mol. wt. 195.22

m.p. 190° [808], 189–190° [1527].

Phenylhydrazone $C_{16}H_{18}N_2O_2$ mol. wt. 270.33

m.p. 191–193° (d) [1128].

2,4-Dinitrophenylhydrazone $C_{16}H_{16}N_4O_6$ mol. wt. 360.33

m.p. 245° [166].

Diacetate $C_{14}H_{16}O_5$ mol. wt. 264.28

-Obtained by reaction of acetic anhydride with resbutyrophenone in the presence of pyridine [2384].

viscous liquid [2384]; b.p. $_{15}$ 170–175° [2384].

Dibenzoate $C_{24}H_{20}O_5$ mol. wt. 388.42

-Obtained by reaction of benzoyl chloride with resbutyrophenone in the presence of pyridine. The mixture was heated on a boiling water bath for 3 h [2384].

oily liquid [2384]; b.p.$_{25}$ 210° [2384].

Dibenzyl ether $C_{24}H_{24}O_3$ mol. wt. 360.45

m.p. 61–62° [2181].

Dimethyl ether [6703-00-0] $C_{12}H_{16}O_3$ mol. wt. 208.26

-Obtained by Friedel-Crafts reaction of butyric anhydride with resorcinol dimethyl ether in the presence of $Hf[N(SO_2C_8H_{17})_2]_4$ in chlorobenzene and SV135 at 70° for 2 h (96 %) [1245].
-Also obtained by Friedel-Crafts reaction of butyryl chloride with resorcinol dimethyl ether,
*in the presence of $Hf[N(SO_2C_8H_{17})_2]_4$ in chlorobenzene and SV135 at 70° for 2 h (94 %) [1245];
*in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].
-Also obtained by reaction of butyronitrile with resorcinol dimethyl ether in the presence of trifluoromethanesulfonic acid at r.t. for 14 days (76 %) [425].
-Also obtained by reaction of butanoic acid with resorcinol dimethyl ether in the presence of polyphosphoric acid and heated on a water bath for 30 min (70 %) [2424].
-Also refer to: [94, 413, 1388].

yellow oil [425];
b.p.$_1$ 140–142° [425], b.p.$_2$ 146–147° [2424], b.p. 156–158° [372];
m.p. 70–71° [57];
^{1}H NMR [425], IR [425], MS [425].

Di(β-D-glucoside) $C_{22}H_{32}O_{12}$ mol. wt. 504.50

-Obtained by treatment of its tetraacetate below with 0.2 M sodium methoxide in methanol for 3 min (30 %) [3243].

$(\alpha)_D^{21} = -109°$ (water) [3243].

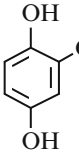
Di(tetraacetyl)-β-D-glucoside $C_{38}H_{48}O_{21}$ mol. wt. 840.80

-Obtained by reaction of α-acetobromoglucose (α-ABG) with resbutyrophenone in the presence of silver oxide in quinoline for 4 h (15–20 %) [3243].

m.p. 152–153° [3243]; $(\alpha)_D^{21} = -36.3°$ (chloroform) [3243].

1-(2,5-Dihydroxyphenyl)-1-butanone

[4693-16-7] $C_{10}H_{12}O_3$ mol. wt. 180.20



Syntheses

-Preparation by reaction of butyric acid with hydroquinone [2102] in the presence of boron trifluoride,
*on a water bath (73 %) [1797];
*at 60° for 2 h in a sealed tube (72 %) [2312].

-Also obtained by reaction of butyryl chloride with hydroquinone [1759] in the presence of aluminium chloride [2374] in nitrobenzene by heating for 3 h in a water bath [1442].
-Also obtained by Fries reaction of hydroquinone dibutyrate at 150–160° for 5 h [1442].
-Also obtained by treatment of 2,5-dimethoxybutyrophenone with hydrobromic acid in refluxing acetic acid for 6 h [1442].
-Also obtained by photoacylation of hydroquinone with butyraldehyde in benzene under nitrogen (82 %) [1759, 1991].
-Also obtained by irradiation of 1,4-benzoquinone and butyraldehyde mixture in benzene containing 5 % ethanol for 3 days (60 %) [2374].
-Also obtained by Fries rearrangement of 4-methoxyphenyl butyrate with aluminium chloride (5 part)/sodium chloride (2 part) mixture at 180–200° (30 %) [1796].
-Also refer to: [1182, 1312, 2781].

$b.p._{.16}$ 193° [1442];
m.p. 175° [1796], 101° [1442], 96° [1797], 94–96° [1759, 1991], 91° [2102], 87–89° [1182], 87–88° [2312], 85° [3204].
N.B.: One of the reported melting point is obviously wrong.

BIOLOGICAL ACTIVITY: Anthelmintic [2781]; Antiprotozoal [1312].

Dimethyl ether [54419-64-6] $C_{12}H_{16}O_3$ mol. wt. 208.26

-Obtained by reaction of butyryl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride,
*in nitrobenzene at r.t. overnight (70 %) [1442];
*in methylene chloride at r.t. for 1 h (70 %) (with carbon disulfide, 61 %) [2878].

-Also obtained by reaction of butanoyl chloride with hydroquinone dimethyl ether in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in a nitrogen flow [352].
-Also obtained by reaction of butyric anhydride with p-dimethoxybenzene in the presence of aluminium chloride in carbon disulfide at −5°, then at r.t. overnight [1159].
-Prepared by Friedel-Crafts acylation (90 %) [1755].
-Also obtained by catalytic hydrogenation of 2,5-dimethoxyphenyl 2-piperidinopropyl ketone over platinum in ethanol under atmospheric pressure at r.t. (50 %) [1217].
-Also refer to: [425, 1159, 1217, 1442, 1755, 1760, 1761, 2874, 2878, 3271].

b.p.$_{.3}$ 121–123° [1755], b.p.$_{0.001}$ 136–138° [1159], b.p.$_{.20}$ 170–178° [2878], b.p.$_{.25}$ 172–175° [1442], b.p.$_{.3}$ 178° [2874];
^{1}H NMR [1755], IR [1217, 1755], MS [1217].

USE: First step of syntheses of Frenolicin B (anticoccidial agent) and Kalafungin (antifungal agent) [1761].

2,4-Dinitrophenylhydrazone of the dimethyl ether

[54419-69-1] $C_{18}H_{20}N_4O_6$ mol. wt. 388.38

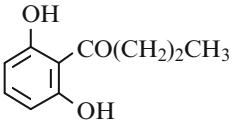
m.p. 174–175° [1442], 154–156° [1217].

Dibenzoate $C_{24}H_{20}O_5$ mol. wt. 388.42

m.p. 110° [1442].

1-(2,6-Dihydroxyphenyl)-1-butanone

[10121-26-3] $C_{10}H_{12}O_3$ mol. wt. 180.20



Syntheses
-Obtained by treatment of 8-butyryl-7-hydroxy-4-methyl-2*H*-1-benzopyran-2-one,
*with 12 % sodium hydroxide on steam a bath for 6 h (80 %) [2670];
*with N sodium hydroxide at reflux for 30 min (55 %) [1882].
-Preparation by treating resorcinol-4,6-dicarboxylic acid dimethyl ester with butyryl chloride in the presence of aluminium chloride, followed by hydrolysis and decarboxylation of the compound obtained (30 %) [862].
-Also obtained from 2,6-dihydroxyacetophenone (59 %) [385].

Isolation from natural sources

-From the culture extract of the endophytic fungus *Nodulisporium* sp. isolated from the plant *Erica arborea*, from Gomera [791].
-Of *Rhizophora apiculata* endophytic fungus 3920 from South China Sea [1391].

-From the extracts of cultures of the *estuarine fungus* [1390].
-From the extracts of cultures of *D. concentrica* strain 26 A1 [91].

m.p. 120° [1882], 116–118° [91], 116–117° [385], 106–107° [862], 106° [2670]; ^{1}H NMR [1390, 1391], ^{13}C NMR [792], IR [792], UV [91], MS [792, 1391]; X-ray data [1390, 1391].

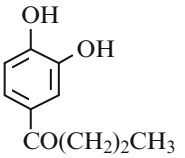
N.B.: Other names of 8-butyryl-7-hydroxy-4-methyl-2*H*-1-benzopyran-2-one:
*8-butyryl-4-methylumbelliferone [1882];
*8-butyryl-7-hydroxy-4-methylcoumarin [2670].

Dimethyl ether $C_{12}H_{16}O_3$ mol. wt. 208.26

b.p.$_{10}$ 150° [1882], 287–290° [2736], 289–291° [1882]; ^{1}H NMR [1887], ^{13}C NMR [1887], MS [1887].

1-(3,4-Dihydroxyphenyl)-1-butanone

[17386-89-9] $C_{10}H_{12}O_3$ mol. wt. 180.20



Syntheses
-Obtained by reaction of butyric acid with pyrocatechol,
*in the presence of zinc chloride at reflux [726];
*in the presence of boron trifluoride for 2.5 h at 150° (61 %) [2312] or for 2–3 h between 65 and 85° [503].

-Also obtained by Fries rearrangement of pyrocatechol dibutyrate,
*in the presence of aluminium chloride [726] in nitrobenzene for 30 min at 100° (35 %) [2646];
*in the presence of aluminium chloride and pyrocatechol (1 mol) in nitrobenzene for 2 h at 80° (70 %) [2646].
-Also obtained by reaction of butyryl chloride with pyrocatechol in the presence of aluminium chloride in nitrobenzene (27 %) [2646].
-Also obtained by treatment of guaiacol butyrate with aluminium chloride in carbon disulfide at 90° for 50 min, then at 135–140° for 2 h after solvent elimination [2075].
-Also obtained by treatment of 4-hydroxy-3-methoxybutyrophenone with boiling pyridinium chloride [505].
-Also refer to: [2127, 3183].

b.p.$_{15}$ 220–230° [726];
m.p. 149° [505], 147° [503], 146–147° [2646], 146° [2312], 139° [2075].

BIOLOGICAL ACTIVITY: Central nervous system depressant [2127].

Dimethyl ether [54419-21-5] $C_{12}H_{16}O_3$ mol. wt. 208.26

-Obtained by Friedel-Crafts reaction of butyric anhydride with veratrole in the presence of $Hf[N(SO_2C_8H_{17})_2]_4$ in chlorobenzene and SV135 at 90° for 1 h (97 %) or with $Hf(OSO_2CF_3)_4$ in the same conditions (66 %) [1244, 1245].
-Also obtained by Friedel-Crafts reaction of butyryl chloride with veratrole,
*in the presence of $Hf[N(SO_2C_8H_{17})_2]_4$ in chlorobenzene and SV135 at 110° for 1 h (94 %) or with $Hf(OSO_2CF_3)_4$ in the same conditions (70 %) [1245];
*in the presence of zinc chloride in refluxing carbon disulfide for 4 h (36.6 %) [1565];
*in the presence of aluminium chloride in carbon disulfide [1602], [1800] (43 %), first at r.t. for 5 h, then heating on a water bath for 30 min (14 %) [1565];
*in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in a nitrogen flow [352].
-Also obtained by reaction of butyric acid with veratrole in the presence of polyphosphoric acid for 2.5 h at 60° (91 %) [1364].
-Also obtained in two steps by reaction of 3,4-dimethoxybenzaldehyde with propylmagnesium bromide followed by pyridinium chlorochromate oxydation (46–54 %) [2557].
-Also obtained by hydrogenation of 3,4-dimethoxyphenyl 2-piperidinopropyl ketone at pH 4.2 with Raney nickel (14 %) [1217].
-Also refer to: [851, 895 (74 %), 1242, 2581, 3056].

White crystalline solid [2557], colourless needles [1565];
b.p.$_4$ 160–165° [1565], b.p.$_9$ 175° [3056], b.p.$_{15}$ 192–196° [1602];
m.p. 63–66° [1602], 61–62° [2557], 59–61° [895], 54.4–55.2° [1364], 54° [1565], 53–54° [1800], 52–53° [1217, 3056];
^{1}H NMR [1217, 1244, 1800, 2557], ^{13}C NMR [1244, 2557],
IR [1217, 1800], UV [2815], MS [2557];
TLC [2557]; GC/MS [1244].

Oxime of the dimethyl ether $C_{12}H_{17}NO_3$ mol. wt. 223.27

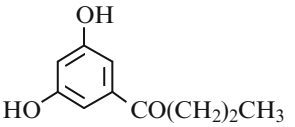
m.p. 73.3–74.5° [1364].

Semicarbazone of the dimethyl ether [106163-57-9] $C_{13}H_{19}N_3O_3$ mol. wt. 265.31

Fine colourless needles [1565];
m.p. 178–180° [895], 135° [1565].
N.B.: One of the reported melting point is obviously wrong.

1-(3,5-Dihydroxyphenyl)-1-butanone

[103323-62-2] $C_{10}H_{12}O_3$ mol. wt. 180.20



Synthesis
-Obtained by treatment of its diacetate with 5 % sodium hydroxide at reflux for 4–5 h (54 %) [1406].
m.p. 107° [1406].

2,4-Dinitrophenylhydrazone $C_{16}H_{16}N_4O_6$ mol. wt. 360.33

m.p. 232° [1406].

Diacetate [100884-40-0] $C_{14}H_{16}O_5$ mol. wt. 264.28

-Preparation by reaction of dipropylcadmium with 3,5-diacetoxybenzoyl chloride in refluxing benzene for 1 h (72 %) [1406].

$b.p._{.0.6}$ 168–174° [1406].

2,4-Dinitrophenylhydrazone of the diacetate

[102158-27-0] $C_{20}H_{20}N_4O_8$ mol. wt. 444.40

m.p. 146° [1406].

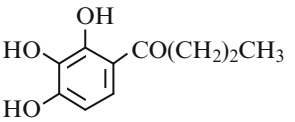
Dimethyl ether [39911-73-4] $C_{12}H_{16}O_3$ mol. wt. 208.26

-Preparation by reaction of propylmagnesium bromide with 3,5-dimethoxybenzamide in refluxing ethyl ether for 5 h (88 %) [2990], or for 70 h under argon (58 %) [2470].

colourless oil [2470];
$b.p._{.11}$ 145° [2470], $b.p._{.7}$ 157–158° [2990];
m.p. 33.5–34° [2990];
^{1}H NMR [2470], IR [2470], MS [2470].

1-(2,3,4-Trihydroxyphenyl)-1-butanone

[2437-61-8] $C_{10}H_{12}O_4$ mol. wt. 196.20



Syntheses
-Obtained by reaction of butyric acid with pyrogallol,
*in the presence of zinc chloride [214, 2678], at 135–140° for 2 h (Nencki reaction) (60 %) [1283];

*in the presence of boron trifluoride in ethyl ether at 0° for 1 h (79 %) [538, 540];
*in the presence of 70 % perchloric acid on boiling during 30 min (25 %) [2070];
*in the presence of cation-exchange resins, sulfonic acid type, Amberlite IR-120 (or Zeokarb) at 160° (70.8 %) [2523];
*in the presence of strongly acidic ion exchanger Amberlyst-15 at 120° for 24 h (52 %) [231].

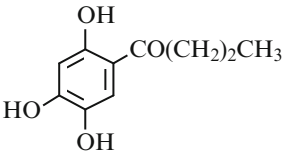
-Also obtained by reaction of butyric anhydride,
*in the presence of polyphosphoric acid or concentrated sulfuric acid (1 drop) at reflux for 10–15 min, according to the method [1470], (64.5 %) [2523];
*in the presence of Amberlite IR-120, (a cation exchange resin, sulfonic acid type), at 160° for 2–3 h (80.5 %) [2523], although Zeokarb 225 was found to be as effective.
-Also obtained by reaction of butyryl chloride with pyrogallol in the presence of aluminium chloride in nitrobenzene (50 %) [58].
-Also refer to: [1260 (36 %), 1361, 1527].

m.p. 109–110° [58], 102° [538, 540], 101–102° [1527], 101° [1260], 100° [214, 215, 2678], 98–99° [2523], 95° [2070], 90–91° [1283];
^{1}H NMR [58, 231], ^{13}C NMR [231], UV [540].

Trimethyl ether [108401-78-1] $C_{13}H_{18}O_4$ mol. wt. 238.28

1-(2,4,5-Trihydroxyphenyl)-1-butanone

[1421-63-2] $C_{10}H_{12}O_4$ mol. wt. 196.20



Syntheses
-Obtained by reaction of 1,2,4-trihydroxybenzene with butyric anhydride,
*in the presence of a catalyst ($ZnCl_2$, $AlCl_3$ or $SOCl_2$) using a mixture of aromatic hydrocarbon and water as binary solvent (80–86 %) [3074];

*in the presence of aluminium chloride in nitrobenzene first at 25°, then at 60° for 45 min (61 %) [292].
-Also obtained by Fries rearrangement of 1,2,4-tributyryloxybenzene (b.p.$_{0.08}$ 153–155°) with aluminium chloride in nitrobenzene [291].
-Also refer to: [78, 165, 333, 347, 376, 495, 666, 899, 961, 1102, 1152, 1310, 1311, 1508, 1570, 1666, 1707, 1896, 2126, 2127, 2257, 2271, 2402, 2712, 2722, 2808, 2809, 2863, 3047, 3229, 3240, 3279, 3425].

Isolation from natural sources

-From urine of rats or dogs [166].

m.p. 151–153° [291, 292], 147–148° [166];
^{13}C NMR [1508], UV [166], MS [1874, 3355];
LC/MS [3047]; HPLC [1874, 2712]; paper chromatography [166].

USE: Preparation of 7-oxabicyclo[4.1.0]heptane *via* epoxidation of cyclohexene catalyzed by vanadium bromoperoxidase from Corallina officinalis (red algae) [3425]; Candesartan cilexetil formulations [2806]; Continuous multi-microencapsulation process for improving stability and storage life of biologically active ingredients in foods, cosmetics and drugs [562]; Excipients in drug delivery vehicles for depot gel [625]; Reducing agent for thermographic imaging composition containing silver behenate and second reducing agent [3279]; Thermostability of synthetic antioxidant for food [3182].

BIOLOGICAL ACTIVITY: Effective inhibitor of the sn-glycerol-3-phosphate oxidase of *Trypanosoma brucei brucei* [1152]; Antioxidant in oils and fats [1874, 2568, 3426]; Antioxidant for fats, oils and paraffin waxes [292]; Antioxidant in foods [2712]; Antioxidant and pesticide [165]; Antioxidant for fats and oils [289, 291]; Antioxidant in estrogen derivatization [3355]; Antioxidant [666, 2295, 3032]; Central nervous system depressant [2127]; Non-permitted phenolic antioxidant [3047]; Antibacterial agent [2722]; Bilirubin stabilization in control serums and calibrators [495]; Antimelanoma activity and skin depigmentation by, *in vitro* method for screening of, [899]; Toxicity [1152]; Cytotoxicity [1393].

Triacetate [145747-19-9] $C_{16}H_{18}O_7$ mol. wt. 322.31

-Obtained by reaction of acetic anhydride with 2,4,5-trihydroxyphenol in the presence of pyridine (**8**) [376].
-Also refer to: [2410].

m.p. 108–110° [376]; ^{1}H NMR [376], IR [376], MS [376].

Trimethyl ether [2020-73-7] $C_{13}H_{18}O_4$ mol. wt. 238.28

-Obtained by heating dimethyl sulfate with 2,4,5-trihydroxybutyrophenone [1250] in the presence of aqueous sodium hydroxide at reflux for 90 min (83 %) [2127].
-Prepared by Friedel-Crafts acylation (88 %) [1755].
-Also obtained by reaction of butyric anhydride with 1,2,4-trimethoxybenzene in the presence of aluminium chloride in methylene chloride at 60° for 1 h (74 %) [772].
-Also obtained by reaction of diazomethane with 4-hydroxy-2,5-dimethoxybutyrophenone in ethyl ether [166].
-Also obtained by reaction of butyryl chloride with 1,2,4-trimethoxybenzene in the presence of aluminium chloride,
*in ethyl ether between 0 and 5° for 7 h 15 min (32 %) [1250];
*without solvent (60–74 %) [771].
-Also obtained by treatment of 1-(2,4,5-trimethoxyphenyl)butane with DDQ in wet dioxane in the presence of silica gel (59 %) [1546].
-Also obtained by reaction of butyric acid with 1,2,4-trimethoxybenzene in the presence of polyphosphoric acid for 4 h at 45–50° [2695].
-Also refer to: [1800 (48 %), 2696].

white crystals [2127], yellow prisms [166], white solid [1546],
white powder [772];
m.p. 79° [1755], 78.5–80° [765, 2127], 77° [766, 1250], 76–77.5° [2695], 76–77° [166], 75–77° [772, 1800], 75–76° [1546];
^{1}H NMR [772, 1546, 1800, 2695], ^{13}C NMR [772],
IR [772, 1800, 2695], MS [772, 2695].

BIOLOGICAL ACTIVITY: Central nervous system depressant [2127].

Triethyl ether [63213-31-0] $C_{16}H_{24}O_4$ mol. wt. 280.36

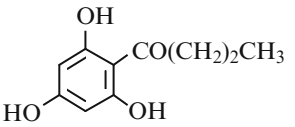
-Obtained by reaction of butyric acid with 1,2,4-triethoxybenzene in the presence of PPA (60–80 %) [2196].

m.p. 50–51° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

1-(2,4,6-Trihydroxyphenyl)-1-butanone

[2437-62-9] $C_{10}H_{12}O_4$ mol. wt. 196.20



Syntheses

-Preparation by reaction of n-butyronitrile with phloroglucinol (Houben-Hoesch reaction) (64 %) [83, 965, (71.7 %) 1375, 1608, 1610].

-Also obtained by reaction of butyryl chloride with phloroglucinol in the presence of aluminium chloride,
*in nitrobenzene [2646], (60–70 %) [421], (53 %) [2618];
*in nitrobenzene and carbon disulfide mixture (56 %) [2113], (53 %) [2620].
-Also obtained by reaction of butyric acid with phloroglucinol in the presence of boron trifluoride etherate [3019, 3020].
-Also obtained by reaction of butyric anhydride with phloroglucinol,
*in the presence of Amberlite IR-120, (a cation exchange resin, sulfonic acid type), at 160° for 2–3 h (32.2 %) [2523];
*in the presence of polyphosphoric acid or concentrated sulfuric acid (1 drop) at reflux for 30 min, according to the method [1470], (32 %) [2523];
*in the presence of boron trifluoride etherate (70–80 %) [2014].
-Also obtained by reaction of butyronitrile with phloroglucinol in the presence of trifluoromethanesulfonic acid at r.t. for 16 days (45 %) [425].
-Also refer to: [180, 205, 544, 763, 1026, 1439, 1916 (**XIIb**), 1942, 2616, 2771, 2860, 3297, 3391].

Isolation from natural sources

-From *Dryopteris lacera* [3299].
-From *Dryopteris sacrosancta* [3299].

m.p. 185–186° [2523, 3297], 183° [544], 182–184° [3391], 181.5–183° [425], 180–181° [1375, 1439], 180° [2113, 2620, 2646], 179–180° [421, 1608, 1610, 2616, 2618], 176° [83];
^{1}H NMR [83, 421, 425, 3019], ^{13}C NMR [205, 3019],
IR [421, 425, 3019], UV [540, 3019], MS [421, 425]; GLC [2531].

BIOLOGICAL ACTIVITY: Antimicrobial activity against *Bacillus subtilis* [3020]; Antimicrobial for *Staphylococcus aureus* [3372]; Antagonist both thromboxane A_2 and Leukotriene D_4 [3019]; Antifungal [2113]; Anthelmintic [1248]; For hepatic and nephritic colic [1813]; Antioxidant in food [2024]; Toxicity [1248].

Monohydrate $C_{10}H_{12}O_4$, H_2O mol. wt. 214.22

-Refer to: [1608, 1610, 2646].

m.p. 110° [1610].

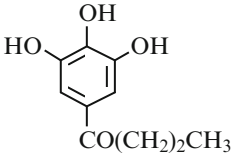
Trimethyl ether [76569-40-9] $C_{13}H_{18}O_4$ mol. wt. 238.28

-Obtained by reaction of butyronitrile with phloroglucinol trimethyl ether in the presence of trifluoromethanesulfonic acid at r.t. for 13 days (67 %) [425].
-Also obtained by reaction of butyryl chloride with 1,3,5-trimethoxybenzene in the presence of stannic chloride in methylene chloride at −15 to −10° for 2 h (96 %) [3068].
-Also refer to: [3070].

yellow oil [425]; b.p.$_1$ 158–160° [425];
^{1}H NMR [425], IR [425], MS [425].

1-(3,4,5-Trihydroxyphenyl)-1-butanone

[3329-02-0] $C_{10}H_{12}O_4$ mol. wt. 196.20



Syntheses
-Refer to: [151, 3280].
Trimethyl ether [170489-31-3]
$C_{13}H_{18}O_4$ mol. wt. 238.28

-Obtained by treatment of ethyl 3-(3,4,5-trimethoxyphenyl)-3-oxo-2-propyl-1-propanoate with 5 % alc. KOH for 1 h at 60° [151].
-Also refer to: [392, 1424–1426].

b.p.$_{20}$ 218–220° [392];
long needles [392]; m.p. 51–52.5° [392];
^{1}H NMR [1894], ^{13}C NMR [1894], IR [1894], MS [1894].

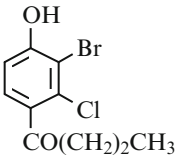
p-Nitrophenylhydrazone of the trimethyl ether $C_{19}H_{23}N_3O_5$ mol. wt. 373.41

dark brownish red needles [392]; m.p. 160° [392].

1.2 Substituted Hydroxyketones

1-(3-Bromo-2-chloro-4-hydroxyphenyl)-1-butanone

[1134-09-4] $C_{10}H_{10}BrClO_2$ mol. wt. 277.54



Syntheses

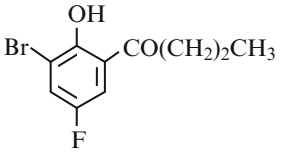
-To n-butyryl chloride, 2-bromo-3-chloroanisole and carbon disulfide was added in small portions at 25°, aluminium chloride; the mixture stirred 1 h at r.t. and 45 min at 55°; pentane and aluminium chloride added, heated 3 h at 80° [2056].

-Also refer to: [2047, 2048, 2766, 2767 (77 %)].

m.p. 107–108.5° [2047, 2048, 2056, 2766, 2767].

1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-butanone

[1957-56-8] $C_{10}H_{10}BrFO_2$ mol. wt. 261.09



Synthesis

-Obtained by Fries rearrangement of 2-bromo-4-fluorophenyl butyrate with aluminium chloride at 130–140° for 3 h (63 %) [1550].

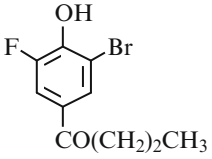
b.p.$_2$ 125–130° [1550].

2,4-Dinitrophenylhydrazone [1995-70-6] $C_{16}H_{14}BrFN_4O_5$ mol. wt. 441.21

m.p. 187–189° [1550].

1-(3-Bromo-5-fluoro-4-hydroxyphenyl)-1-butanone

[586-03-8] $C_{10}H_{10}BrFO_2$ mol. wt. 261.09



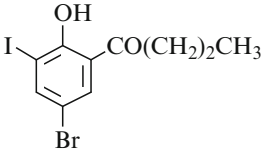
Synthesis

-Obtained by reaction of bromine with 3-fluoro-4-hydroxybutyrophenone in acetic acid [516].

m.p. 97° [516].

1-(5-Bromo-2-hydroxy-3-iodophenyl)-1-butanone

[883566-10-7] $C_{10}H_{10}BrIO_2$ mol. wt. 368.99



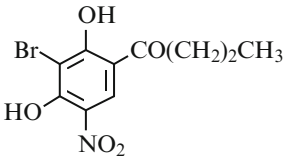
Synthesis

-Obtained by iodination of 2-hydroxy-5-bromo-butyrophenone in the presence of iodine and iodic acid in 95 % ethanol at 35–40° for 1.5 h (78 %) [2422].

m.p. 127° [2422]; ^{1}H NMR [2422], IR [2422], MS [2422].

1-(3-Bromo-2,4-dihydroxy-5-nitrophenyl)-1-butanone

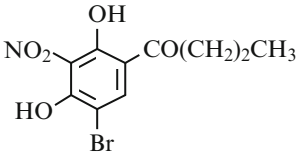
[103274-59-5] $C_{10}H_{10}BrNO_5$ mol. wt. 304.10



Synthesis
-Obtained by reaction of bromine with 2,4-dihydroxy-5-nitrobutyrophenone in hot acetic acid for 1 h [799].
m.p. 120–121° [799].

1-(5-Bromo-2,4-dihydroxy-3-nitrophenyl)-1-butanone

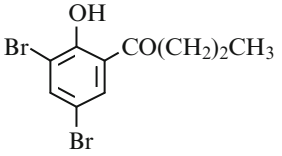
[103273-98-9] $C_{10}H_{10}BrNO_5$ mol. wt. 304.10



Synthesis
-Obtained by reaction of bromine with 2,4-dihydroxy-3-nitrobutyrophenone in acetic acid at r.t. for 2 h [799].
yellow needles [799]; m.p. 104–105° [799].

1-(3,5-Dibromo-2-hydroxyphenyl)-1-butanone

[22362-68-1] $C_{10}H_{10}Br_2O_2$ mol. wt. 322.00



Syntheses
-Obtained by Fries rearrangement of 2,4-dibromophenyl butyrate in the presence of aluminium chloride at 160–165° for 30 min (68 %) [647] or at 150° for 2 h (43 %) [659].
-Also obtained by reaction of butyric anhydride with 2,4-dibromophenol in the presence of aluminium chloride in nitrobenzene at 120° [659].

-Also refer to: [375, 998].

b.p.$_{3.5}$ 155–160° [659]; m.p. 71–72° [647].

Benzoate [101602-22-6] $C_{17}H_{14}Br_2O_3$ mol. wt. 426.10

m.p. 56–58° [659].

Oxime [99070-35-6] $C_{10}H_{11}Br_2NO_2$ mol. wt. 337.01

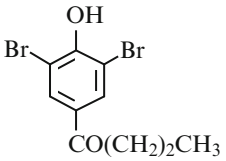
m.p. 178° (d) [659].

Semicarbazone [105041-43-8] $C_{11}H_{13}Br_2N_3O_2$ mol. wt. 379.05

m.p. $>$ 280° [659].

1-(3,5-Dibromo-4-hydroxyphenyl)-1-butanone

[2904-87-2] $C_{10}H_{10}Br_2O_2$ mol. wt. 322.00



Syntheses
-Obtained by reaction of bromine with 4-hydroxy-butyrophenone in dilute acetic acid [516].
-Also obtained by adding an aqueous solution of bromine and potassium bromide to a solution of 4-hydroxy-butyrophenone in acetone at r.t. [2001].

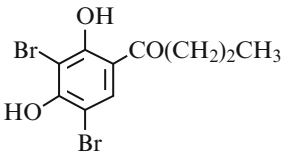
m.p. 117° [516, 1762, 2001]; UV [1995].

Methyl ether $C_{11}H_{12}Br_2O_2$ mol. wt. 336.02

-Refer to: [516]; m.p. 53° [516].

1-(3,5-Dibromo-2,4-dihydroxyphenyl)-1-butanone

$C_{10}H_{10}Br_2O_3$ mol. wt. 338.00



Syntheses
-Obtained by direct bromination of 2,4-dihydroxy-butyrophenone with bromine,
*in acetic acid for 2 h at r.t. [1128] or in 80 % acetic acid solution (10 %) [449];
*in chloroform [860].

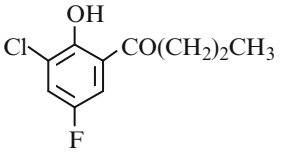
yellow needles [860];
m.p. 113° [1128], 108–109° [449], 100° [860].

Phenylhydrazone $C_{16}H_{16}Br_2N_2O_2$ mol. wt. 428.12

m.p. 155° [1128].

1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-butanone

[2585-70-8] $C_{10}H_{10}ClFO_2$ mol. wt. 216.64



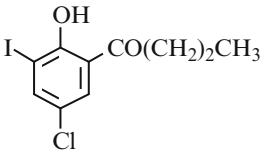
Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-fluoro-phenyl butyrate with aluminium chloride at 130–140° for 3 h (94 %) [1550].
$b.p._{\cdot 0.5}$ 122° [1550].

2,4-Dinitrophenylhydrazone [1995-74-0] $C_{16}H_{14}ClFN_4O_5$ mol. wt. 396.76

m.p. 187–189° [1550].

1-(5-Chloro-2-hydroxy-3-iodophenyl)-1-butanone

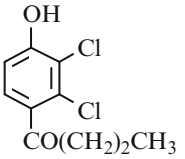
[883566-09-4] $C_{10}H_{10}ClIO_2$ mol. wt. 324.54



Synthesis
-Obtained by iodination of 2-hydroxy-5-chloro-butyrophenone in the presence of iodine and iodic acid in 95 % ethanol at 35–40° for 1.5 h (76 %) [2422].
m.p. 163° [2422];
^{1}H NMR [2422], IR [2422], MS [2422].

1-(2,3-Dichloro-4-hydroxyphenyl)-1-butanone

[2350-46-1] $C_{10}H_{10}Cl_2O_2$ mol. wt. 233.10



Syntheses
-To n-butyryl chloride, 2,3-dichloroanisole and carbon disulfide was added aluminium chloride, in small portions at 25°. The mixture stirred 1 h at r.t. and 45 min at 55°. Pentane and aluminium chloride added, heated 3 h at 80° (**IVa**) (78 %) [2056], (**IV**) (69 %) [2059].

-Also refer to: [940, 1339, 2047, 2049, 2050, 2054, 2055, 2060, 2061, 2767 (85 %), 2929].

b.p.$_{0.5}$ 140–142° [2929];
m.p. 109–110.5° [2047, 2049, 2050, 2056, 2767],
109–110° [2054, 2055, 2059–2061], 105–107° [940], 85–86° [2929].

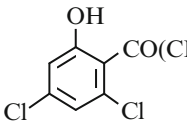
Methyl ether [41715-70-2] $C_{11}H_{12}Cl_2O_2$ mol. wt. 247.12

-Preparation by reaction of butyryl chloride with 2,3-dichloroanisole in the presence of aluminium chloride (77 %) [3333], (90 %) [742].
-Also refer to: [732, 734–736, 738, 739, 2052].

m.p. 43–44° [3333], 42–44° [732, 734–736, 738, 739, 2052].

1-(2,4-Dichloro-6-hydroxyphenyl)-1-butanone

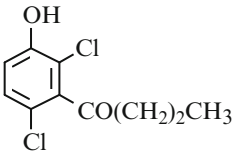
[1133-34-2] $C_{10}H_{10}Cl_2O_2$ mol. wt. 233.10



Syntheses
-Refer to: [2060, 2767 (51 %)].
b.p.$_{0.15}$ 101–102° [2047, 2767];
m.p. 47–48.5° [2047, 2048, 2058, 2060, 2766, 2767].

1-(2,6-Dichloro-3-hydroxyphenyl)-1-butanone

[1441-41-4] $C_{10}H_{10}Cl_2O_2$ mol. wt. 233.10



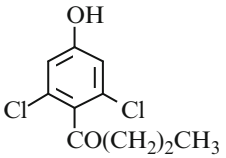
Syntheses
-Refer to: [2060, 2767].
b.p.$_{1.5}$ 148–150° [2047, 2048, 2058, 2060, 2766, 2767];
$n_D^{20} = 1.5558$ [2047, 2048, 2058, 2060, 2767].

Methyl ether [5862-11-3] $C_{11}H_{12}Cl_2O_2$ mol. wt. 247.12

yellowish oil [2767].

1-(2,6-Dichloro-4-hydroxyphenyl)-1-butanone

[1133-33-1] $C_{10}H_{10}Cl_2O_2$ mol. wt. 233.10



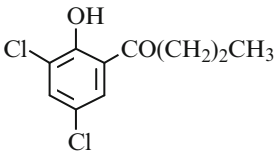
Syntheses
-To n-butyryl chloride, 3,5-dichloroanisole and carbon disulfide was added aluminium chloride, in small portions at 25°. The mixture stirred 1 h at r.t. and 45 min at 55°. Pentane and aluminium chloride added, heated 3 h at 80° [2056].

-Also refer to: [2047, 2048, 2766, 2767 (10 %)].

b.p.$_{0.10}$ 162–163° [2047, 2767];
m.p. 75.5–76.5° [2047, 2048, 2056, 2766, 2767].

1-(3,5-Dichloro-2-hydroxyphenyl)-1-butanone

[81141-14-2] $C_{10}H_{10}Cl_2O_2$ mol. wt. 233.10



Syntheses
-Obtained by Fries rearrangement of 2,4-dichlorophenyl butyrate with aluminium chloride at 170° for 40 min (68 %) [646].
-Also refer to: [563 (70 %), 564, 1159, 1372, 2956].

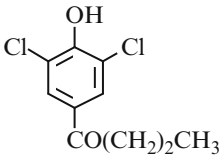
m.p. 49–50° [646], 47–48° [1159], 47° [563];
^{1}H NMR [563], IR [563, 2957], UV [2956].

2,4-Dinitrophenylhydrazone $C_{16}H_{14}Cl_2N_4O_5$ mol. wt. 413.22

m.p. 226–227° [1159].

1-(3,5-Dichloro-4-hydroxyphenyl)-1-butanone

[129527-09-9] $C_{10}H_{10}Cl_2O_2$ mol. wt. 233.10

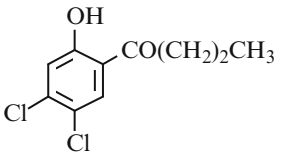


Synthesis
-Obtained by Fries rearrangement of 2,6-dichlorophenyl butyrate with aluminium chloride for 1 h at 140–150° (59 %) [3079].
m.p. 96–97° [3079].

Na salt [129527-10-2] $C_{10}H_9Cl_2O_2Na$ mol. wt. 255.07

1-(4,5-Dichloro-2-hydroxyphenyl)-1-butanone

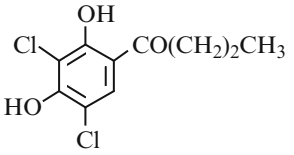
[71290-02-3] $C_{10}H_{10}Cl_2O_2$ mol. wt. 233.10



Synthesis
-Obtained by condensation of butyryl chloride on 3,4-dichlorophenol [2958].
m.p. 75–76° [2958].

1-(3,5-Dichloro-2,4-dihydroxyphenyl)-1-butanone

$C_{10}H_{10}Cl_2O_3$ mol. wt. 249.10

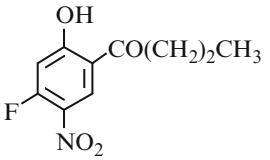


Syntheses
-Obtained by reaction of an excess of chlorine with 2,4-dihydroxybutyrophenone in 80 % acetic acid (21 %) [449].
-Also obtained by treatment of 4-chloro-6-butyrylresorcinol in ether with a slow stream of chlorine gas for 1 h (36 %) [2141].

m.p. 124–125° [2141], 110.5–111° [449].

1-(4-Fluoro-2-hydroxy-5-nitrophenyl)-1-butanone

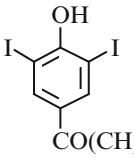
[120259-64-5] $C_{10}H_{10}FNO_4$ mol. wt. 227.19



Synthesis
-Refer to: [958].

1-(4-Hydroxy-3,5-diiodophenyl)-1-butanone

[340317-30-8] $C_{10}H_{10}I_2O_2$ mol. wt. 415.99



Syntheses

-Obtained by reaction of iodine with 4-hydroxy-butyrophenone in ethanol in the presence of yellow mercuric oxide [516].

-Also refer to: [2741].

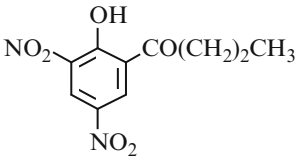
m.p. 115° [2741], 106° [516].

Methyl ether $C_{11}H_{12}I_2O_2$ mol. wt. 430.02

colourless prisms [516]; m.p. 79° [516].

1-(2-Hydroxy-3,5-dinitrophenyl)-1-butanone

$C_{10}H_{10}N_2O_6$ mol. wt. 254.20



Syntheses

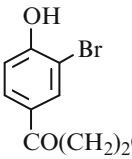
-Obtained by slowly adding a cold solution of 90 % HNO_3 in acetic anhydride to a cold solution of o-hydroxy-butyrophenone in acetic anhydride at below 15°. The mixture was then stirred for 1 h at r.t. (10 %) [116].

-Also refer to: [1078].

yellow needles [116]; m.p. 118–120° [116];
^{1}H NMR [116], IR [116];
TLC [116, 1078]; HPLC [1078].

1-(3-Bromo-4-hydroxyphenyl)-1-butanone

$C_{10}H_{11}BrO_2$ mol. wt. 243.10



Synthesis

-Obtained (by-product) by reaction of butyryl chloride with 2-bromoanisole or 2-bromophenetole in the presence of aluminium chloride (**XIX**) [1334].

m.p. 122° [1334].

Methyl ether $C_{11}H_{13}BrO_2$ mol. wt. 257.13

-Preparation by reaction of butyryl chloride with 2-bromoanisole in the presence of aluminium chloride (**X**) [1334].

m.p. 71° [1334].

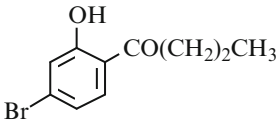
Ethyl ether $C_{12}H_{15}BrO_2$ mol. wt. 271.15

-Preparation by reaction of butyryl chloride with 2-bromophenetole in the presence of aluminium chloride (**XIII**) [1334].

m.p. 57° [1334].

1-(4-Bromo-2-hydroxyphenyl)-1-butanone

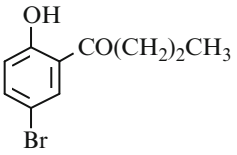
$C_{10}H_{11}BrO_2$ mol. wt. 243.10



Synthesis
-Refer to: [132].
m.p. 31–32° [132]; ^{1}H NMR [132].

1-(5-Bromo-2-hydroxyphenyl)-1-butanone

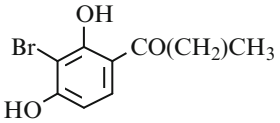
[105211-80-1] $C_{10}H_{11}BrO_2$ mol. wt. 243.10



Syntheses
-Obtained by Fries rearrangement of 4-bromophenyl butyrate with aluminium chloride [1701, 2797], [1640] (56 %).
b.p.$_{0.35}$ 104–106° [1640], b.p.$_3$ 127–132° [1701];
m.p. 53.6° [1701]; IR [1640].

1-(3-Bromo-2,4-dihydroxyphenyl)-1-butanone

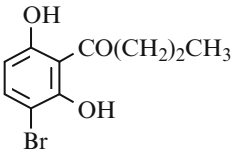
[1204738-04-4] $C_{10}H_{11}BrO_3$ mol. wt. 259.10



Synthesis
-Refer to: [1672].
MS [1672].

1-(3-Bromo-2,6-dihydroxyphenyl)-1-butanone

[99070-24-3] $C_{10}H_{11}BrO_3$ mol. wt. 259.10

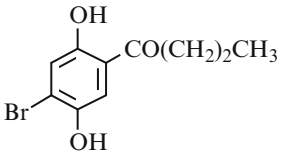


Synthesis
-Obtained by decarboxylation of 1-[5-bromo-2,4-dihydroxy-3-(1-oxobutyl)]benzoic acid [2811].

yellow fibrous needles [2811];
m.p. 108–109° [2811].

1-(4-Bromo-2,5-dihydroxyphenyl)-1-butanone

[52376-23-5] $C_{10}H_{11}BrO_3$ mol. wt. 259.10



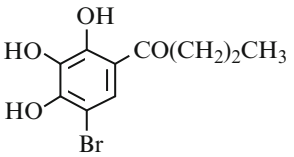
Synthesis
-Obtained by Fries rearrangement of 2-bromohydroquinone dibutyrate with aluminium chloride at 170–180° for 2 h [1105].
m.p. 98–99° [1105].

Semicarbazone [52376-24-6] $C_{11}H_{14}BrN_3O_3$ mol. wt. 316.15

m.p. 198° [1105].

1-(5-Bromo-2,3,4-trihydroxyphenyl)-1-butanone

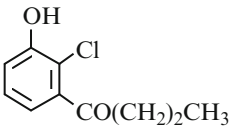
$C_{10}H_{11}BrO_4$ mol. wt. 275.10



Synthesis
-Obtained by reaction of bromine with 4-butyroylpyrogallol in acetic acid [506].
m.p. 137° [506].

1-(2-Chloro-3-hydroxyphenyl)-1-butanone

[1201-04-3] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



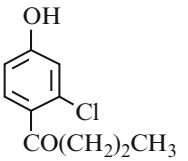
Syntheses
-Refer to: [2047, 2048, 2766, 2767 (88 %)].
$b.p._{0.3}$ 110–120° [2047, 2048, 2766, 2767].

Methyl ether [1133-58-0] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

$b.p._{22}$ 174–180° [2047, 2048, 2767];
$n_D^{23} = 1.5375$ [2047, 2048, 2767].

1-(2-Chloro-4-hydroxyphenyl)-1-butanone

[1130-98-9] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



Syntheses
-To n-butyryl chloride, 3-chloroanisole and carbon disulfide was added aluminium chloride, in small portions at 25°. The mixture stirred 1 h at r.t. and 45 min at 55°. Pentane and aluminium chloride added, heated 3 h at 80° [2056].

-Also obtained from its 2-propynyl ether by palladium-catalyzes deprotection [2378].
-Also refer to: [2047, 2048, 2055, 2058, 2060, 2765–2767].

b.p.$_{0.1}$ 100–110° [2061], b.p.$_{0.2}$ 155–175° [2054], b.p.$_{0.03}$ 160–178° [2767]; m.p. 82.5–84° [2047, 2048, 2055, 2056, 2058, 2060, 2765–2767].

Methyl ether [4070-68-2] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

-Refer to: [2047, 2767].

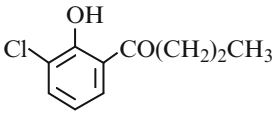
b.p.$_{1.5–2.9}$ 122–138° [2047].

2-Propynyl ether [500127-72-0] $C_{13}H_{13}ClO_2$ mol. wt. 236.70

-Obtained by reaction of propargyl bromide with 2-chloro-4-hydroxybutyrophenone [2378].

1-(3-Chloro-2-hydroxyphenyl)-1-butanone

[60474-43-3] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



Syntheses
-Obtained by Fries rearrangement of o-chlorophenyl butyrate with aluminium chloride for 2 h at 110° (36.5 %) [2799].
-Also refer to: [2423].

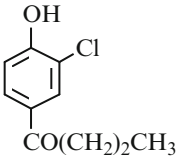
m.p. 118° [2799].

Semicarbazone [100130-01-6] $C_{11}H_{14}ClN_3O_2$ mol. wt. 255.70

m.p. 142° [2799].

1-(3-Chloro-4-hydroxyphenyl)-1-butanone

[500127-73-1] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



Syntheses
-Obtained (by-product) by reaction of butyryl chloride with 2-chloroanisole or 2-chlorophenetole in the presence of aluminium chloride (**XVI**) [1334].
-Also refer to: [2767].

m.p. 123.5–124° [2378], 122° [1334], 82.5–84° [2061];
^{1}H NMR [2378], IR [2378].

Methyl ether [868075-01-8] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

-Preparation by reaction of butyryl chloride with 2-chloroanisole in the presence of aluminium chloride (**III**) [1334].

m.p. 71° [1334].

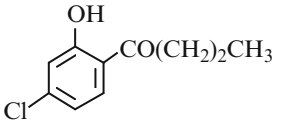
Ethyl ether $C_{12}H_{15}ClO_2$ mol. wt. 226.70

-Preparation by reaction of butyryl chloride with 2-chlorophenetole in the presence of aluminium chloride (**VI**) [1334].

m.p. 72° [1334].

1-(4-Chloro-2-hydroxyphenyl)-1-butanone

[4133-95-3] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



Syntheses

-Preparation by Fries rearrangement of m-chlorophenyl butyrate with aluminium chloride,

*without solvent for 2 h at 130° (80 %) [2802] or for 3 h at 140–150° (87 %) [2432];

*in nitrobenzene at 25° for 6 h (83 %) [2802].

-Also refer to: [2428, 2429, 2767].

$b.p._{\cdot 0.03}$ 145° [2047, 2767], $b.p._{\cdot 0.03}$ 160–178° [2055];
m.p. 51° [2432, 2802]; ^{1}H NMR [2432], IR [2432].

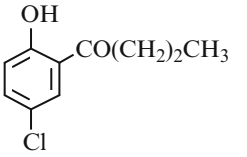
Methyl ether [4070-69-3] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

-Obtained by methylation of the above ketone in the usual way (90 %) [2802].
-Also refer to: [2767].

$b.p._{\cdot 45}$ 135° [2802].

1-(5-Chloro-2-hydroxyphenyl)-1-butanone

[51978-33-7] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



Syntheses

-Preparation by Fries rearrangement of 4-chlorophenyl butyrate with aluminium chloride [3170], (59.5 %) [1640],

*without solvent [3325] at 155° for 30 min [1702] or at 150–160° for 30 min [1701];

*in nitrobenzene, first at r.t. overnight, then at 50–60° for 8 h [1702].

-Also obtained by reaction of butyric acid with 4-chlorophenol in the presence of boron trifluoride at 150° for 5 h (86 %) [1684].
-Also refer to: [1686, 2956].

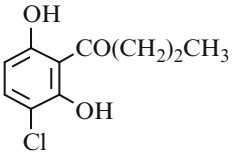
b.p.$_{.3}$ 108–112° [1702], b.p.$_{0.8}$ 115–118° [1640],
b.p.$_{.3}$ 127–132° [1701], b.p.$_{18}$ 151–152° [1684];
m.p. 55° [1684], 53.6° [1701], 50.5° [1702, 3170], 49–50° [3325];
IR [1640, 1684, 2957], (Sadtler standard N° 8982), UV [2956, 3170].

Methyl ether $C_{11}H_{13}ClO_2$ mol. wt. 212.68

b.p. 98–105° [1166].

1-(3-Chloro-2,6-dihydroxyphenyl)-1-butanone

[99070-83-4] $C_{10}H_{11}ClO_3$ mol. wt. 214.65



Syntheses
-Obtained by decarboxylation of 1-[5-chloro-2,4-dihydroxy-3-(1-oxobutyl)]benzoic acid [2811].
-Also obtained by hydrolysis of 8-butyryl-7-hydroxy-6-chloro-4-methylcoumarin with 12 % sodium hydroxide [2811].

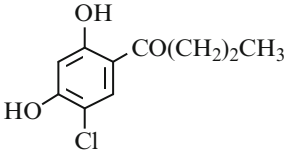
yellow needles [2811]; m.p. 115° [2811].

Dibenzoate [102665-28-1] $C_{24}H_{19}ClO_5$ mol. wt. 422.86

colourless plates [2811]; m.p. 123° [2811].

1-(5-Chloro-2,4-dihydroxyphenyl)-1-butanone

[90919-46-3] $C_{10}H_{11}ClO_3$ mol. wt. 214.65



Syntheses
-Obtained by treatment of 2,4-dihydroxybutyrophenone in ether with sulfuryl chloride (75 %) [2141].
-Also obtained by reaction of butyric acid with 4-chloro-resorcinol in the presence of zinc chloride, *at 125–135° for 2 h (62 %) [2141];

*at 140–145° for 3 min [586].
-Also refer to: [1052].

b.p.$_{.22}$ 180–195° [2141]; m.p. 96° [586], 84–85° [2141].

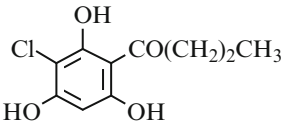
BIOLOGICAL ACTIVITY: Bactericide [1052].

2,4-Dinitrophenylhydrazone [92907-10-3] $C_{16}H_{15}ClN_4O_6$ mol. wt. 394.77

m.p. 235° [586].

1-(3-Chloro-2,4,6-trihydroxyphenyl)-1-butanone

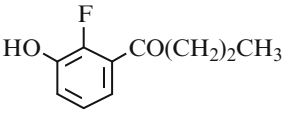
[1245818-23-8] $C_{10}H_{11}ClO_4$ mol. wt. 230.65



Synthesis
-Obtained by reaction of 2,4,6-trihydroxy-1-butanone with sulfuryl dichloride in ethanol/chloroform at 0° for 0.5 h [2141].
^{1}H NMR [1676], ^{13}C NMR [1676]; MS [1676].

1-(2-Fluoro-3-hydroxyphenyl)-1-butanone

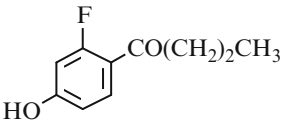
$C_{10}H_{11}FO_2$ mol. wt. 182.20



Synthesis
-Refer to: [1516].
m.p. 85–87° [1516].

1-(2-Fluoro-4-hydroxyphenyl)-1-butanone

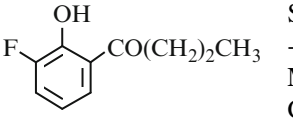
$C_{10}H_{11}FO_2$ mol. wt. 182.20



Synthesis
-Refer to: [2233].
^{1}H NMR [2233]; MS [2233].

1-(3-Fluoro-2-hydroxyphenyl)-1-butanone

[949902-14-1] $C_{10}H_{11}FO_2$ mol. wt. 182.20

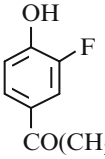


Syntheses
-Refer to: [310, 311].
Methyl ether [949902-16-3]
$C_{11}H_{13}FO_2$ mol. wt. 196.22

-Refer to: [310, 311].

1-(3-Fluoro-4-hydroxyphenyl)-1-butanone

[586-18-5] $C_{10}H_{11}FO_2$ mol. wt. 182.20



Syntheses
-Obtained by total demethylation of 3-fluoro-4-methoxy-butyrophenone by treatment in boiling pyridinium chloride (62 %) [517].
-Also obtained by reaction of butyryl chloride with 2-fluoroanisole in the presence of aluminium chloride [918].

m.p. 91° [918], 90° [517]; ^{1}H NMR [918].

Methyl ether [347-65-9] $C_{11}H_{13}FO_2$ mol. wt. 196.22

-Obtained by reaction of butyryl chloride with o-fluoroanisole in the presence of aluminium chloride,
*in carbon disulfide (90 %) [517];
*in nitrobenzene at 110° [671].
-Also refer to: [672, 3158].

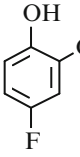
b.p.$_{16}$ 161–162° [517];
m.p. 57–58° [671, 672], 55° [517].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{17}H_{17}FN_4O_6$ mol. wt. 392.34

m.p. 188° [517].

1-(5-Fluoro-2-hydroxyphenyl)-1-butanone

[575-67-7] $C_{10}H_{11}FO_2$ mol. wt. 182.20



Syntheses
-Obtained by Fries rearrangement of p-fluorophenyl butyrate with aluminium chloride,
*without solvent at 155° for 30 min (83 %) [2991];
*in 1,2-dichloroethane at 100° for 2 h (80–85 %) (**2**) [1998].

N.B.: Industrial preparation from 500 kg of the ester (Sanofi industries, Aramon, Fr.).
-Also obtained by reaction of butyric acid with 4-fluorophenol in the presence of boron trifluoride in a sealed tube for 3 h at 125° (80 %) [1684].
-Also obtained by reaction of p-fluorophenetole, first treated with aluminium chloride in benzene, with butyryl chloride in the presence of aluminium chloride at 150–160° for 60–90 min (25 %) [2991].
-Also refer to: [1686].

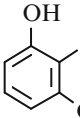
b.p.$_{8}$ 105–114° [2991], b.p.$_{14}$ 116–118° [2991], b.p.$_{20}$ 130–131° [1684];
m.p. 39° [1998], 38–39° [1684, 2991];
^{1}H NMR [1998], IR [1998], UV [1998], MS [1998].

2,4-Dinitrophenylhydrazone [100697-02-7] $C_{16}H_{15}FN_4O_5$ mol. wt. 362.32

m.p. 216° [1998].

1-(3-Hydroxy-2-iodophenyl)-1-butanone

$C_{10}H_{11}IO_2$ mol. wt. 290.10



Synthesis
-Refer to: [73].

Methyl ether [213387-03-2]
$C_{11}H_{13}IO_2$ mol. wt. 304.13

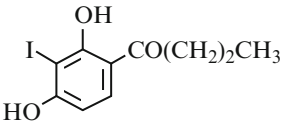
-Refer to: [73] (76 %).

N.B.: Regioselective directed *meta*-acylation of aromatic compounds *via* cycloaddition of nitriles to benzyne-zirconocene complexes.

reddish orange oil [73];
^{1}H NMR [73], ^{13}C NMR [73], IR [73], MS [73].

1-(2,4-Dihydroxy-3-iodophenyl)-1-butanone

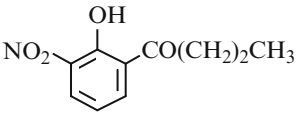
[1204737-62-1] $C_{10}H_{11}IO_3$ mol. wt. 306.10



Synthesis
-Refer to: [1672].
MS [1672].

1-(2-Hydroxy-3-nitrophenyl)-1-butanone

[91992-00-6] $C_{10}H_{11}NO_4$ mol. wt. 209.20



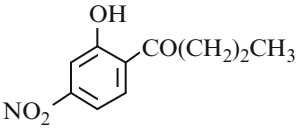
Syntheses
-Obtained by treatment of 3-ethyl-8-nitrochromone with potassium hydroxide [785].

-Also obtained by slowly adding a cold solution of 90 % HNO_3 in acetic anhydride to a cold solution of o-hydroxybutyrophenone in acetic anhydride at below 15°. The mixture was then stirred for 1 h at r.t. (30 %) [116].
-Also refer to: [116, 786, 1078].

yellow needles [116];
m.p. 108–110° [785, 786], 43–45° [116];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [116], IR [116]; TLC [116, 1078]; HPLC [1078].

1-(2-Hydroxy-4-nitrophenyl)-1-butanone

[90922-78-4] $C_{10}H_{11}NO_4$ mol. wt. 209.20



Syntheses
-Obtained by Fries rearrangement of 3-nitrophenyl butyrate with aluminium chloride at 135–140° for 150 min (3.5–5 %) [3009].
-Also refer to: [2921].

m.p. 63.5–64° [3009].

Phenylhydrazone [94708-70-0] $C_{16}H_{17}N_3O_3$ mol. wt. 299.33

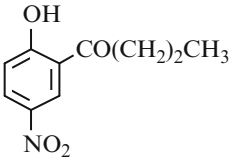
m.p. 179–180° [3009].

Benzyl ether [1192824-04-6] $C_{17}H_{17}NO_4$ mol. wt. 299.33

-Obtained by reaction of benzyl chloride with 2-butanoyl-5-nitrophenol [2921].

1-(2-Hydroxy-5-nitrophenyl)-1-butanone

$C_{10}H_{11}NO_4$ mol. wt. 209.20



Syntheses

-Obtained by slowly adding a cold solution of 90 % HNO_3 in acetic anhydride to a cold solution of o-hydroxy-butyrophenone in acetic anhydride at below 15°. The mixture was then stirred for 1 h at r.t. (60 %) [116].

-Also refer to: [1078, 2415].

yellow needles [116]; m.p. 108–110° [116];
^{1}H NMR [116], IR [116]; TLC [116, 1078]; HPLC [1078].

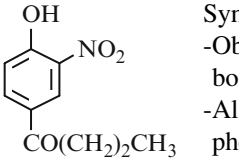
USE: Formation of chelates with Cu(II), Ni(II), Co(II) and Zn(II) [2415].

Diphenylmethyl ether [508210-78-4] $C_{23}H_{21}NO_4$ mol. wt. 375.42

-Refer to: [2020]; ^{1}H NMR [2019].

1-(4-Hydroxy-3-nitrophenyl)-1-butanone

[82350-83-2] $C_{10}H_{11}NO_4$ mol. wt. 209.20



Syntheses

-Obtained by treatment of 4-chloro-3-nitrobutyrophenone with boiling 6 % aqueous potassium hydroxide [2147].

-Also obtained by reaction of butyryl chloride with o-nitrophenol in the presence of aluminium chloride in nitrobenzene for 2.5 h at 55–60°, then at r.t. overnight (43 %) [465].

pale yellow needles [2147]; m.p. 47.6–48.2° [465], 46° [2147].

2,4-Dinitrophenylhydrazone $C_{16}H_{15}N_5O_7$ mol. wt. 389.32

m.p. 192.4–192.8° [465].

4-Nitrophenylhydrazone $C_{16}H_{16}N_4O_5$ mol. wt. 344.33

masses of orange crystals [2147]; m.p. 203–204° [2147].

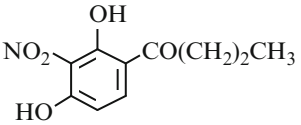
Methyl ether [1032174-10-9] $C_{11}H_{13}NO_4$ mol. wt. 223.23

-Obtained by adding potassium nitrate to an ice-cold solution of 4-methoxybutyrophenone in sulfuric acid, then the reaction was run at r.t. for 8–15 h (61 %) [2243].

white solid [2243]; m.p. 69–70° [2243]; ^{1}H NMR [2243].

1-(2,4-Dihydroxy-3-nitrophenyl)-1-butanone

[103205-61-4] $C_{10}H_{11}NO_5$ mol. wt. 225.20



Syntheses

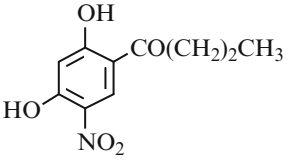
-Obtained by reaction of butyric anhydride (1.1 mol) with 2-nitroresorcinol (1 mol) in the presence of aluminium chloride (3.3 mol) in nitrobenzene at 100° [105].

-Also obtained by reaction of butyric anhydride with 2-nitroresorcinol in the presence of aluminium chloride in nitrobenzene on a boiling water bath for 3 h (46 %) [799].

m.p. 90–91° [799], 90° [105].

1-(2,4-Dihydroxy-5-nitrophenyl)-1-butanone

[103204-42-8] $C_{10}H_{11}NO_5$ mol. wt. 225.20



Syntheses

-Obtained by reaction of nitric acid (d = 1.40–1.42) with resbutyrophenone,

*without solvent, first at 0°, then at r.t. (92 %) [166];

*in acetic acid, first at 0°, then at 45° (40 %) [799].

pale yellow needles [799], yellow needles [166];
m.p. 121.5–122° [166], 120–121° [799].

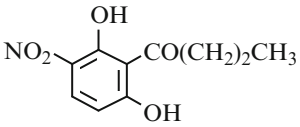
Dimethyl ether [100137-55-1] $C_{12}H_{15}NO_5$ mol. wt. 253.25

-Obtained by reaction of dimethyl sulfate with 2,4-dihydroxy-5-nitrobutyrophenone in the presence of potassium carbonate in refluxing acetone for 12 h (70 %) [166].

m.p. 113–114° [166].

1-(2,6-Dihydroxy-3-nitrophenyl)-1-butanone

[103204-43-9] $C_{10}H_{11}NO_5$ mol. wt. 225.20



Syntheses

-Obtained by Fries rearrangement of 4-nitroresorcinol butyrate (1 mol) with aluminium chloride (3.3 mol) in nitrobenzene at 110–120° for 2 h or at r.t. for 72 h [104].

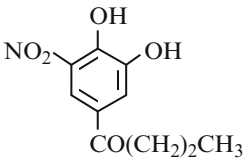
-Also obtained by heating a mixture of butyric anhydride and 4-nitroresorcinol in the presence of aluminium chloride in nitrobenzene for 3 h in a water bath [2224].

-Also obtained by reaction of nitric acid (d = 1.42) with 2,6-dihydroxybutyrophenone at 0° for 10 min [2224].

m.p. 78° [104, 2223, 2224].

1-(3,4-Dihydroxy-5-nitrophenyl)-1-butanone

[134610-36-9] $C_{10}H_{11}NO_5$ mol. wt. 225.20



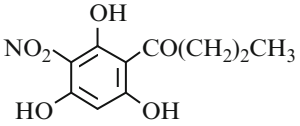
Synthesis

-Obtained by treatment of 4-hydroxy-3-methoxy-5-nitrobutyrophenone with pyridinium chloride at 200° for 40 min [324].

m.p. 88–90° [324].

1-(2,4,6-Trihydroxy-3-nitrophenyl)-1-butanone

[119691-93-9] $C_{10}H_{11}NO_6$ mol. wt. 241.20



Synthesis

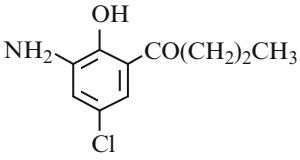
-Obtained by adding hexane, then a mixture of concentrated sulfuric acid and fuming nitric acid at 0° to a solution of phlorobutyrophenone in concentrated sulfuric acid below 0° (70–80 %) [3414].

bright yellow needles [3414]; m.p. 93–94° [3414];
^{1}H NMR [3414], IR [3414], MS [3414].

BIOLOGICAL ACTIVITY: Germination inhibitory activity [3414]; PET inhibition [3414].

1-(3-Amino-5-chloro-2-hydroxyphenyl)-1-butanone

$C_{10}H_{12}ClNO_2$ mol. wt. 213.66

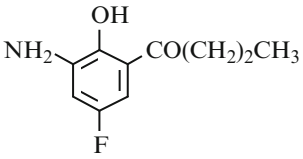


Synthesis

-Refer to: [2105].

1-(3-Amino-5-fluoro-2-hydroxyphenyl)-1-butanone

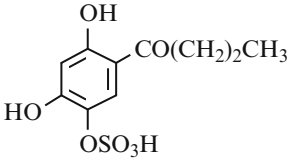
$C_{10}H_{12}FNO_2$ mol. wt. 197.21



Synthesis
-Refer to: [2105].

1-[2,4-Dihydroxy-5-(sulfooxy)phenyl]-1-butanone

$C_{10}H_{12}O_7S$ mol. wt. 276.27



Synthesis
-Obtained by hydrolysis of its potassium salt with 3 N HCl at 95° for 30 min (41 %) [166].
yellow prisms [166]; m.p. 147–148° [166].

Isolation from natural sources
-From urines of dogs and rats [166].

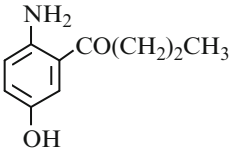
K salt
Potassium 5-butyryl-2,4-dihydroxyphenylsulfate

[116956-62-8] $C_{10}H_{11}O_7SK$ mol. wt. 314.36

colourless plates [166]; m.p. 230–232° [166];
UV [166]; paper chromatography [166].

1-(2-Amino-5-hydroxyphenyl)-1-butanone

[404919-01-3] $C_{10}H_{13}NO_2$ mol. wt. 179.22

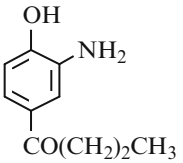


Synthesis
-Refer to: [3331].

USE: Preparation of indazoles having an action similar to that of a thyroid hormone and method for the production thereof, and their use in medicaments [3331].

1-(3-Amino-4-hydroxyphenyl)-1-butanone

$C_{10}H_{13}NO_2$ mol. wt. 179.22

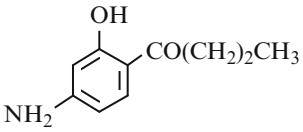


Synthesis
-Obtained by treatment of 4-hydroxy-3-nitrobutyrophenone in solution of aqueous sodium carbonate with sodium hydrosulfite at reflux [254].
white leaflets [254]; m.p. 115–116° (d) [254].

BIOLOGICAL ACTIVITY: Antibacterial [254].

1-(4-Amino-2-hydroxyphenyl)-1-butanone

$C_{10}H_{13}NO_2$ mol. wt. 179.22



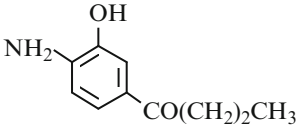
Syntheses
-Obtained by hydrolysis of 1-(4-acetylamino-2-hydroxy-phenyl)-1-butanone (SM) (m.p. 102°) with boiling 50 % HCl [1552]. **SM** was prepared,

*by Friedel-Crafts reaction of n-butyryl chloride with m-acetylaminoanisole in the presence of an excess of aluminium chloride in refluxing 1,2-dichloroethane for 2 h (58 %) [1552];
*or by Fries rearrangement of m-acetylaminophenyl n-butyrate (m.p. 85°) with aluminium chloride (2 mol) for 4 h at 180° (46 %) [1552].

m.p. 139° [1552].

1-(4-Amino-3-hydroxyphenyl)-1-butanone

[123172-47-4] $C_{10}H_{13}NO_2$ mol. wt. 179.22

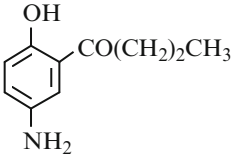


Syntheses
-Obtained by treatment [424] of 6-butyryl-benzoxazolinone with boiling 10 % aqueous sodium hydroxide for 4 h (60 %) [2161].
-Also refer to: [2162].
m.p. 118–120° [2161].

USE: Preparation of acylbenzoxazinon acetates [2162].

1-(5-Amino-2-hydroxyphenyl)-1-butanone

[99075-34-0] $C_{10}H_{13}NO_2$ mol. wt. 179.22



Syntheses
-Obtained by hydrolyzing 5-acetamido-2-hydroxy-butyro-phenone with boiling 50 % HCl [1449].
-Also refer to: [2029].
m.p. 53° [1449].

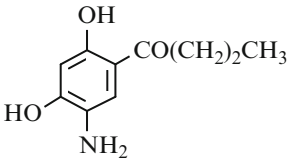
Acetate $C_{12}H_{15}NO_3$ mol. wt. 221.26

m.p. 134° [1449].

BIOLOGICAL ACTIVITY: Glycosuric [1449]; Toxicity [1449].

1-(5-Amino-2,4-dihydroxyphenyl)-1-butanone

$C_{10}H_{13}NO_3$ mol. wt. 195.22



Synthesis

-Refer to: [166].

Dimethyl ether [100370-41-0]

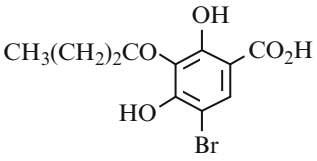
$C_{12}H_{17}NO_3$ mol. wt. 223.27

-Obtained from 2,4-dimethoxy-5-nitrobutyrophenone by treatment with clean mossy zinc and HCl on the water bath (52 %) [166].

m.p. 75–76° [166].

1-[5-Bromo-2,4-dihydroxy-3-(1-oxobutyl)]benzoic acid

[99853-34-6] $C_{11}H_{11}BrO_5$ mol. wt. 303.11



Syntheses

-Obtained by adding butyric anhydride to a cold solution of methyl 2,4-dihydroxy-5-bromobenzoate and aluminium chloride in nitrobenzene. The mixture was left overnight at r.t., and then heated at 100–105° for 4 h [2811].

-Also obtained by Friedel-Crafts butyrylation of 5-bromo-β-resorcylic acid [2811].
-Also obtained by hydrolysis of the methyl ester with 10 % NaOH on a water bath for 1 h and then kept overnight at r.t. [2811].
-Also obtained by heating 2-hydroxy-4-butyroxy-5-bromobenzoic acid (m.p. 146°) with aluminium chloride at 170–175° for 1 h [2811].

needles [2811]; m.p. 211° (d) [2811].

Methyl ester [104780-38-3] $C_{12}H_{13}BrO_5$ mol. wt. 317.14

-Obtained at the same time in the first reaction above mentioned (21 %) [2811].

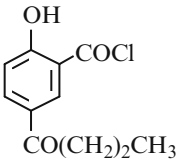
yellow needles [2811]; m.p. 107° [2811].

Oxime of the methyl ether [100116-12-9] $C_{12}H_{14}BrNO_5$ mol. wt. 332.15

colourless granules [2811]; m.p. 166° (d) [2811].

5-(1-Oxobutyl)-2-hydroxybenzoyl chloride

$C_{11}H_{11}ClO_3$ mol. wt. 226.66



Synthesis
-Refer to: [523].

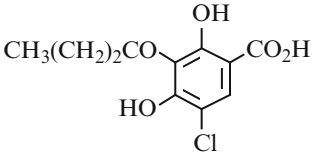
Methyl ether [64808-72-6]
$C_{12}H_{13}ClO_3$ mol. wt. 240.68

-Obtained by chlorination of 5-butyryl-2-methoxybenzoic acid [523].

m.p. 65° [523]; IR [523].

1-[5-Chloro-2,4-dihydroxy-3-(1-oxobutyl)]benzoic acid

[99854-28-1] $C_{11}H_{11}ClO_5$ mol. wt. 258.66



Syntheses
-Obtained by adding butyric anhydride to a cold solution of methyl 2,4-dihydroxy-5-chlorobenzoate and aluminium chloride in nitrobenzene. The mixture was left overnight at r.t., and then heated at 100–105° for 4 h [2811].

-Also obtained Fries rearrangement of 2-hydroxy-4-butyroxy-5-chlorobenzoic acid (m.p. 145°) with aluminium chloride at 145° for 1 h [2811].
-Also obtained by hydrolysis of the methyl ester with 10 % NaOH on a water bath for 1 h and then kept overnight at r.t. [2811].

pale yellow needles [2811]; m.p. 203° (d) [2811].

Methyl ester [104851-85-6] $C_{12}H_{13}ClO_5$ mol. wt. 272.68

-Obtained at the same time in the first reaction above mentioned [2811].

yellow silky needles [2811]; m.p. 100° [2811].

Oxime of the methyl ester [100116-82-3] $C_{12}H_{14}ClNO_5$ mol. wt. 287.70

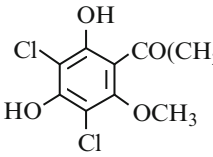
shining needles; m.p. 167° (d) [2811].

Dibenzoate of the methyl ester [102949-16-6] $C_{26}H_{21}ClO_7$ mol. wt. 480.90

colourless truncated needles; m.p. 101° [2811].

1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-butanone

$C_{11}H_{12}Cl_2O_4$ mol. wt. 279.12

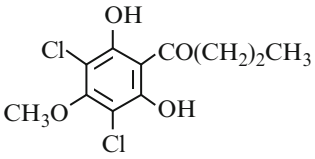


Synthesis
-Obtained by reaction of chlorine with 2,4-dihydroxy-6-methoxybutyrophenone in water [2012].
^{1}H NMR [2012], MS [2012].

BIOLOGICAL ACTIVITY: Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-butanone
(DIF-1) (−2)

[118222-70-1] $C_{11}H_{12}Cl_2O_4$ mol. wt. 279.12



Syntheses
-Obtained by reaction of sulfuryl chloride (1.5 equiv.) with 2,6-dihydroxy-4-methoxybutyrophenone in a methylene chloride/ethanol mixture at r.t. [1129].

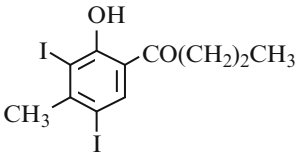
-Also obtained by reaction of chlorine with 2,6-dihydroxy-4-methoxybutyrophenone in water [2012].
-Also refer to: [1772, 1773, 2341].

Yellow amorphous solid [1129]; ^{1}H NMR [2012], MS [1129, 2012].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of *Dictyostelium* differentiation-inducing factors for their stalk-cell-inducing activity in *Dictyostelium* cells and antiproliferative activity in K562 human leukemic cells [1129]; Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

1-(2-Hydroxy-3,5-diiodo-4-methylphenyl)-1-butanone

[883566-08-3] $C_{11}H_{12}I_2O_2$ mol. wt. 430.02

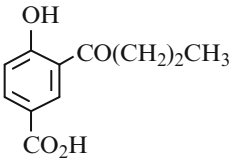


Synthesis
-Obtained by iodination of 2-hydroxy-4-methylbutyrophenone in the presence of iodine and iodic acid in 95 % ethanol at 35–40° for 1.5 h (81 %) [2422].
m.p. 98° [2422];

^{1}H NMR [2422], ^{13}C NMR [2422], IR [2422], MS [2422].

3-Butyryl-4-hydroxybenzoic acid

[25065-15-0] $C_{11}H_{12}O_4$ mol. wt. 208.21



Synthesis
-Obtained by hydrolysis of its ethyl ester [967].
m.p. 202° [967].

Acetate [23298-90-0]
$C_{13}H_{14}O_5$ mol. wt. 250.24

-Obtained by acetylation of 3-butyryl-4-hydroxybenzoic acid [967].

m.p. 113° [967].

Methyl ether [258273-25-5] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by methylation of 3-butyryl-4-hydroxybenzoic acid [967].

m.p. 185° [967].

Ethyl ether [258273-42-6] $C_{13}H_{16}O_4$ mol. wt. 236.27

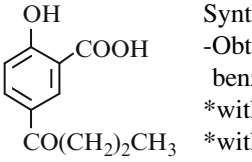
Ethyl ester $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by reaction of butyryl chloride with ethyl 4-hydroxybenzoate in the presence of aluminium chloride in tetrachloroethane, then the reaction mixture was heated at 120° for 3–4 h [967].

$b.p._{.35}$ 180° [967]; $n_D^{34} = 1.5268$ [967].

5-Butyryl-2-hydroxybenzoic acid

[106393-53-7] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Obtained by hydrolysis of methyl 5-butyryl-2-hydroxybenzoate,
*with boiling 20 % solution of potassium hydroxide [730];
*with boiling dilute solution of sodium hydroxide for 2.5 h (81 %) [107].

-Also obtained by alkaline hydrolysis of 5-butyrylsalicylamide [1158].

m.p. 168–170° [107], 153° [1158], 152–153° [730].

Methyl ester [36481-17-1] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by Fries rearrangement of methyl 2-(butyryloxy)benzoate with aluminium chloride [523] in boiling carbon disulfide for 2 h, then the reaction mixture heated for a few min after solvent elimination [730].
-Also refer to: [107, 689 (91 %), 700] (79 %)].

m.p. 73° [730], 70.5–71.5° [689], 70–71° [700], 70° [523];
IR [523].

Methyl ether of the methyl ester [64808-71-5] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by methylation of the above methyl ester [523].

m.p. 72° [523]; IR [523].

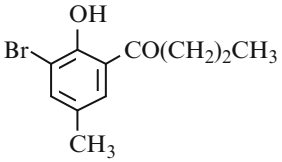
Methyl ether [64779-96-0] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by saponification of its above methyl ester [523].

m.p. 105–106° [523]; IR [523].

1-(3-Bromo-2-hydroxy-5-methylphenyl)-1-butanone

[727687-84-5] $C_{11}H_{13}BrO_2$ mol. wt. 257.13



Synthesis

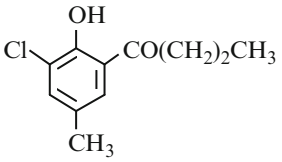
-Obtained by reaction of bromine with 2-hydroxy-5-methyl-butyrophenone in refluxing dilute acetic acid (69 %) [375].

yellow crystals [375]; m.p. 71–72° [375];

^{1}H NMR [375], IR [375].

1-(3-Chloro-2-hydroxy-5-methylphenyl)-1-butanone

$C_{11}H_{13}ClO_2$ mol. wt. 212.68



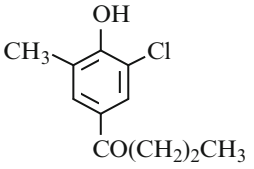
Synthesis

-Preparation by Fries rearrangement of 2-chloro-4-methyl-phenyl butyrate with aluminium chloride at 120° for 10 min (quantitative yield) [2647].

m.p. 62° [2647].

1-(3-Chloro-4-hydroxy-5-methylphenyl)-1-butanone

$C_{11}H_{13}ClO_2$ mol. wt. 212.68

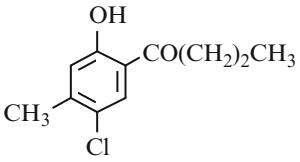


Synthesis

-Obtained from wastes in manufacturing of 4-chloro-2-methylphenol [2762].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-butanone

[408309-74-0] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



Syntheses

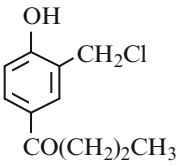
-Obtained by reaction of butyric acid with 4-chloro-3-methylphenol in the presence of boron trifluoride,
*at 100° for 1 h in a sealed tube (82 %) [1684];
*at 70–80° for 2 h (80 %) [1684].

-Also obtained by Fries rearrangement of 4-chloro-3-methylphenyl butyrate in the presence of aluminium chloride at 120° for 10 min (92 %) [2647].

m.p. 61–62° [2647], 61° [1684]; IR (Sadtler standard N° 8987) [1684].

1-[(3-Chloromethyl)-4-hydroxyphenyl]-1-butanone

[56490-86-9] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



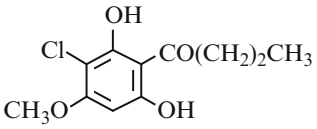
Synthesis

-Obtained by adding 4-hydroxybutyrophenone in dioxane to a 37 % formaldehyde solution and 11 N hydrochloric acid. Then, the mixture was heated at 50–60° for 1 h (55 %) [1573].

m.p. 121–123° [1573]; ^{1}H NMR [1573].

1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-1-butanone
(DIF-3) (−2)

[861889-88-5] $C_{11}H_{13}ClO_4$ mol. wt. 244.67



Syntheses

-Obtained by reaction of sulfuryl chloride (1.5 equiv.) with 2,6-dihydroxy-4-methoxybutyrophenone in a methylene chloride/ethanol mixture at r.t. [1129].

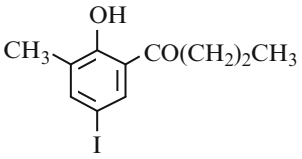
-Also refer to: [1772].

colourless amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2-Hydroxy-5-iodo-3-methylphenyl)-1-butanone

[883566-11-8] $C_{11}H_{13}IO_2$ mol. wt. 304.13



Syntheses

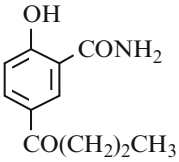
-Obtained by iodination of 2-hydroxy-3-methylbutyrophenone in the presence of iodine and iodic acid in 95 % ethanol at 35–40° for 1.5 h (80 %) [2422].

-Also refer to: [374].

m.p. 119° [2422];
^{1}H NMR [2422], IR [2422], MS [2422].

2-Hydroxy-5-butyrylbenzamide

$C_{11}H_{13}NO_3$ mol. wt. 207.23



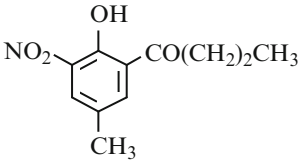
Synthesis

-Obtained by Fries rearrangement of salicylamide butyrate in the presence of aluminium chloride in nitrobenzene for 3 h at 20° [1158].

m.p. 183° [1158].

1-(2-Hydroxy-5-methyl-3-nitrophenyl)-1-butanone

[70978-45-9] $C_{11}H_{13}NO_4$ mol. wt. 223.23



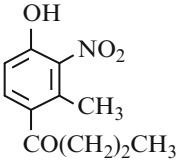
Synthesis

-Preparation by nitration of 2-hydroxy-5-methylbutyrophenone at −20° using standard reagents (55 %) [1017].

m.p. 72–74° [1017].

1-(4-Hydroxy-2-methyl-3-nitrophenyl)-1-butanone

[1210-91-9] $C_{11}H_{13}NO_4$ mol. wt. 223.23



Syntheses

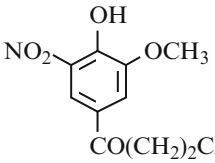
-To n-butyryl chloride, 3-methyl-2-nitroanisole and carbon disulfide was added aluminium chloride, in small portions at 25°. The mixture stirred 1 h at r.t. and 45 min at 55°. Pentane and aluminium chloride added, heated 3 h at 80° [2056].

-Also refer to: [2047, 2048, 2766, 2767 (16.5 %)].

m.p. 133–134° [2047, 2048, 2056, 2766, 2767].

1-(4-Hydroxy-3-methoxy-5-nitrophenyl)-1-butanone

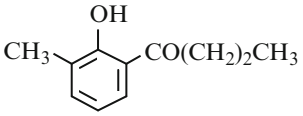
[134610-35-8] $C_{11}H_{13}NO_5$ mol. wt. 239.23



Synthesis
-Obtained by reaction of 11.2 N nitric acid with 4-hydroxy-3-methoxybutyrophenone in acetic acid at r.t. [324].
m.p. 92–93° [324].

1-(2-Hydroxy-3-methylphenyl)-1-butanone

[36375-38-9] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses
-Obtained by Fries rearrangement of 2-methylphenyl butyrate with aluminium chloride,
*at 160–180° for 30 min (60 %) [726], (45 %) [1644];
*at 100° (40 %) [726].

-Also obtained by reaction of butyric acid with o-cresol in the presence of zinc chloride at reflux for 2 h (Nencki reaction) (8 %) [317].
-Also refer to: [195].

$b.p._{.10}$ 142–143° [317], $b.p._{.11}$ 143° [726, 1644]; IR [2777].

Phenylhydrazone $C_{17}H_{20}N_2O$ mol. wt. 268.36

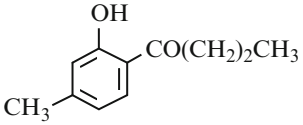
m.p. 157–158° [726].

2,4-Dinitrophenylhydrazone $C_{17}H_{18}N_4O_5$ mol. wt. 358.35

m.p. 190–192° [317].

1-(2-Hydroxy-4-methylphenyl)-1-butanone

[40991-98-8] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses
-Obtained from 2-difluoroboryloxy-4-methylbutyrophenone (**III**) by refluxing in dilute ethanol (**X**) [2500]. 2-Difluoroboryloxy-4-methylbutyrophenone (**III**), still named in (Chem. Abstr., **124**, 145544 u):

Difluoro[1-(2-hydroxy-4-methylphenyl)-1-butanonato-O,O′] boron (T-4) [173380-47-7] $C_{11}H_{13}BF_2O_2$ mol. wt. 226.03

-Compound (**III**) was obtained by reaction of butyric acid with m-cresol in the presence of boron trifluoride etherate at r.t. for 30 min (39 %) [2500].

m.p. 75–76° [2500]; IR [2500].

-Also obtained by reaction of butyric acid with m-cresol,
*in the presence of zinc chloride, then boil for five min (17 %) [726];
*in the presence of boron trifluoride for 2 h at 70° (84 %) [1685].
-Also obtained by Fries rearrangement of m-tolyl butyrate with aluminium chloride,
-without solvent,
*for 2 h at 160° (88 %) [726];
*for 10–20 min at 120–140° (75 %) [243];
*for 30 min at 120–148° (48 %) [1644];
*at 140–150° [906].
-in the presence of solvent,
*in nitrobenzene for 24 h at 25° (66 %) [243], for 66 h at 25–30° (70 %) [244] or for 10 days at + 2° (72 %) [243];
*first in carbon disulfide, then at 60–70° for 1 h and 20° for 24 h after carbon disulfide elimination (71 %) [515, 2089].
-Also obtained by reaction of butyryl chloride with m-cresol methyl ether in the presence of aluminium chloride in carbon disulfide [1602].
-Also obtained (**8**) by irradiation of 2-methoxy-5-methylphenyl butyrate in 90 % ethanol solution with the American Hanovia 450 W high pressure mercury arc amp in a water-cooled immersion photo-chemical reactor for 2.5 h (10 %) [599].
-Also refer to: [2633].

pale yellow liquid [599];
b.p.$_{0.4}$ 45° [599], b.p.$_{1}$ 92–93° [244], b.p.$_{4}$ 112–115° [243], b.p.$_{4}$ 114° [906], b.p.$_{17}$ 130–131° [2500], b.p.$_{10}$ 136° [1602], b.p.$_{15}$ 141–143° [1685], b.p.$_{15}$ 142–144° [726, 1644], b.p.$_{17}$ 144–146° [515, 2089];
m.p. 17° [726, 1644], 14.5° [1685], 12–13° [1602];
^{1}H NMR [599], IR [599, 2500], UV [2500], MS [599];
ESR [2940].

Methyl ether $C_{12}H_{16}O_2$ mol. wt. 192.26

-Obtained by reaction of butyryl chloride with 3-methylanisole in the presence of aluminium chloride in carbon disulfide at r.t. for 24 h [2088].

Oxime $C_{11}H_{15}NO_2$ mol. wt. 193.25

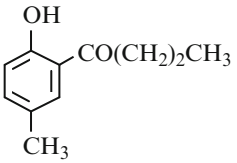
m.p. 74–75° [726].

Phenylhydrazone $C_{17}H_{20}N_2O$ mol. wt. 268.36

m.p. 97–98° [243], 95–97° [726].

1-(2-Hydroxy-5-methylphenyl)-1-butanone

[24323-47-5] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses

-Obtained by Fries rearrangement of 4-methylphenyl butyrate with aluminium chloride for 2 h at 170° (90 %) [1348], for 3 h at 120–130° [194], for 1 h at 100° (60 %) [1644] or for 2 h at 150° [726].

-Also obtained by dealkylation of its ethyl ether with aluminium chloride in carbon disulfide for 8 h at 60–70° [191].

-Also obtained by reaction of butyric acid with p-cresol in the presence of,

*zinc chloride at reflux for 2 h (27 %) [317];

*zinc chloride under microwave irradiation with 600 W for 3 min (95 %) [2211];

*stannic chloride under microwave irradiation with 700 W for 2 min at 50° and atmospheric pressure conditions (95 %) [2212];

*boron trifluoride etherate under microwave irradiation for 2 min at r.t. (95 %) [2210].

-Also obtained by reaction of butyryl chloride with p-cresol in the presence of aluminium chloride in ethylene chloride at 110–120° for 8 h (66 %) [1769].

-Also obtained by adding aluminium chloride, then butyryl chloride to a solution of aluminium p-cresylate in benzene. After standing 15 h, the mixture was refluxed 2 h (84.3 %) [1802].

-Also refer to: [375, 1822, 2516, 2932, 3028].

oil [2210–2212];
b.p.$_{15}$ 132–133° [194], b.p.$_{15}$ 132° [317], b.p. 246° [2516];
m.p. 34° [191, 1644], 33° [1802], 32–33° [194], 30–31.5° [1769];
^{1}H NMR [2210–2212], IR [2210–2212];
TLC [2210, 2211]; GLC [1348].
Cryoscopic study [182].

STUDIES: Stability constants of bivalent metal complexes with 2-hydroxy-5-methyl-butyrophenone Cu(II), Ni(II), Co(II), UO_2(II), Zn(II) and Mn(II) [2516].

Oxime [103582-37-2] $C_{11}H_{15}NO_2$ mol. wt. 193.25

m.p. 97.5–98.5° [1769];
^{1}H NMR [1769], ^{13}C NMR [1769], IR [1769], UV [1769], MS [1921].

USE: Extraction of copper [1769].

2,4-Dinitrophenylhydrazone [127699-71-2] $C_{17}H_{18}N_4O_5$ mol. wt. 358.35

m.p. 218–219° [1769].

p-Nitrophenylhydrazone $C_{17}H_{19}N_3O_3$ mol. wt. 313.36

m.p. 184–186° [194].

Methyl ether [5340-05-6] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Obtained by reaction of butyric anhydride with 4-methylanisole in the presence of aluminium chloride in boiling carbon disulfide for 30 min (84 %) [2297].
-Obtained by methylation of 2-hydroxy-5-methylbutyrophenone [1602].

b.p.$_{.3}$ 123° [2297], b.p.$_{21}$ 166–168° [1602, 2296], b.p.$_{739}$ 276.5° [2297]; m.p. 86° [2297].

Ethyl ether $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by Friedel-Crafts reaction of butyryl chloride with 4-methylphenetole in the presence of aluminium chloride [191].

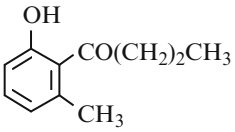
oil [191]; b.p.$_{100}$ 205° [191].

isoAmyl ether $C_{16}H_{24}O_2$ mol. wt. 248.37

b.p.$_{13}$ 150° [823].

1-(2-Hydroxy-6-methylphenyl)-1-butanone

[1200-95-9] $C_{11}H_{14}O_2$ mol. wt. 178.23



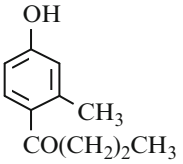
Syntheses
-Refer to: [2047, 2048, 2766, 2767].
b.p.$_{20}$ 155–158° [2047, 2048, 2766, 2767].

Methyl ether $C_{12}H_{16}O_2$ mol. wt. 192.26

-Refer to: [2767].

1-(4-Hydroxy-2-methylphenyl)-1-butanone

[104174-31-4] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses
-Obtained by Fries rearrangement of 3-methylphenyl butyrate with aluminium chloride,
*without solvent for 2 h at 160° [726];
*in carbon disulfide and diphenyl oxide, at 100–110° for 15–20 min, after elimination of carbon disulfide (≤40 %) [730];
*in nitrobenzene at + 2° for 10 days (3 %) [243], at r.t. (2 %) [726] or at 25–30° for 66 h (11 %) [244].

-Also obtained by reaction of butyric acid with m-cresol in the presence of boron trifluoride for 2 h at 70° (8 %) [1685].
-Also obtained by reaction of butyryl chloride with 3-methylanisole in the presence of aluminium chloride in carbon disulfide [1602] at r.t. for 24 h (2 %) [2088].
-Also obtained by treatment of its methyl ether with boiling pyridinium chloride for 15 min (79 %) [221].
-Also obtained by treatment of 4-hydroxy-2-methyl-5-isopropylbutyrophenone with aluminium chloride in chlorobenzene, first at r.t. for 20 h, then at 50° for 4 h (55 %) [1523].

b.p.$_{15}$ 175–200° [730];
m.p. 115° [1602], 104° [1523], 102° [1685], 98–99° [243], 98° [2088], 97–98° [726], 88° [730].

Methyl ether [54696-06-9] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Obtained by reaction of butyryl chloride with 3-methylanisole in the presence of aluminium chloride in carbon disulfide for 24 h at r.t. (70 %) or without solvent first 1 h at 70°, then 24 h at r.t. (52 %) [2088].
-Also obtained by reaction of butyric anhydride with 3-methylanisole (78 %) [2297].
-Also obtained by reaction of dimethyl sulfate with 4-hydroxy-2-methylbutyrophenone in the presence of sodium hydroxide (50 %) [1602].
-Also refer to: [221].

b.p.$_{12}$ 156° [1602], b.p.$_{15}$ 161–163° [2088], b.p. 270° [823];
m.p. 13–14° [1602]; $n_D^{21} = 1.5376$ [2088].

Propyl ether $C_{14}H_{20}O_2$ mol. wt. 220.31

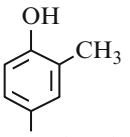
b.p.$_{13}$ 197–199° [823].

Butyl ether $C_{15}H_{22}O_2$ mol. wt. 234.34

b.p.$_{18}$ 205° [823].

1-(4-Hydroxy-3-methylphenyl)-1-butanone

[52780-68-4] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses
-Obtained by Fries rearrangement of o-tolyl butyrate in the presence of aluminium chloride (47 %) [184], at 100° (55 %) [726] or at 160–180° for 30 min (23 %) [1644].
-Also obtained by reaction of butyric acid with o-cresol in the presence,

*of boron trifluoride (84 %) [1685];
*of zinc chloride at reflux for 1 h (10 %) [317].
-Also obtained by reaction of butyronitrile with o-cresol in the presence of trifluoromethane-sulfonic acid for 21 days at r.t. (75 %) [425].
-Also obtained by treatment of 4-hydroxy-3-methyl-6-isopropylbutyrophenone with aluminium chloride in chlorobenzene, first at r.t. for 20 h, then at 50° for 4 h (64 %) [1522, 1523].

b.p.$_{15}$ 195–200° [726, 1644], b.p.$_{20}$ 220–240° [184];
m.p. 133° [1522, 1523], 132–133° [317, 726], 130–131° [184], 130° [1685], 129–130° [1967], 127–129° [425];
^{1}H NMR [425, 1967], IR [425, 1967], MS [425, 1967].

Methyl ether [29665-52-9] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Refer to: [683, 718, 823, 1602, 3049].

b.p.$_{0.08}$ 105–107° [718], b.p.$_{11}$ 162–163° [1602], b.p.$_{13}$ 168–171° [823];
m.p. 48° [1602]; $n_D^{20} = 1.5392$ [718].

Semicarbazone of the methyl ether $C_{13}H_{19}N_3O_2$ mol. wt. 249.31

m.p. 168° [823].

Ethyl ether $C_{13}H_{18}O_2$ mol. wt. 206.28

b.p. 284–286° [823].

Semicarbazone of the ethyl ether $C_{14}H_{21}N_3O_2$ mol. wt. 263.34

m.p. 174° [823].

Butyl ether $C_{15}H_{22}O_2$ mol. wt. 234.34

b.p.$_{15}$ 200° [823].

Semicarbazone of the butyl ether $C_{16}H_{25}N_3O_2$ mol. wt. 291.39

m.p. 160° [823].

isoAmyl ether $C_{16}H_{24}O_2$ mol. wt. 248.37

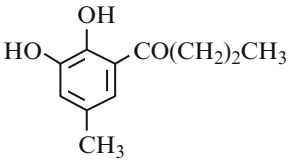
b.p.$_{13}$ 197° [823].

Semicarbazone of the isoamyl ether $C_{17}H_{27}N_3O_2$ mol. wt. 305.42

m.p. 139° [823].

1-(2,3-Dihydroxy-5-methylphenyl)-1-butanone

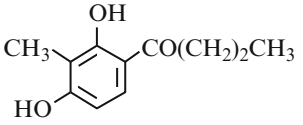
[91970-63-7] $C_{11}H_{14}O_3$ mol. wt. 194.23



Synthesis
-Obtained from creosol [784].
yellow crystals [784];
m.p. 86–88° [784].

1-(2,4-Dihydroxy-3-methylphenyl)-1-butanone

[93970-93-5] $C_{11}H_{14}O_3$ mol. wt. 194.23



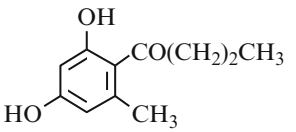
Syntheses
-Obtained by treatment of 2-hydroxy-4-methoxy-3-methyl-butyrophenone with hydriodic acid in refluxing acetic anhydride at 125–135° for 2 h (43 %) [2822].

-Also obtained by reaction of n-butyronitrile with 2-methylresorcinol (Houben-Hoesch reaction) [2821, 2822].
-Also obtained by reaction of butyryl chloride with 2-methylresorcinol in the presence of aluminium chloride,
*in methylene chloride first at 0°, then at r.t. for 16 h [2486];
*in nitrobenzene (50 %) [58].
-Also refer to: [773, 1240, 1957].

straw [2821];
m.p. 155–157° [2821, 2822], 154–155° [1515], 113–114° [58];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [58, 1515], ^{13}C NMR [1240, 1515], MS [1515].

1-(2,4-Dihydroxy-6-methylphenyl)-1-butanone

[154921-40-1] $C_{11}H_{14}O_3$ mol. wt. 194.23



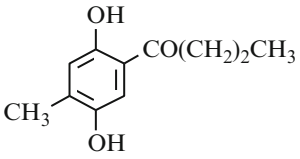
Synthesis
-Obtained from 2-difluoroboryloxy-4-hydroxy-6-methyl-butyrophenone by refluxing in dilute ethanol (70 %) [2938].

-Compound 2-difluoroboryloxy-4-hydroxy-6-methylbutyrophenone, still named difluoro[1-(2,4-dihydroxy-6-methylphenyl)-1-butanonato-O,O′] boron (70 %).

m.p. 118° [2938]; IR [2938], UV [2938].

1-(2,5-Dihydroxy-4-methylphenyl)-1-butanone

$C_{11}H_{14}O_3$ mol. wt. 194.23



Synthesis

-Refer to: [1755].

Dimethyl ether [83893-20-3]

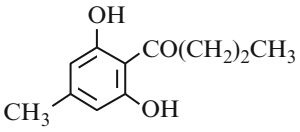
$C_{13}H_{18}O_3$ mol. wt. 222.28

-Prepared by Friedel-Crafts acylation (96 %) [1755].

b.p.$_{.3}$ 129–130° [1755]; m.p. 46–46.5° [1755]; ^{1}H NMR [1755], IR [1755].

1-(2,6-Dihydroxy-4-methylphenyl)-1-butanone

[4390-93-6] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses

-Obtained by treatment of 2,4-dibutyrylorcinol with 85 % sulfuric acid for 4 h (quantitative yield) [855].

-Also obtained by reaction of butyric anhydride with orcinol,

*in the presence of aluminium chloride (40 %) [854];

*in the presence of Amberlite IR-120, (a cation exchange resin, sulfonic acid type), at 160° for 2–3 h [2523];

*in the presence of polyphosphoric acid or concentrated sulfuric acid (1 drop) at reflux for 30 min, according to the method [1470], (16 %) [2523].

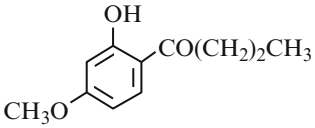
m.p. 120–122° [2523], 120–121° [854].

4-Nitrophenylhydrazone $C_{17}H_{19}N_3O_4$ mol. wt. 329.36

m.p. 180° [854].

1-(2-Hydroxy-4-methoxyphenyl)-1-butanone

[20800-24-2] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses

-Preparation by reaction of butyric anhydride with resorcinol monomethyl ether in the presence of concentrated sulfuric acid (2 drops) at 130° for few min [1469].

-Also obtained by reaction of butyryl chloride with resorcinol dimethyl ether in the presence of aluminium chloride in cooled ethyl ether for 4 h [57].

-Also obtained by partial methylation of resbutyrophenone [1469],

*with dimethyl sulfate in the presence of sodium hydroxide solution by heating the mixture on water bath for about half an hour (60 %) [799];

*with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 4–6 h (85–90 %) [2501];
*with methyl bromide in refluxing acetone [284].
-Also refer to: [60, 1787].

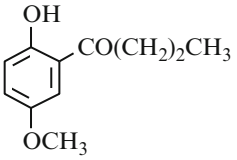
yellow oil [57];
b.p.$_2$ 124–125° [787], b.p.$_5$ 143–145° [674], b.p.$_8$ 162–164° [284, 799];
m.p. 32.5° [1469], 32–33° [674], 30–31° [787];
^{1}H NMR [57].

Oxime [143286-57-1] $C_{11}H_{15}NO_3$ mol. wt. 209.25

m.p. 64–67° [284]

1-(2-Hydroxy-5-methoxyphenyl)-1-butanone

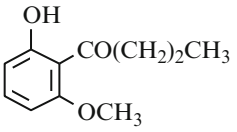
[57314-81-5] $C_{11}H_{14}O_3$ mol. wt. 194.23



Synthesis
-Obtained by reaction of butyryl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in methylene chloride at r.t. for 1 h (0.4 %) [2878].
oil [2878].

1-(2-Hydroxy-6-methoxyphenyl)-1-butanone

$C_{11}H_{14}O_3$ mol. wt. 194.23

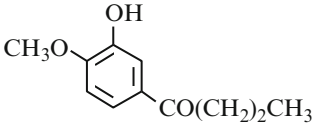


Synthesis
-Refer to: [1882].
m.p. 44–45° [1882]; ^{1}H NMR [792], ^{13}C NMR [792], IR [792], MS [792].

BIOLOGICAL ACTIVITY: Phytotoxicity [792]; Antifungal [792].

1-(3-Hydroxy-4-methoxyphenyl)-1-butanone

[91970-65-9] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Obtained by reaction of butyric acid with guaiacol in the presence of phosphorous oxychloride on steam bath for 3 h [726].

-Also obtained by treatment of 3-hydroxy-4-methoxy-phenyl monochloroacetate with sodium acetate in refluxing methanol for 3 h [3163].
-Also obtained by treatment of 3-butyloxy-4-methoxybutyrophenone with sodium methoxide in methanol at r.t. overnight (82 %) [3220].

m.p. 81–82° [726, 3220], 78–79° [3163].

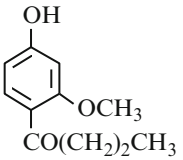
Butyrate [92655-68-0] $C_{15}H_{20}O_4$ mol. wt. 264.32

-Obtained by reaction of butyric anhydride with guaiacol in the presence of polyphosphoric acid by heating at reflux for 5 h (21 %) [3220].

b.p.$_1$ 185–190° [3220]; m.p. 42–43° [3220].

1-(4-Hydroxy-2-methoxyphenyl)-1-butanone

$C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses

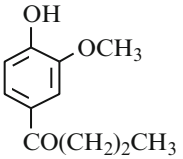
-Preparation by reaction of butyric anhydride with resorcinol monomethyl ether in the presence of concentrated sulfuric acid (2 drops) at 130° for few min [1469].

-Also obtained by partial methylation of resbutyrophenone [1469].

m.p. 69° [1469].

1-(4-Hydroxy-3-methoxyphenyl)-1-butanone

[64142-23-0] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses

-Obtained by reaction of butyric acid with guaiacol,

*in the presence of fused zinc chloride for 3 h at reflux (Nencki reaction) [726];

*in the presence of a boron trifluoride and hydrogen fluoride mixture in xylene at 60–70° [505].

-Also obtained by Fries rearrangement of 2-methoxyphenyl butyrate with aluminium chloride in nitrobenzene [1990], at 80° for 30–60 min (50 %) [726].

-Also obtained by reaction of butyric anhydride with guaiacol in the presence of zinc chloride at 155° for 3 min [324].

-Also obtained by adding DDQ to 1-(4-hydroxy-3-methoxyphenyl)-1-butanol in benzene and the reaction mixture stirred for 4 h at r.t. [2989].

-Also obtained by hydrolysis of its benzoate (90 %) [1377].

-Also refer to: [526, 527, 978, 1616].

Isolation from natural sources

-From 1988 to 1989 vintage Chardonnay juices (butyrovanillone N° 98) [614, 2783].

-Varietal aroma compounds of some grapes grown in Southern Italy [3054].

-Volatile compound evolution in Spanish oak wood (Quercus petraea and Quercus pyrenaica) during natural seasoning. [528].

-In oak wood chips [3222].

-Volatile of oak heartwood [832], volatile compound in grapes from 18 Italian Malvasia grapevine cultivars [430].

-Aroma precursors of non-floral grapes of Vitis vinifera L. Bombino n. and Uva di Troia varieties [3053].
-In oak wood used for aging of wines and spirits [2454].
-Identification of volatile compounds with a "Toasty" aroma in heated Oak used in Barrel making [780].

monoclinic and triclinic crystals [1377];
b.p.$_{15}$ 185–195° [726, 1990], b.p.$_{12}$ 202° [505];
m.p. 62.9° [1377], 55° [2989], 54–55° [726, 1990], 45° [505], 40–41° [324];
^{1}H NMR [2989], MS [2783, 3222];
GC-MS [780, 2454, 2783, 3222].

BIOLOGICAL ACTIVITY: Choleretic [2989].

Phenylhydrazone $C_{17}H_{20}N_2O_2$ mol. wt. 284.36

m.p. 91–92° [726], 79° [1377].

Benzoate $C_{18}H_{18}O_4$ mol. wt. 298.34

-Refer to: [1129, 1377 (92 %)].

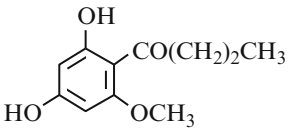
shiny triclinic crystals [1377]; m.p. 88.1° [1377], 75–77° [726].

Phenylhydrazone of the benzoate $C_{24}H_{24}N_2O_3$ mol. wt. 388.47

m.p. 175.5° [1377].

1-(2,4-Dihydroxy-6-methoxyphenyl)-1-butanone
(o-Desaspidinol)

[21185-39-7] $C_{11}H_{14}O_4$ mol. wt. 210.23



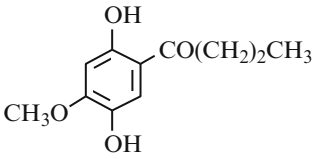
Syntheses
-Preparation by reaction of n-butyronitrile with phloroglucinol monomethyl ether (Houben-Hoesch reaction) (**XIX**) [1610].

-Also obtained by acylation of methyl 2,6-dihydroxy-4-methoxybenzoate with butyric acid and boron trifluoride and hydrolysis and decarboxylation [3296].
-Also refer to: (**II**) [205, 2448].

m.p. 130° [1610], 127–128° [3296];
^{13}C NMR [205], UV [2448]; GLC [2531].

1-(2,5-Dihydroxy-4-methoxyphenyl)-1-butanone

[2015-80-7] $C_{11}H_{14}O_4$ mol. wt. 210.23



Synthesis

-Preparation by Fries rearrangement of methoxyhydroquinone with aluminium chloride in nitrobenzene (64 %) [1250].

m.p. 109–110° [1250].

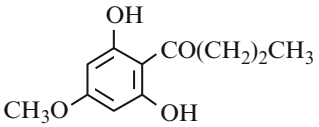
Dibenzyl ether [2017-96-1] $C_{25}H_{26}O_4$ mol. wt. 390.48

-Obtained by reaction of benzyl chloride with title ketone in the presence of potassium hydroxide (74 %) [1250].

m.p. 92° [1250].

1-(2,6-Dihydroxy-4-methoxyphenyl)-1-butanone
(Desaspidinol B)

[437-72-9] $C_{11}H_{14}O_4$ mol. wt. 210.23



Syntheses

-Preparation by reaction of butyryl chloride with phloroglucinol monomethyl ether in the presence of aluminium chloride in methylene chloride at r.t. [1129].

-Preparation by reaction of n-butyronitrile with phloroglucinol monomethyl ether (Houben-Hoesch reaction) (**XX**) [1610].

-Also obtained by partial methylation of phlorobutyrophenone with diazomethane [3296].

-Also refer to: [205, 567, 1045, 2303, 3447, 3448].

Isolation from natural sources

-From the roots of *Dryopteris championii* [3480].

-From kochia (*Kochia scoparia* L.) Schrad. KOCSC [817].

-From giant foxtail (*Setaria faberi*) SEFTA [817].

-From yellow foxtail (*Setaria glauca* L.) Beauv. SETLU [817].

-From field pennycress (*Thlaspi arvense* L.) THLAR [817].

-From the fern of *Elaphoglossum spathulatum* [2917].

-Of *Populus tritis* bud exudate [955].

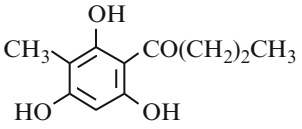
-In bud exudate of *Populus koreana*, *Populus maximowiczii* and *Populus suaveolens* (Salicaceae) [1164].

m.p. 127–128° [2444, 3301], 125–127° [1151], 121–123° [37], 113° [1610]; ^{13}C NMR [205], UV [37]; GC-MS [1164]; GLC [2531].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2,4,6-Trihydroxy-3-methylphenyl)-1-butanone
(Aspidinol-B)

[1509-06-4] $C_{11}H_{14}O_4$ mol. wt. 210.23



Syntheses

-Preparation by reaction of n-butyronitrile with 2-methyl-phloroglucinol (Houben-Hoesch reaction) (**XVI**) [1610].

-Also obtained by mild alkaline hydrolysis of the flavaspidic acid AB (m.p. 102–106°) (**VI**) from *Dryopteris goldiana* (Hook.) A. Gray [3294] according to [2449].
-Also obtained by reaction of butyryl chloride with 2-methylphloroglucinol in the presence of aluminium chloride in carbon disulfide/nitrobenzene mixture [2618], (41 %) [2617, 2620].
-Also refer to: [35, 205, 1916 (**XIII**), 1917, 2033, 2305, 2911 (19 %), 3297, 3372].

Isolation from natural sources

-From absolute oil of *Lysimachia foenum-graecum* [3429].
-From the roots of *Dryopteris championii* [3480].
-From *Dryopteris caucasica* (A. Br.) [3298].
-From *Dryopteris bissetiana* [3299].
-From *Dryopteris lacera* [3299].
-From *Dryopteris sacrosancta* [3299].

m.p. 166–167° [1917, 3297], 162° [2617], 160–162° [3296], 155° [2620], 154–155° [1610];
^{13}C NMR [205], UV [540], MS [1917, 3429];
TLC [3294, 3298]; paper chromatography [2449]; GC [3429];
GC/MS [2305]; GLC [2531].

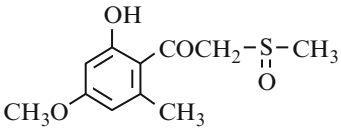
BIOLOGICAL ACTIVITY: Insecticide [3429]; Antimicrobial for *Staphylococcus aureus* [3372]; Toxicity [3429].

Monohydrate $C_{11}H_{14}O_4, H_2O$ mol. wt. 228.25

m.p. 154–155° [1610].

1-(2-Hydroxy-4-methoxy-6-methylphenyl)-2-(methylsulfinyl)-1-ethanone

[104783-89-3] $C_{11}H_{14}O_4S$ mol. wt. 242.30

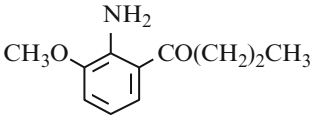


Synthesis
-A mixture of DMSO and sodium hydride (70 % in oil) in benzene was stirred at 80° for 1 h, then cooled to 35° and treated dropwise with ethyl 2-hydroxy-4-methoxy-6-methylbenzoate (85 %) [1157].

m.p. 146–148° [1157]; ^{1}H NMR [1157], IR [1157].

1-(2-Amino-3-methoxyphenyl)-1-butanone

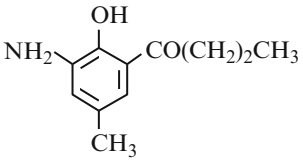
$C_{11}H_{15}NO_2$ mol. wt. 193.25



Synthesis
-Refer to: [81].
b.p.$_{0.02}$ 82–84° [81].

1-(3-Amino-2-hydroxy-5-methylphenyl)-1-butanone

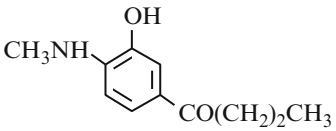
[70978-64-2] $C_{11}H_{15}NO_2$ mol. wt. 193.25



Synthesis
-Preparation by hydrogenation of 2-hydroxy-5-methyl-3-nitrobutyrophenone using 5 % Pd/C as catalyst in ethanol (77 %) [1017].
m.p. 79–81° [1017].

1-(3-Hydroxy-4-methylaminophenyl)-1-butanone

[123172-48-5] $C_{11}H_{15}NO_2$ mol. wt. 193.25

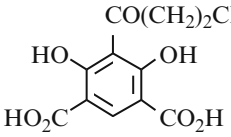


Syntheses
-Obtained by treatment [424] of 6-butyryl-3-methylbenzoxazolinone with boiling 10 % aqueous sodium hydroxide for 4 h (70 %) [2161].
-Also refer to: [2160].

m.p. 130° [2160, 2161].

[4,6-Dihydroxy-5-(1-oxobutyl)phenyl]-1,3-dicarboxylic acid

$C_{12}H_{12}O_7$ mol. wt. 268.22



Synthesis
-Refer to: [862].

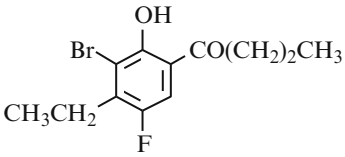
Dimethyl ester [13937-24-1]
$C_{14}H_{16}O_7$ mol. wt. 296.28

-Preparation by treating resorcinol-4,6-dicarboxylic acid dimethyl ester with butyryl chloride in the presence of aluminium chloride (75 %) [862].

m.p. 115–116° [862].

1-(3-Bromo-4-ethyl-5-fluoro-2-hydroxyphenyl)-1-butanone

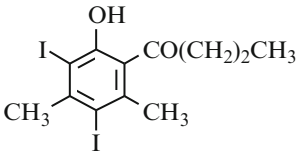
$C_{12}H_{14}BrFO_2$ mol. wt. 289.15



Synthesis
-Refer to: [2002].
m.p. 50° (Sadtler standard N° 76413K);
^{1}H NMR (Sadtler standard N° 49340M),
IR (Sadtler standard N° 76413K).

1-(2-Hydroxy-3,5-diiodo-4,6-dimethylphenyl)-1-butanone

[883566-12-9] $C_{12}H_{14}I_2O_2$ mol. wt. 444.04

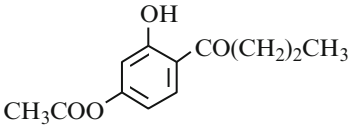


Synthesis
-Obtained by iodination of 2-hydroxy-4,6-dimethyl-butyrophenone in the presence of iodine and iodic acid in 95 % ethanol at 35–40° for 1.5 h (75 %) [2422].

m.p. 181° [2422];
^{1}H NMR [2422], IR [2422], MS [2422].

1-[4-(Acetyloxy)-2-hydroxyphenyl]-1-butanone

[91497-29-9] $C_{12}H_{14}O_4$ mol. wt. 222.24

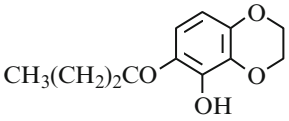


Synthesis
-Obtained by reaction of acetic anhydride with resbutyrophenone in the presence of sodium acetate at r.t. for 24–30 h (70–80 %) [3243].

m.p. 47.5–48° [3243].

5-Hydroxy-6-(1-oxobutyl)-1,4-benzodioxane

$C_{12}H_{14}O_4$ mol. wt. 222.24



Syntheses
-Obtained by Fries rearrangement of 5-butyryloxy-1,4-benzodioxane in the presence of aluminium chloride in nitrobenzene at 20° (90 %) [801].
-Also refer to: [2558].

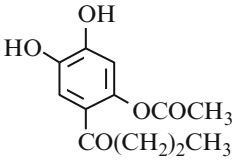
m.p. 82.5–83° [801]; UV [801].

Oxime $C_{12}H_{15}NO_4$ mol. wt. 237.26

USE: Photometric determination of titanium [2558].

1-(2-Acetyloxy-4,5-dihydroxyphenyl)-1-butanone

[145747-23-5] $C_{12}H_{14}O_5$ mol. wt. 238.24



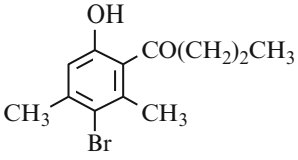
Syntheses
-Obtained by partial enzymatic deacylation of 2,4,6-triacetoxybutyrophenone (**8**) at 42–45° for 40 h [376, 2410],
*with **PPL** (porcine pancreatic lipase),
-in THF (tetrahydrofuran) (10 %) (**17**) [376];
-in DIPE (diisopropyl ether) (15 %) (**17**) [376];
-in acetone (15 %) (**17**) [376].

*with **CCL** (Candida cylindracea lipase),
-in THF (tetrahydrofuran) (20 %) (**17**) [376], (20 %) (**14**) [2412];
-in a THF and n-butanol mixture (20 %) (**20**) [2410];
-in DIPE (diisopropyl ether) (10 %) (**17**) [376];
-in acetone (10 %) (**17**) [376].

m.p. 118–120° [376];
^{1}H NMR [376], MS [376], IR [376], UV [376]; TLC [376].

1-(3-Bromo-6-hydroxy-2,4-dimethylphenyl)-1-butanone

$C_{12}H_{15}BrO_2$ mol. wt. 271.15

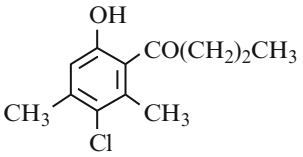


Syntheses
-Obtained by reaction of bromine (1 mol) with 2-hydroxy-4,6-dimethylbutyrophenone in carbon disulfide [189].
-Also obtained by reaction of butyryl chloride with 4-bromo-3,5-dimethylanisole in the presence of aluminium chloride in carbon disulfide [189].

b.p.$_{12}$ 170–182° [189]; m.p. 106–106.5° [189].

1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-butanone

[100388-73-6] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

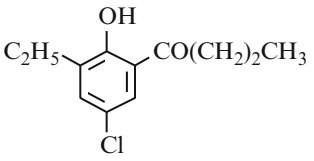


Synthesis
-Preparation by Fries rearrangement of 4-chloro-3,5-dimethylphenyl butyrate with aluminium chloride in carbon disulfide at 80° for 2 h, then at 110° for 2 h after solvent elimination (96 %) [3114].

m.p. 76° [3114].

1-(5-Chloro-3-ethyl-2-hydroxyphenyl)-1-butanone

[53347-08-3] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

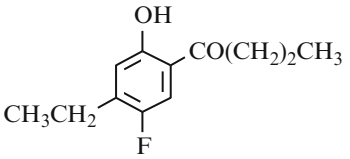


Synthesis
-Obtained by Fries rearrangement of 4-chloro-2-ethylphenyl butyrate in the presence of aluminium chloride at 120° for 1.5 h (86.4 %) [2763].

b.p.$_{18}$ 173.5–174° [2763]; $n_D^{20} = 1.5470$ [2763].

1-(4-Ethyl-5-fluoro-2-hydroxyphenyl)-1-butanone

[98841-70-4] $C_{12}H_{15}FO_2$ mol. wt. 210.25



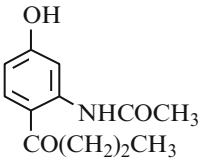
Syntheses
-Isolated on Fries rearrangement (by-product) of 4-fluorophenyl butyrate with aluminium chloride in 1,2-dichloroethane at 100° for 2 h (0.2 %) (**6**) [1998].

N.B.: In tar of the industrial preparation from 500 kg of the ester (Sanofi industries, Aramon, Fr.).
-Obtained (**6**) by Fries rearrangement of 4-fluorophenyl butyrate with aluminium chloride in bromoethane, first at 0°, then at r.t. for 2 days (30 %) [1998].
-Refer to: [2002].

m.p. 50° (Sadtler standard N° 68953K) [1998];
H NMR (Sadtler standard N° 41516M) [1998],
IR (Sadtler standard N° 68953K) [1998], UV [1998], MS [1998].

1-[2-(Acetylamino)-4-hydroxyphenyl]-1-butanone

[1211-07-0] $C_{12}H_{15}NO_3$ mol. wt. 221.26



Syntheses

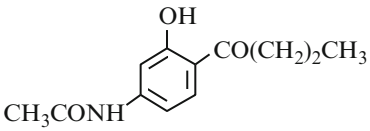
-To n-butyryl chloride, 3-methoxy-N-phenylacetamide and carbon disulfide was added in small portions at 25°, aluminium chloride; the mixture stirred 1 h at r.t. and 45 min at 55°; pentane and aluminium chloride added, heated 3 h at 80° [2056].

-Also refer to: [2047, 2048, 2766, 2767 (61 %)].

m.p. 94–96° [2047, 2048, 2056, 2766, 2767].

1-[4-(Acetylamino)-2-hydroxyphenyl]-1-butanone

[28583-62-2] $C_{12}H_{15}NO_3$ mol. wt. 221.26



Syntheses

-Obtained by *Friedel-Crafts reaction of butyryl chloride with m-acetylaminoanisole in the presence of an excess of aluminium chloride in refluxing 1,2-dichloroethane for 2 h (58 %) [1552];

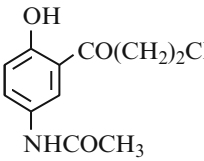
*or by Fries rearrangement of m-acetylaminophenyl butyrate (m.p. 85°) with aluminium chloride (2 mol) for 4 h at 180° (46 %) [1552].

-Also refer to: [2117].

m.p. 115–117° [2117], 102° [1552]; ^{1}H NMR [767], ^{13}C NMR [767].

1-[5-(Acetylamino)-2-hydroxyphenyl]-1-butanone

[28583-76-8] $C_{12}H_{15}NO_3$ mol. wt. 221.26



Syntheses

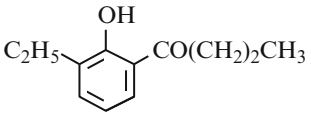
-Obtained by Fries rearrangement of p-acetamidophenyl butyrate with aluminium chloride, first at 110–120°, then for 3 h at 160° [1449].

-Also refer to: [2117].

m.p. 100.5–102° [2117], 99.5–99.8° [2117].

1-(3-Ethyl-2-hydroxyphenyl)-1-butanone

$C_{12}H_{16}O_2$ mol. wt. 192.26

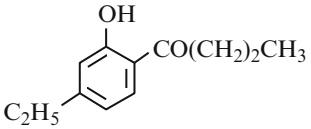


Synthesis
-Obtained by Fries rearrangement of 2-ethylphenyl butyrate with aluminium chloride at 120° (71 %) [2955].

b.p.$_1$ 170–175° [2955]; m.p. 91–92° [2955].

1-(4-Ethyl-2-hydroxyphenyl)-1-butanone

$C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses
-Obtained by Fries rearrangement of 3-ethylphenyl n-butyrate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (89 %) [2801];
*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (88 %) [2801];
*in the presence of aluminium chloride (1.3 equiv.) without solvent at 140–150° [906].

b.p.$_4$ 126–128° [906], b.p.$_{15}$ 180° [2801]; ESR [2940].

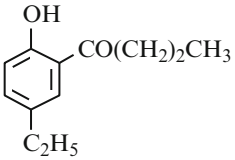
Methyl ether $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of dimethyl sulfate with 1-(4-ethyl-2-hydroxyphenyl)-1-butanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (80 %) [2801].

b.p.$_{35}$ 150° [2801].

1-(5-Ethyl-2-hydroxyphenyl)-1-butanone

$C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses
-Obtained by Fries rearrangement of 4-ethylphenyl butyrate with aluminium chloride at 100° for 2 h (75 %) [2800] or at 120° (50 %) [2955].
b.p.$_1$ 112–113° [2955], b.p.$_{10}$ 145° [2800].

Methyl ether [3781-76-8] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of butyryl chloride with p-ethylanisole in the presence of aluminium chloride in carbon disulfide at r.t. for 1 h (75.5 %) [845].

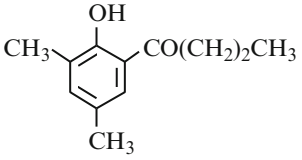
b.p.$_{24}$ 170–172° [845]; $n_D^{24} = 1.5239$ [845].

2,4-Dinitrophenylhydrazone $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 184° [2801].

1-(2-Hydroxy-3,5-dimethylphenyl)-1-butanone

[873989-36-7] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses
-Preparation by Fries rearrangement of 2,4-dimethylphenyl butyrate,
*with aluminium chloride (2 mol) at 110–115° for 6.5 h (84 %) [1016];
*with aluminium chloride at 120° (45 %) [2955].

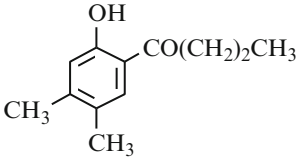
oil [2955]; b.p.$_2$ 121° [2955], b.p.$_{30}$ 145–150° [1016];
m.p. 57–58° [2061], 30° [1016].

Phenylhydrazone $C_{18}H_{22}N_2O$ mol. wt. 282.39

m.p. 168–170° [2955].

1-(2-Hydroxy-4,5-dimethylphenyl)-1-butanone

[91667-38-8] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses
-Obtained by Fries rearrangement of 3,4-dimethylphenyl butyrate with aluminium chloride at 110° without solvent (85 %) [3117].
-Also obtained by reaction of butyric acid with 3,4-dimethylphenol in the presence of boron trifluoride etherate (74 %) [2939, 2956].

b.p.$_{10}$ 116° [3117]; m.p. 52–53° [2939], 40–41° [2955];
^{1}H NMR [2939], IR [2939], UV [2939, 2956].

Methyl ether $C_{13}H_{18}O_2$ mol. wt. 206.28

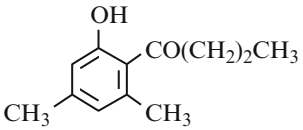
b.p.$_{13}$ 171° [824]; m.p. 54° [824].

isoAmyl ether $C_{17}H_{26}O_2$ mol. wt. 262.39

b.p.$_{13}$ 182° [824]; m.p. 54° [824].

1-(2-Hydroxy-4,6-dimethylphenyl)-1-butanone

[1639-85-6] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Obtained by Fries rearrangement of 3,5-dimethylphenyl n-butyrate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (90 %) [2801];
*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (86 %) [2801].

-Also obtained by reaction of butyryl chloride with 3,5-dimethylanisole in the presence of aluminium chloride [189].

-Also obtained from 2-difluoroboryloxy-4,6-dimethylbutyrophenone (**VII**) by refluxing in dilute ethanol (**XIV**). **VII** was obtained by reaction of butyric acid with 3,5-dimethylphenol in the presence of boron trifluoride etherate at r.t. for 30 min ($C_{12}H_{15}BF_2O_2$, mol. wt. 240.06, 60 %, m.p. 121–122°, IR) [2500].

-Also obtained by reaction of butyric acid with 3,5-dimethylphenol in the presence of boron trifluoride for 2 h at 70° (85 %) [1685].

-Also refer to: [2767].

b.p.$_{15}$ 157.5–158° [1685];
colourless solid [146];
m.p. 60° [1685], 59° [189], 57–58° [2061, 2500, 2767], 51° [2801];
IR [146, 2500], UV [2500].

4-Nitrophenylhydrazone $C_{18}H_{21}N_3O_3$ mol. wt. 327.38

m.p. 162–162.5° [189].

2,4-Dinitrophenylhydrazone $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 185° [2801].

Acetate $C_{14}H_{18}O_3$ mol. wt. 234.30

-Obtained by reaction of acetyl chloride with 2-hydroxy-4,6-dimethylbutyrophenone [189].

oil; b.p.$_{17}$ 173–175° [189].

Methyl ether $C_{13}H_{18}O_2$ mol. wt. 206.28

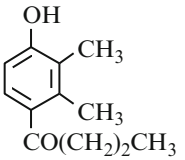
-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxy-4,6-dimethylphenyl)-1-butanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (85 %) [2801].

-Also obtained by reaction of butyryl chloride with 3,5-dimethylanisole in the presence of aluminium chloride [189].

oil; b.p.$_{17}$ 162° [189]; m.p. 44° [2801].

1-(4-Hydroxy-2,3-dimethylphenyl)-1-butanone

[5862-05-5] $C_{12}H_{16}O_2$ mol. wt. 192.26



Synthesis

-Obtained by treatment of 4-methoxy-2,3-dimethyl-butyrophenone with aluminium chloride (2 mol) in refluxing heptane [2060].

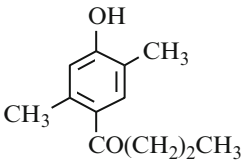
m.p. 100–102° [2060].

Methyl ether $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of butyryl chloride with 2,3-dimethylanisole in the presence of aluminium chloride in petroleum ether at r.t. [2060].

1-(4-Hydroxy-2,5-dimethylphenyl)-1-butanone

[575487-37-5] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Preparation by Fries rearrangement of 2,5-dimethylphenyl butyrate with aluminium chloride in nitrobenzene at 25° (70 %) [2955], at r.t. for 24 h (40 %) [844].

m.p. 131–132° [2955], 129° [844].

Propyl ether $C_{15}H_{22}O_2$ mol. wt. 234.34

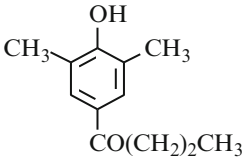
b.p.$_{12}$ 187–190° [824].

Butyl ether $C_{16}H_{24}O_2$ mol. wt. 248.37

b.p.$_{13}$ 198° [824]; m.p. 40° [824].

1-(4-Hydroxy-3,5-dimethylphenyl)-1-butanone

[104008-42-6] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Obtained by Fries rearrangement of 2,6-dimethylphenyl n-butyrate (*vic-m-Xylenyl butyrate*) (b.p. 248–250°) in the presence of aluminium chloride (67 %) [184] in nitrobenzene at r.t. for 24 h [2008].

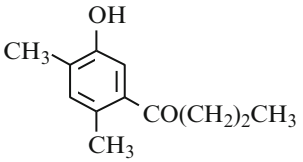
m.p. 127–127.5° [2008], 124–125° [184].

Methyl ether $C_{13}H_{18}O_2$ mol. wt. 203.29

^{1}H NMR [1267].

1-(5-Hydroxy-2,4-dimethylphenyl)-1-butanone

[1203-88-9] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

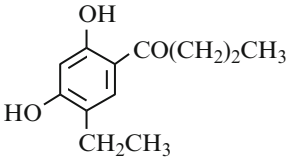
-Preparation by diazotization of 5-amino-2,4-dimethyl-butyrophenone and hydrolysis of the obtained diazonium salt [2060].

-Also refer to: [2767].

m.p. 100.5–102° [2060], 95–100° [2767].

1-(2,4-Dihydroxy-5-ethylphenyl)-1-butanone

[859939-56-3] $C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis

-Obtained by Fries rearrangement of 3-ethylresorcinol dibutyrate (1 mol) in the presence of 3-ethylresorcinol (1 mol) with aluminium chloride (2 mol) in nitrobenzene at 50–60° for 3–4 h [2651].

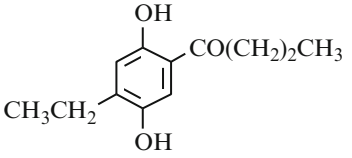
m.p. 100° [2651].

Phenylhydrazone $C_{18}H_{22}N_2O_2$ mol. wt. 298.38

m.p. 142.5° [2651].

1-(4-Ethyl-2,5-dihydroxyphenyl)-1-butanone

$C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis

-Refer to: [2441].

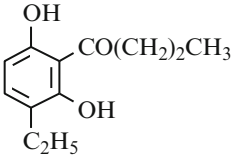
Dimethyl ether [153756-51-5]

$C_{14}H_{20}O_3$ mol. wt. 236.31

-Obtained by acylation of 2-ethyl-1,4-dimethoxybenzene with butyric acid in the presence of trifluoroacetic anhydride [2441].

1-(2,6-Dihydroxy-3-ethylphenyl)-1-butanone

[100256-99-3] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses

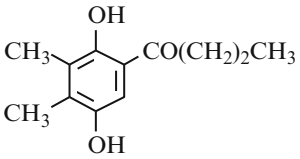
-Obtained by decarboxylation of 1-[5-ethyl-2,4-dihydroxy-3-(1-oxobutyl)]benzoic acid with conc. HCl (few drops) in boiling acetic acid for 20 h (25 %) [2811].

-Also obtained by hydrolysis of 8-butyryl-7-hydroxy-6-ethylcoumarin [2811].

m.p. 80° [2811].

1-(2,5-Dihydroxy-3,4-dimethylphenyl)-1-butanone

$C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis
-Refer to: [1755].

Dimethyl ether

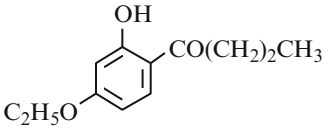
$C_{14}H_{20}O_3$ mol. wt. 236.31

-Prepared by Friedel-Crafts acylation (88 %) [1755].

b.p.$_3$ 140–143° [1755], m.p. 48–48.5° [1755];
^{1}H NMR [1755], IR [1755].

1-(4-Ethoxy-2-hydroxyphenyl)-1-butanone

[23187-42-0] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses
-Obtained by ethylation of 2,4-dihydroxybutyrophenone [1587].

-Also obtained by reaction of butanoyl chloride with m-diethoxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°.

The temperature was then raised to 80° and stirring was continued at that temperature for 5 h (60 %) [1194].
-Also refer to: [852].

b.p.$_5$ 155° [1587]; m.p. 51.5–52.5° [1194]; UV [1194].

USE: UV absorber [1194]; Light-stabilizer of polymeric materials [1194].

Oxime [173959-45-0] $C_{13}H_{17}NO_3$ mol. wt. 235.28

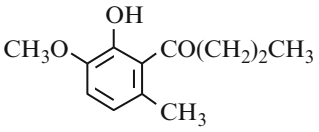
USE: As analytical reagent for palladium determination by gravimetry and spectrophotometry [852].

2,4-Dinitrophenylhydrazone $C_{18}H_{20}N_4O_6$ mol. wt. 388.38

m.p. 187° [1587].

1-(2-Hydroxy-3-methoxy-6-methylphenyl)-1-butanone

[40991-99-9] $C_{12}H_{16}O_3$ mol. wt. 208.26



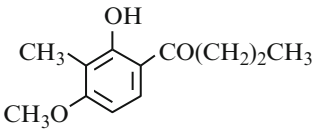
Synthesis

-Obtained (**7**) by irradiation of 2-methoxy-5-methylphenyl butyrate in 90 % ethanol solution with the American Hanovia 450 W high pressure mercury arc amp in a water cooled immersion photo-chemical reactor for 2.5 h (23 %) [599].

pale yellow liquid [599]; $b.p._{\cdot 0.6}$ 71° [599];
^{1}H NMR [599], IR [599], UV [599], MS [599].

1-(2-Hydroxy-4-methoxy-3-methylphenyl)-1-butanone

[92755-95-8] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses

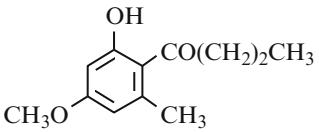
-Obtained by reaction of methyl iodide with resbutyrophenone in the presence of potash in methanol first at r.t. overnight, then refluxing for 6 h (24 %) [2822].

-Also obtained by adding butyryl chloride to a cooled solution of 1,3-dimethoxy-2-methylbenzene in ethyl ether and aluminium chloride for 1 h. The stirring continued for a further 4 h (70 %) [60].

m.p. 82–84° [2822], 65–66° [60]; ^{1}H NMR [60].

1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1-butanone

[92755-96-9] $C_{12}H_{16}O_3$ mol. wt. 208.26



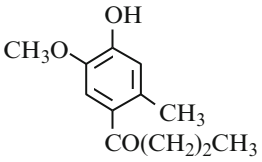
Synthesis

-Obtained by adding butyryl chloride to a cooled solution of 1,3-dimethoxy-5-methylbenzene in ethyl ether and aluminium chloride for 1 h. The stirring continued for a further 4 h (50 %) [60].

m.p. 68–69° [60]; ^{1}H NMR [60].

1-(4-Hydroxy-5-methoxy-2-methylphenyl)-1-butanone

[41082-97-7] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses

-Obtained (**6**) by Fries rearrangement of 2-methoxy-5-methylphenyl butyrate with titanium tetrachloride in nitrobenzene at 60–67° for 4 h (43 %) [599].

-Also obtained (**6**) by irradiation of 2-methoxy-5-methylphenyl butyrate in 90 % ethanol solution with the American Hanovia 450 W high pressure mercury arc amp in a water cooled immersion photochemical reactor for 2.5 h (16 %) [599].

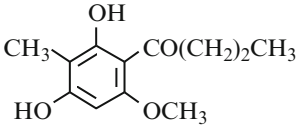
pale yellow crystals [599]; m.p. 63–64° [599];
^{1}H NMR [599], IR [599], UV [599], MS [599].

Methyl ether [3307-03-7] $C_{13}H_{18}O_3$ mol. wt. 222.28

b.p.$_7$ 180° [305]; m.p. 45° [305].

1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-1-butanone
(Isoaspidinol B)

[479-96-9] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses

-Preparation by reaction of n-butyronitrile with 2-methyl-5-methoxyresorcinol (Houben-Hoesch reaction) (**XXI**) [1610].

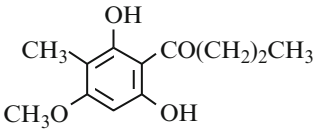
-Also refer to: [205, 325, 326, 1609, 2448 (**IX**)].

m.p. 152–153° [3301], 151.5° [1609, 1610];
^{13}C NMR [205], UV [2448], MS [2531]; GLC [2531].

BIOLOGICAL ACTIVITY: Inhibitor of angiogenesis using human antiangiogenic assay [326]; Inhibition of endothelial cell functions by novel potential cancer chemopreventive agents [325].

1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-1-butanone
(Aspidinol) (Aspidinol B)

[519-40-4] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses

-Obtained by reaction of butyryl chloride with 5-methoxy-4-methylresorcinol in the presence of aluminium chloride in carbon disulfide/nitrobenzene mixture (71.5 %) [2620].

-Also obtained from 5-methoxy-4-methylresorcinol (**I**) [1609, 2611].

-Also obtained by partial methylation of 3-methyl-2,4,6-trihydroxybutyrophenone with diazomethane [3296].
-Also refer to: [35, 205, 2393, 3302].

Isolation from natural sources

-Occurs in extracts of male fern [388, 1276].
-From *Dryopteris austriaca* (Jacq.) Woynar (Polypodiaceae) [36].
-From *Dryopteris fragrans* [1471, 2851, 2854, 2855, 3453].
-From industrial Eucalyptus globulus kraft black liquor [2258].
-In essential oil from aromatic plants [2922].
-From the rose cell liquid [1187].
-From the leaves and twigs of *Calyptranthes pallens* [1898].
-From the fern of *Elaphoglossum spathulatum* [2917].
-From the leaves of *Dryopteris villarii* and *Dryopteris arguta* (Pteridaceae) [3328].
-From the leaves of *Currania robertiana* (Pteridaceae) [3328].
-From the rhizomes of *Dryopteris crassirhizoma* (Dryopteridaceae) [2208].
-Also refer to: [386, 1270, 1610, 2414, 2612, 2713, 3102, 3297].

yellow needles [1898];
m.p. 156–161° [3102], 144–145° [1898], 143° [386], 142–143° [2713, 3297], 141–143° [3302], 141° [2620], 140–141° [36, 1609];
^{1}H NMR [1898, 2208, 3328], ^{13}C NMR [204, 205, 1898, 3328], IR [1898, 3302], UV [35, 1898], MS [1898, 2208, 2258, 3328];
GLC [2531]; HPLC [3328].

N.B.: There are two different representations of the Aspidinol:
*1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-1-butanone (**847**) [3102] page 140.
*1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-1-butanone (**I**) [1610] page 466.

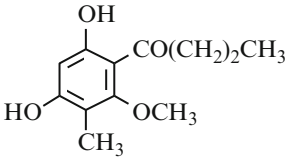
BIOLOGICAL ACTIVITY: Antiinfective ointment containing *Dryopteris fragrans*. The *Dryopteris fragrans* extract comprises dryofragin, aspidin AB, aspidin PB, aspidin BB, aspidinol and albicanol [2852]; QSAR vasodilatory activity relationship of resveratrol-coumarin hybrids [3225]; Cytotoxicity [1898]; Antitumor [1471]; Fatty acid synthase inhibitory activity [2208].

Diacetate $C_{16}H_{20}O_6$ mol. wt. 308.33

m.p. 68° [2630], 64–66° [2133].

1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-1-butanone
(Pseudoaspidinol B)

[478-48-8] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Obtained by reductive alkaline cleavage of Aspidin BB (**VII**) from *Dryyoteris assimilis* [1916] (**IVd**).
-Also obtained by reaction of butyryl chloride with methyl 2,6-dihydroxy-4-methoxy-3-methylbenzoate in the presence of aluminium chloride [2436].

-Also obtained by reaction of butyronitrile with 5-methoxy-4-methylresorcinol (Hoesch reaction) [1609].
-Also obtained by hydrolysis of 1-[4,6-bis(1,1-dimethylethoxy)-2-methyl-3-methoxyphenyl]-1-butanone with hydrochloric acid in ethanol [1213].
-Also refer to: [2448 (**X**), 2534, 2612 (**VIII**), 2860, 3302].

Isolation from natural sources

-From the roots of *Dryopteris championii* [3480].

colourless plates;
m.p. 116.5° [1609], 79–80° [2534], 72–73° [3302], 70–72° [1916, 2436].
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [1916, 2436, 2534, 3302], ^{13}C NMR [205], IR [2436, 3302], UV [2436, 2448], MS [1916, 2534]; GLC [2531].

Monohydrate $C_{12}H_{16}O_4$, H_2O mol. wt. 242.27

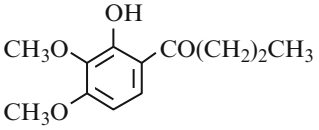
-Refer to: [2611, 2612 (**VIII**)].

4,6-Dimethylethyl ether [172219-19-1] $C_{20}H_{32}O_4$ mol. wt. 336.47

-Obtained by oxidation of 1-[4,6-bis(1,1-dimethylethoxy)-2-methoxy-3-methylphenyl]-1-butanol with NACAA (nicotinic-chromic anhydride) in methylene chloride in the presence of pyridine [1213].

1-(2-Hydroxy-3,4-dimethoxyphenyl)-1-butanone

[75218-94-9] $C_{12}H_{16}O_4$ mol. wt. 224.26



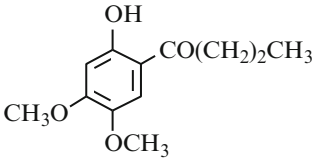
Syntheses
-Preparation by reaction of butyryl chloride with pyrogallol trimethyl ether in the presence of aluminium chloride in cooled ethyl ether for 4 h (30 %) [57].

-Also refer to: [60, 1787].

pale yellow plates [57]; m.p. 53–54° [57]; ^{1}H NMR [57].

1-(2-Hydroxy-4,5-dimethoxyphenyl)-1-butanone

[91555-34-9] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Obtained by reaction of dimethyl sulfate with 2,4,5-trihydroxybutyrophenone in the presence of potassium carbonate in refluxing benzene for 15.5 h (25 %) [2127].

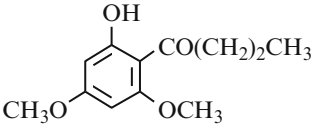
-Also obtained by reaction of n-butyronitrile with 3,4-dimethoxyphenol in the presence of zinc chloride (Houben-Hoesch reaction) (poor yield) [1537].
-Also refer to: [166, 1787].

white crystals [2127], nadeln [1537];
m.p. 81° [166, 1537], 77–78° [2127];
^{1}H NMR [2127], IR [2127].

BIOLOGICAL ACTIVITY: Central nervous system depressant [2127].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-butanone

[2999-37-3] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Preparation by reaction of butyryl chloride with phloroglucinol trimethyl ether in the presence of aluminium chloride in cooled ethyl ether for 4 h (53 %) [57].

-Also obtained by reaction of butyronitrile with 3,5-dimethoxyphenol [544, 1547].
-Also obtained by reaction of dimethyl sulfate with phlorobutyrophenone in the presence of potassium carbonate in refluxing acetone for 30–40 min (80–90 %) [2014].
-Also obtained by treatment of 2,4,6-trimethoxybutyrophenone with boron trichloride in methylene chloride at 0–5° for 2.5 h (85 %) [3068].
-Also obtained by degradation of dimethyllathodoratin (5,7-dimethoxy-3-ethylchromone) with potassium hydroxide in refluxing 50 % aqueous ethanol for 3 h (51 %) [83].
-Also refer to: [60, 545, 1464, 3069].

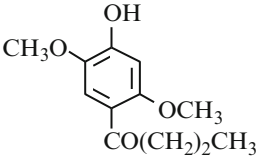
Isolation from natural sources

-From *Dysophylla stellata* Benth. (Labiatae) [1547].
-From *Dysophylla tomentosa* (Labiatae) [2242].

yellow flakes [57];
m.p. 72–74° [2242], 72–73° [1547], 70–71° [57, 83], 70° [544], 68° [203];
^{1}H NMR [57, 83, 1547, 2242], ^{13}C NMR [204],
IR [1547, 2242], UV [1547, 2242], MS [1547, 2242]; GLC [2531].

1-(4-Hydroxy-2,5-dimethoxyphenyl)-1-butanone

[105476-01-5] $C_{12}H_{16}O_4$ mol. wt. 224.26

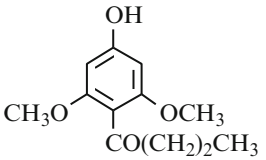


Syntheses
-Obtained by reaction of n-butyronitrile with 2,5-dimethoxyphenol (Hoesch reaction) (4 %) [166].
-Also obtained from 4-butyryl-2,5-dihydroxyphenyl glucosiduronic acid (compound **A**) [166].

elongated plates [166];
b.p.$_{0.1}$ 120–140° [166]; m.p. 86–88° [166], 85–86° [166],
IR [166], UV [166].

1-(4-Hydroxy-2,6-dimethoxyphenyl)-1-butanone

$C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Obtained by reaction of butyronitrile with phloroglucinol dimethyl ether (Hoesch reaction) (6 %) [544].
-Also obtained by treatment of 4-(benzoyloxy)-2,6-dimethoxybutyrophenone with 6 % potassium hydroxide in methanol at r.t. for 24 h [544].

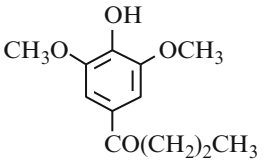
m.p. 107° [544].

Benzoate $C_{19}H_{20}O_5$ mol. wt. 328.36

m.p. 86° [544].

1-(4-Hydroxy-3,5-dimethoxyphenyl)-1-butanone
(Butyrylsyringone)

[69271-91-6] $C_{12}H_{16}O_4$ mol. wt. 224.26



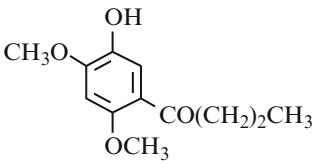
Syntheses
-Refer to: [1180, 1514, 2738, 2887].
Isolation from natural sources
-In oak wood chips [3222].
-In liquid smoke flavoring preparations [1179].

m.p. 80–82° [2887];
MS [1179, 2887, 3222]; GC-MS [1179, 3222].

BIOLOGICAL ACTIVITY: Antioxidant and organoleptic properties [1179].
-Also refer to: [2738].

1-(5-Hydroxy-2,4-dimethoxyphenyl)-1-butanone

[105475-57-8] $C_{12}H_{16}O_4$ mol. wt. 224.26

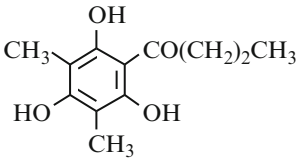


Syntheses
-Obtained by treatment of potassium 5-butyryl-2,4-di-hydroxyphenylsulphate (compound **B**) in methanol with an excess of ethereal diazomethane for 12 h (23 %) [166].
-Preparation by diazotization of 5-amino-2,4-dimethoxy-butyrophenone (22 %) [166].

pink plates [166]; m.p. 87–88° [166]; UV [166].

1-(2,4,6-Trihydroxy-3,5-dimethylphenyl)-1-butanone

[84633-27-2] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses

-Preparation by reaction of n-butyronitrile with 2,4-dimethylphloroglucinol (Houben-Hoesch reaction) [539, 1610] (**XVII**)].

-Also refer to: [724, 2414, 2451].

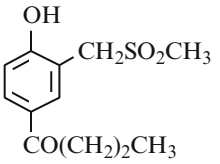
Isolation from natural sources

-From *Dryopteris abbreviata* (DC) NEWMAN (Aspidiaceae) [724].

yellow needles [724];
m.p. 140–141° [2451], 140° [539, 1610], 135–137° [724];
^{1}H NMR [724], IR [724], UV [540, 724], MS [724];
TLC [724]; HPLC [724].

1-[4-Hydroxy-3-(methylsulfonylmethyl)phenyl]-1-butanone

[56490-66-5] $C_{12}H_{16}O_4S$ mol. wt. 256.32



Synthesis

-Obtained by reaction of 3-chloromethyl-4-hydroxy-butyrophenone with magnesium methylsulfinate in refluxing dilute methanol for 18 h (50 %) [1573].

m.p. 130–132° [1573].

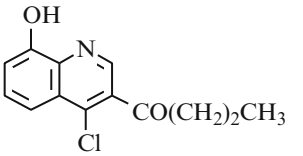
Benzyl ether [56490-73-4] $C_{19}H_{22}O_4S$ mol. wt. 346.45

-Obtained by treatment of the title ketone with benzyl chloride in the presence of potassium carbonate and sodium iodide in refluxing acetone for 18 h (61 %) [1573].

m.p. 120–122° [1573]; ^{1}H NMR [1573].

1-(4-Chloro-8-hydroxy-3-quinolinyl)-1-butanone

[125500-45-0] $C_{13}H_{12}ClNO_2$ mol. wt. 249.70



Synthesis

-Refer to: [1099].

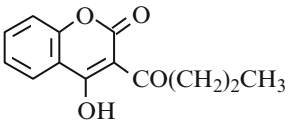
Methyl ether [115607-76-6]
$C_{14}H_{14}ClNO_2$ mol. wt. 263.72

-Refer to: [170, 1099, 1420, 1579, 1841].

m.p. 114–116° [1420, 1841]; ^{1}H NMR [1420].

4-Hydroxy-3-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[4139-74-6] $C_{13}H_{12}O_4$ mol. wt. 232.24



Syntheses

-Obtained by Fries rearrangement of 4-butyryloxycoumarin in the presence of several metal halides as catalysts at 100–150° for 30–60 min. Similarly the conversion was accomplished in nitrobenzene [1705].

The yields of 3-acyl-4-hydroxycoumarin were as follows:

$TiCl_4$ (74 %); $AlBr_3$ (50 %); $AlCl_3$ (43 %); $SnCl_4$ (25 %); $FeCl_3$ (23 %), $CrCl_3$ (21 %).

N.B.: $SnCl_2$, $SiCl_4$, $HgPh_2$; $AlPh_3$, $HgCl_2$, $ZnCl_2$, Ph_3SnCl and PhHgCl were unreactive [1705].

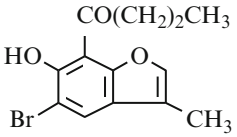
-Also obtained by reaction of butyryl chloride with 4-hydroxycoumarin in pyridine containing one drop of piperidine for 3 h on a water bath (42 %) [3174].

-Also refer to: [525, 610, 2306, 3144].

m.p. 120–121° [3174].

1-(5-Bromo-6-hydroxy-3-methyl-7-benzofuranyl)-1-butanone

[106320-28-9] $C_{13}H_{13}BrO_3$ mol. wt. 297.15



Synthesis

-Obtained by decarboxylation of 5-bromo-6-hydroxy-3-methyl-7-(1-oxobutyl)-2-benzofurancarboxylic acid on heating for 10 min at 255° [2827].

m.p. 103° [2827].

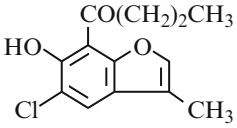
Oxime [100380-49-2] $C_{13}H_{14}BrNO_3$ mol. wt. 312.16

-Refer to: [2827].

m.p. 196° [2827].

1-(5-Chloro-6-hydroxy-3-methyl-7-benzofuranyl)-1-butanone

[100712-42-3] $C_{13}H_{13}ClO_3$ mol. wt. 252.70



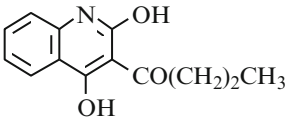
Synthesis

-Obtained by decarboxylation of 5-chloro-6-hydroxy-3-methyl-7-(1-oxobutyl)-2-benzofurancarboxylic acid on heating for 10 min at 255° [2827].

m.p. 102° [2827].

1-(2,4-Dihydroxy-3-quinolinyl)-1-butanone

$C_{13}H_{13}NO_3$ mol. wt. 231.24



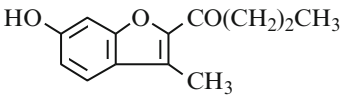
Synthesis
-Obtained by reaction of butyryl chloride with 2,4-dihydroxyquinoline in the presence of aluminium chloride in nitrobenzene on the steam bath for 3 h (25 %) [3123].

m.p. 218–219° [3123]; UV [3123].

BIOLOGICAL ACTIVITY: Antibacterial properties (Staphylococcus aureus and Escherichia coli) [3123].

1-(6-Hydroxy-3-methyl-2-benzofuranyl)-1-butanone

[99245-46-2] $C_{13}H_{14}O_3$ mol. wt. 218.25



Syntheses
-Obtained by Fries rearrangement of 6-butyryloxy-3-methylbenzofuran (m.p. 45°) with aluminium chloride in nitrobenzene at r.t. overnight [2825].

-Also refer to: [2826].

m.p. 124° [2825, 2826].

Acetate [100976-33-8] $C_{15}H_{16}O_4$ mol. wt. 260.29

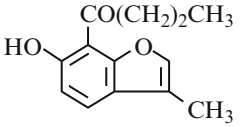
m.p. 85–86° [2825, 2826].

Methyl ether [56397-48-9] $C_{14}H_{16}O_3$ mol. wt. 232.28

m.p. 93–94° [2825, 2826].

1-(6-Hydroxy-3-methyl-7-benzofuranyl)-1-butanone

[107623-54-1] $C_{13}H_{14}O_3$ mol. wt. 218.25

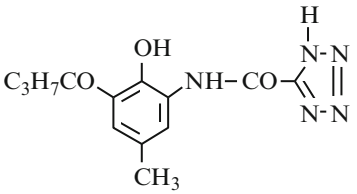


Syntheses
-Obtained by decarboxylation of 6-hydroxy-7-butyryl-3-methylcoumarilic acid [2826].
-Also obtained by alkaline hydrolysis of 3-bromo-7-hydroxy-8-butyryl-4-methylcoumarin (m.p. 146°) [2826].

m.p. 83° [2826].

N-(3-Butanoyl-2-hydroxy-5-methylphenyl)-1*H*-tetrazole-5-carboxamide

[70977-53-6] $C_{13}H_{15}N_5O_3$ mol. wt. 289.30

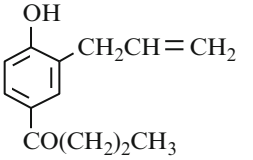


Synthesis
-Refer to: [1017 (37 %)].
m.p. 231–233° (d) [1017].

BIOLOGICAL ACTIVITY: Antiallergic [1017].

1-[4-Hydroxy-3-(2-propenyl)phenyl]-1-butanone

[97023-54-6] $C_{13}H_{16}O_2$ mol. wt. 204.27

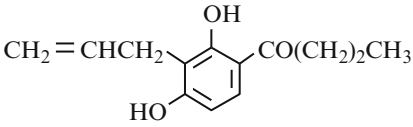


Syntheses
-Obtained by Claisen rearrangement of 4-allyloxy-butyrophenone in boiling dimethylaniline for 5–6 h [511].
-Also refer to: [467].
b.p.$_{16}$ 206–207° [511]; m.p. 64° [511].

USE: As intermediate for squalene synthase inhibitors [467].

1-[2,4-Dihydroxy-3-(2-propenyl)phenyl]-1-butanone

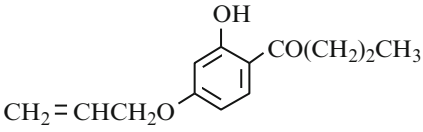
[194792-30-8] $C_{13}H_{16}O_3$ mol. wt. 220.27



Synthesis
-Refer to: [22].

1-[2-Hydroxy-4-(2-propenyloxy)phenyl]-1-butanone

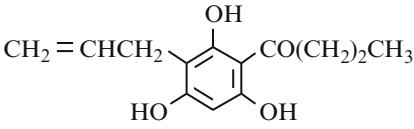
[194792-29-5] $C_{13}H_{16}O_3$ mol. wt. 220.27



Synthesis
-Refer to: [22].

1-[2,4,6-Trihydroxy-3-(2-propenyl)phenyl]-1-butanone
2-Butyryl-4-(propen-2-yl)phloroglucinol (**16**) [1026]

$C_{13}H_{16}O_4$ mol. wt. 236.27



Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and allyl chloride to a solution of phlorobutyrophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

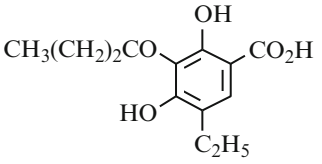
-Also refer to: [1501, 1502].

^{1}H NMR [1026], ^{13}C NMR [1026], IR [1026].

BIOLOGICAL ACTIVITY: Antimicrobial [1026, 1501, 1502].

1-[5-Ethyl-2,4-dihydroxy-3-(1-oxobutyl)]benzoic acid

[106214-14-6] $C_{13}H_{16}O_5$ mol. wt. 252.27



Syntheses

-Obtained by adding butyric anhydride to a cold solution of methyl 2,4-dihydroxy-5-ethylbenzoate and aluminium chloride in nitrobenzene. The mixture was left overnight at r.t., and then heated at 100–105° for 4 h (16 %) [2811].

-Also obtained by hydrolysis of the methyl ester with 10 % NaOH on a water bath for 1 h and then kept overnight at r.t. [2811].

m.p. 181° [2811].

Methyl ester [108125-65-1] $C_{14}H_{18}O_5$ mol. wt. 266.29

-Obtained at the same time in the first reaction above mentioned (20 %) [2811].

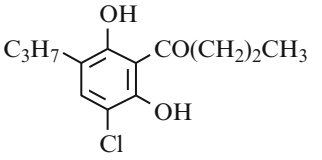
m.p. 66° [2811].

Dibenzoate of the methyl ester [103098-69-7] $C_{28}H_{26}O_7$ mol. wt. 474.51

m.p. 108° [2811].

1-(3-Chloro-2,6-dihydroxy-5-propylphenyl)-1-butanone

[120058-71-1] $C_{13}H_{17}ClO_3$ mol. wt. 256.73

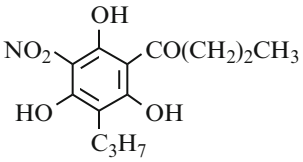


Synthesis

-Refer to: [1836 (**1 h**)].

1-(2,4,6-Trihydroxy-3-nitro-5-propylphenyl)-1-butanone

[119691-99-5] $C_{13}H_{17}NO_6$ mol. wt. 283.28



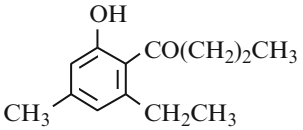
Synthesis
-Obtained by adding a mixture of fuming nitric acid and acetic acid to the solution of 1-(2,4,6-trihydroxy-3-propylphenyl)-1-butanone in acetic acid at 60° for 30 min (30–40 %) [3414].

m.p. 67–69° [3414]; ^{1}H NMR [3414], IR [3414], MS [3414].

BIOLOGICAL ACTIVITY: Germination inhibitory activity [3414]; PET inhibition [3414].

1-(2-Ethyl-6-hydroxy-4-methylphenyl)-1-butanone

$C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses
-Preparation by Fries rearrangement of 3-ethyl-5-methyl-phenyl butyrate with aluminium chloride,
*without solvent at 130° for 2 h (79 %) [2802];
*in nitrobenzene at 25° for 6 h (80 %) [2802].

m.p. 58° [2802].

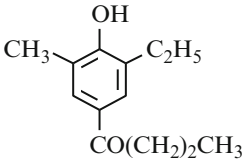
Methyl ether $C_{14}H_{20}O_2$ mol. wt. 220.31

-Obtained by methylation of the above ketone in the usual way [2802].

b.p.$_{28}$ 175° [2802].

1-(3-Ethyl-4-hydroxy-5-methylphenyl)-1-butanone

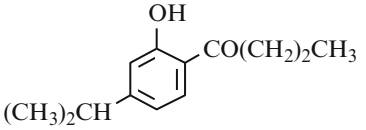
$C_{13}H_{18}O_2$ mol. wt. 206.28



Synthesis
-Obtained by Fries rearrangement of 2-ethyl-6-methylphenyl n-butyrate (b.p. 258–261°) in the presence of aluminium chloride (53 %) [184].
m.p. 86–87° [184].

1-[2-Hydroxy-4-(1-methylethyl)phenyl]-1-butanone

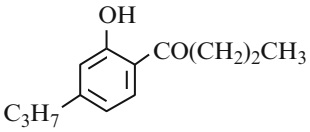
$C_{13}H_{18}O_2$ mol. wt. 206.28



Synthesis
-Refer to: [2940].
ESR [2940].

1-(2-Hydroxy-4-propylphenyl)-1-butanone

$C_{13}H_{18}O_2$ mol. wt. 206.28



Synthesis
-Obtained by reaction of butyric acid with 3-propylphenol in the presence of zinc chloride (Nencki reaction) (30–40 %) [728].

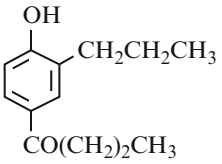
$b.p._{0.7}$ 87–88° [728], $b.p._{19}$ 130–132° [728].

Semicarbazone $C_{14}H_{21}N_3O_2$ mol. wt. 263.34

yellow solid [728]; m.p. 175° [728].

1-(4-Hydroxy-3-propylphenyl)-1-butanone

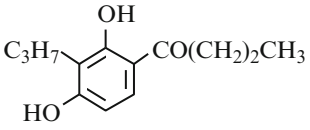
$C_{13}H_{18}O_2$ mol. wt. 206.28



Synthesis
-Obtained by reaction of butyryl chloride with 2-propylphenol in the presence of aluminium chloride in nitrobenzene at r.t. overnight [2648].
$b.p._{14}$ 210° [2648]; m.p. 54° [2648].

1-(2,4-Dihydroxy-3-propylphenyl)-1-butanone

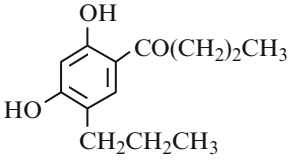
[194792-31-9] $C_{13}H_{18}O_3$ mol. wt. 222.28



Syntheses
-Refer to: [20, 22, 307].

1-(2,4-Dihydroxy-5-propylphenyl)-1-butanone

$C_{13}H_{18}O_3$ mol. wt. 222.28



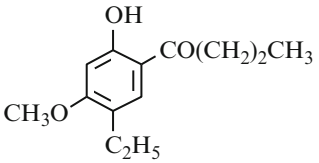
Synthesis
-Obtained by Fries rearrangement of 4-propylresorcinol dibutyrate/4-propylresorcinol mixture with aluminium chloride in nitrobenzene at 50° for 4 h [2651].
$b.p._{9}$ 190° [2651]; m.p. 64° [2651].

Phenylhydrazone $C_{19}H_{24}N_2O_2$ mol. wt. 312.41

m.p. 139–140° [2651].

1-(5-Ethyl-2-hydroxy-4-methoxyphenyl)-1-butanone

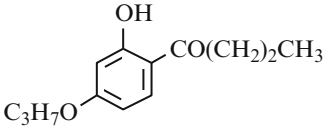
[178754-67-1] $C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Obtained by acylation of 4-ethylresorcinol with butyric acid in the presence of zinc chloride and phosphorous oxychloride, followed by methylation of the non-chelated hydroxy group [2397].

1-(2-Hydroxy-4-propoxyphenyl)-1-butanone

$C_{13}H_{18}O_3$ mol. wt. 222.28

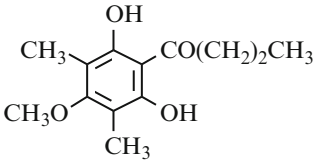


Synthesis
-Refer to: [851].
Oxime [168978-08-3]
$C_{13}H_{19}NO_3$ mol. wt. 237.30

USE: Reagent for copper determination by gravimetry and spectrophotometry [851].

1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-1-butanone
(Methylaspidinol) (**V**)

[4069-47-0] $C_{13}H_{18}O_4$ mol. wt. 238.28

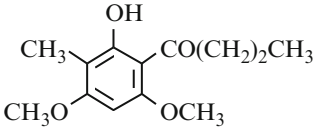


Syntheses
-Obtained by alkaline cleavage of *para*-aspidin (**I**) with zinc dust in 5 % sodium hydroxide on a water bath for 5 min [2445].
-Also refer to: [37, 2442, 2451, 3113].

m.p. 111° [2445, 3113], 109–111° [2451], 108–110° [37]; UV [37].

1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-1-butanone

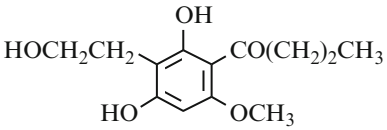
[69480-08-6] $C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses
-Refer to: [203, 2531, 2630].
m.p. 111–112° [2630], 108–110° [203]; ^{13}C NMR [203]; GLC [2531].

1-[2,4-Dihydroxy-3-(2-hydroxyethyl)-6-methoxyphenyl]-1-butanone
(Phomalone)

[159768-89-5] $C_{13}H_{18}O_5$ mol. wt. 254.28

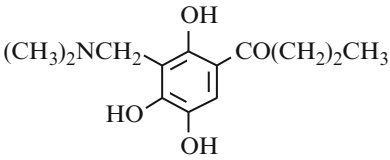


Synthesis
-Refer to: [202].
m.p. 126–127° [201];
^{1}H NMR [201], ^{13}C NMR [201], UV [201].

USE: Wood and lawn fungicide [202].

1-[3-[(Dimethylamino)methyl]-2,4,5-trihydroxyphenyl]-1-butanone

[50113-09-5] $C_{13}H_{19}NO_4$ mol. wt. 253.30

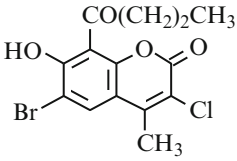


Synthesis
-Refer to: [2787].

USE: Photostabilizer for polymers [2787]; Polydentate ligand for copper [2787].

6-Bromo-3-chloro-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

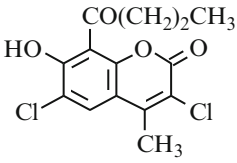
$C_{14}H_{12}BrClO_4$ mol. wt. 359.60



Synthesis
-Obtained by Fries rearrangement of 6-bromo-7-butyryloxy-3-chloro-4-methylcoumarin (m.p. 138°) with aluminium chloride for 1.5 h at 155° [2827].
m.p. 171–172° [2827].

3,6-Dichloro-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

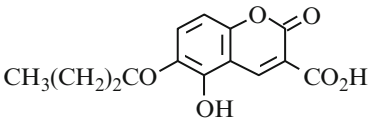
$C_{14}H_{12}Cl_2O_4$ mol. wt. 315.15



Synthesis
-Obtained by Fries rearrangement of 7-butyryloxy-3,6-dichloro-4-methylcoumarin with aluminium chloride for 1.5 h at 155° [2827].

5-Hydroxy-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one-3-carboxylic acid

$C_{14}H_{12}O_6$ mol. wt. 276.25

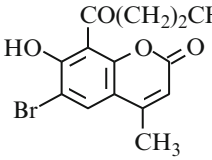


Synthesis
-Preparation by the condensation of the 2,4-dihydroxy-3-formylbutyrophenone with cyanoacetic acid [2821].

straw-coloured needles [2821]; m.p. 198–200° (d) [2821].

6-Bromo-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[110029-30-6] $C_{14}H_{13}BrO_4$ mol. wt. 325.16



Syntheses

-Obtained by Pechmann condensation of 1-(2,6-dihydroxy-3-bromophenyl)-1-butanone with ethyl acetoacetate in presence of 80 % sulfuric acid [2811].

-Also obtained by Fries rearrangement of 7-butyryloxy-6-bromo-4-methylcoumarin (m.p. 120°) with aluminium chloride at 145–150° for an hour (40 %) [2811].

yellow needles [2811]; m.p. 157° [2811].

Semicarbazone [109262-64-8] $C_{15}H_{16}BrN_3O_4$ mol. wt. 382.21

colourless granules; m.p. 231° (d) [2811].

Acetate [109602-86-0] $C_{16}H_{15}BrO_5$ mol. wt. 367.20

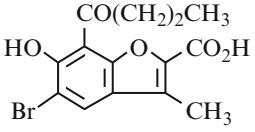
colourless needles [2811]; m.p. 128° [2811].

Benzoate [112222-68-1] $C_{21}H_{17}BrO_5$ mol. wt. 429.27

colourless lustrous cubes [2811]; m.p. 151° [2811].

5-Bromo-6-hydroxy-3-methyl-7-(1-oxobutyl)-2-benzofurancarboxylic acid

[108955-15-3] $C_{14}H_{13}BrO_5$ mol. wt. 341.16



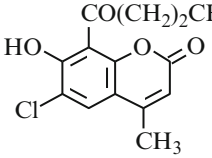
Synthesis

-Obtained by Fries rearrangement of 5-bromo-6-butyryloxy-3-methylcoumarilic acid (m.p. 261°) with aluminium chloride for 1 h at 150–160° [2827].

m.p. 268° [2827].

6-Chloro-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[109103-09-5] $C_{14}H_{13}ClO_4$ mol. wt. 280.78



Syntheses

-Obtained by Pechmann condensation of 1-(2,6-dihydroxy-3-chlorophenyl)-1-butanone with ethyl acetoacetate in presence of 80 % sulfuric acid [2811].

-Also obtained by Fries rearrangement of 7-butyryloxy-6-chloro-4-methylcoumarin (m.p. 119°) (33 %) [2811].

yellow fibrous needles [2811]; m.p. 153° [2811].

Oxime $C_{14}H_{14}ClNO_4$ mol. wt. 295.72

colourless needles [2811]; m.p. 197° (d) [2811].

Acetate $C_{16}H_{15}ClO_5$ mol. wt. 322.74

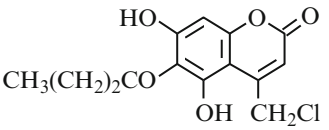
colourless needles [2811]; m.p. 139° [2811].

Benzoate [112222-67-0] $C_{21}H_{17}ClO_5$ mol. wt. 384.82

colourless lustrous cubes [2811]; m.p. 144° [2811].

4-(Chloromethyl)-5,7-dihydroxy-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[98498-60-3] $C_{14}H_{13}ClO_5$ mol. wt. 296.71

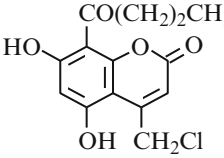


Syntheses
-Obtained by condensation of 2-butyrylphloroglucinol with ethyl 4-chloro-3-oxobutanoate (61 %) [763].
-Also obtained from a Pechmann reaction (low yield) [766].

yellow solid [763]; m.p. 225–230° (d) [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

4-(Chloromethyl)-5,7-dihydroxy-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

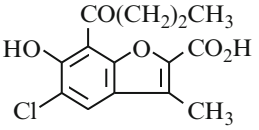
[111249-71-9] $C_{14}H_{13}ClO_5$ mol. wt. 296.71



Synthesis
-Obtained by condensation of 2-butyrylphloroglucinol with ethyl 4-chloro-3-oxobutanoate (3 %) [763].
m.p. 210–212° (d) [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

5-Chloro-6-hydroxy-3-methyl-7-(1-oxobutyl)-2-benzofurancarboxylic acid

[109103-12-0] $C_{14}H_{13}ClO_5$ mol. wt. 296.71

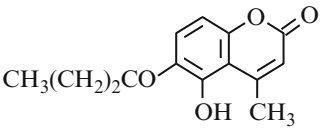


Synthesis
-Obtained by Fries rearrangement of 5-chloro-6-butyryloxy-3-methylcoumarilic acid with aluminium chloride for 1 h at 150–160° [2827].

m.p. 255° [2827].

5-Hydroxy-4-methyl-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[855159-27-2] $C_{14}H_{14}O_4$ mol. wt. 246.26



Syntheses

-Obtained by condensation of resbutyrophenone with ethyl acetoacetate in the presence of aluminium chloride in nitrobenzene for 1 h at 120–130° (37 %) [841].

-Also obtained by Fries transformation of 5-butyroxy-4-methylcoumarin (m.p. 100–101°) with aluminium chloride [841].
-Also refer to: [2824].

m.p. 141–142° [841, 2824].

Acetate $C_{16}H_{16}O_5$ mol. wt. 288.30

-Preparation by means of acetic anhydride in pyridine with the title ketone [841].

m.p. 167° [841].

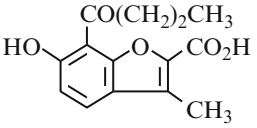
Methyl ether $C_{15}H_{16}O_4$ mol. wt. 260.29

-Obtained by reaction of methyl iodide with the title ketone in the presence of potassium carbonate in refluxing acetone for 24 h [841].

m.p. 83–84° [841].

6-Hydroxy-7-(1-oxobutyl)-3-methylcoumarilic acid

[109564-87-6] $C_{14}H_{14}O_5$ mol. wt. 262.26



Synthesis

-Obtained by Fries rearrangement of 6-butyryloxy-3-methyl-coumarilic acid [m.p. 197° (d)] with aluminium chloride for 1 h at 150–160° [2826].

m.p. 218° [2826].

Acetate [130907-67-4] $C_{16}H_{16}O_6$ mol. wt. 304.30

m.p. 211° [2826].

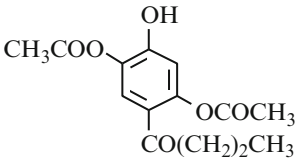
Methyl ether [109641-80-7] $C_{15}H_{16}O_5$ mol. wt. 276.29

-Refer to: [2826].

m.p. 107–108° [2826].

1-[2,5-Bis(acetyloxy)-4-hydroxyphenyl]-1-butanone

[145747-22-4] $C_{14}H_{16}O_6$ mol. wt. 280.28

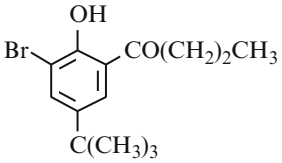


Syntheses
-Obtained by partial enzymatic deacylation of 2,4,5-triacetoxybutyrophenone (**8**) at 42–45° for 40 h [376, 2410],
*with **PPL** (Porcine pancreatic lipase),
-in THF (tetrahydrofuran) (40 %) (**16**) [376];
-in DIPE (diisopropyl ether) (40 %) (**16**) [376];
-in acetone (30 %) (**16**) [376].
*with **CCL** (Candida cylindracea lipase),
-in THF (tetrahydrofuran) (65 %) (**16**) [376], (65 %) (**13**) [2412];
-in a THF and n-butanol mixture (65 %) (**19**) [2410];
-in DIPE (diisopropyl ether) (50 %) (**16**) [376];
-in acetone (30 %) (**16**) [376].

m.p. 142–143° [376];
^{1}H NMR [376], MS [376], UV [376]; TLC [376].

1-[3-Bromo-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-butanone

[100792-29-8] $C_{14}H_{19}BrO_2$ mol. wt. 299.21



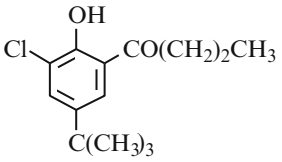
Synthesis
-Obtained by Fries rearrangement of 2-bromo-4-tert-butylphenyl butyrate with aluminium chloride at 110° for 2 h (65 %) [3113].
b.p.$_{.2}$ 150° [3113].

2,4-Dinitrophenylhydrazone $C_{20}H_{23}BrN_4O_5$ mol. wt. 479.33

m.p. 175° [3113].

1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-butanone

[106321-41-9] $C_{14}H_{19}ClO_2$ mol. wt. 254.76



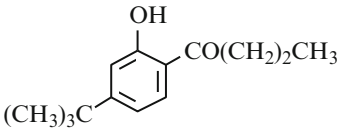
Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-tert-butylphenyl butyrate with aluminium chloride at 110° (80 %) [3119].
b.p.$_{10}$ 152° [3119].

2,4-Dinitrophenylhydrazone $C_{20}H_{23}ClN_4O_5$ mol. wt. 434.88

m.p. 176° [3119].

1-[4-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-butanone

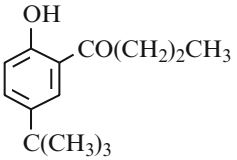
$C_{14}H_{20}O_2$ mol. wt. 220.31



Synthesis
-Refer to: [2940].
ESR [2940].

1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-butanone

[75060-53-6] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses
-Obtained by Fries rearrangement of 4-tert-butylphenyl butyrate with aluminium chloride in carbon disulfide at r.t., then at 120° for 1 h after solvent elimination (57 %) [2796].

-Also obtained by treatment of 2-methoxy-5-tert-butyl-butyrophenone with 47 % hydrobromic acid/57 % hydriodic acid mixture in refluxing acetic acid for 2 h (81 %) [1475].

b.p.$_{20}$ 150° [2796]; ^{1}H NMR [1475]; ESR [2940]; TLC [1475].

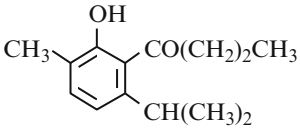
Methyl ether [75060-46-7] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Obtained by reaction of butyryl chloride with 4-tert-butylanisole in the presence of aluminium chloride in methylene chloride under nitrogen, first at 0°, then at 20° for 30 min (85 %) [1475].

^{1}H NMR [1475]; TLC [1475].

1-[2-Hydroxy-3-methyl-6-(1-methylethyl)phenyl]-1-butanone

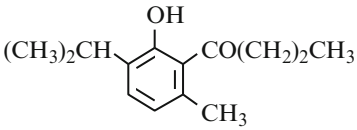
$C_{14}H_{20}O_2$ mol. wt. 220.31



Synthesis
-Preparation by Fries rearrangement of carvacryl butyrate with aluminium chloride at 120° (70 %) [2798].
b.p.$_3$ 142° [2798].

1-[2-Hydroxy-3-(1-methylethyl)-6-methylphenyl]-1-butanone

[106476-93-1] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses

-Obtained by Fries rearrangement of thymyl butyrate with aluminium chloride without solvent at 120° (85 %) [2803].

-Also obtained by reaction of butyric acid with thymol in the presence of aluminium chloride on heating at reflux for 12 h (81 %) [2960].
-Also refer to: [2961].

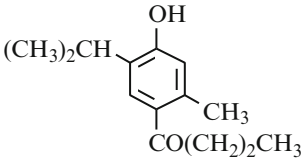
b.p.$_2$ 190° [2803], b.p.$_{12}$ 120–121° [2960, 2961].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 216° [2803].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-butanone

[95185-72-1] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses

-Obtained by Fries rearrangement of thymyl butyrate with aluminium chloride in nitrobenzene,
*first 2 h at 30°, then at r.t. for 24 h [2704];
*for 12 h at 30° (86 %) [2647].

-Also obtained by refluxing its methyl ether with pyridinium chloride (205–215°) for 40 min (40 %) [2660].

b.p.$_{14}$ 204° [2648], b.p.$_{14}$ 203–205° [2660]; m.p. 94° [2660], 93–94° [2647].

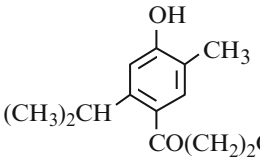
Methyl ether [854870-33-0] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Obtained by reaction of butyryl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (50 %) [2660].
-Also refer to: [1652, 2647].

b.p.$_{16}$ 175–178° [2660]; m.p. 50° [2647, 2660].

1-[4-Hydroxy-5-methyl-2-(1-methylethyl)phenyl]-1-butanone

$C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses

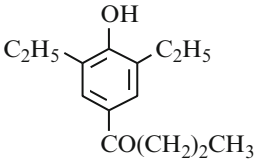
-Obtained by reaction of butyryl chloride with carvacrol in the presence of aluminium chloride in nitrobenzene at r.t. for 48 h (16 %) [1522] or first at $\leq 50°$, then at r.t. overnight [2650].

-Also obtained by Fries rearrangement of carvacryl butyrate with aluminium chloride in nitrobenzene for 24 h at 25° (88 %) [2647].

b.p.$_{15}$ 200° [2650]; m.p. 66° [1522, 2647, 2650].

1-(3,5-Diethyl-4-hydroxyphenyl)-1-butanone

[104008-48-2] $C_{14}H_{20}O_2$ mol. wt. 220.31

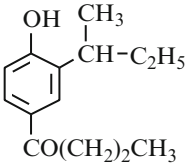


Syntheses

-Refer to: [3005, 3006].

1-[4-Hydroxy-3-(1-methylpropyl)phenyl]-1-butanone

[16648-70-7] $C_{14}H_{20}O_2$ mol. wt. 220.31



Synthesis

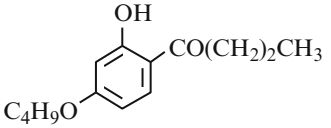
-Refer to: [1205].

b.p.$_1$ 170–175° [1205];

m.p. 96–97° [1205].

1-(4-Butyloxy-2-hydroxyphenyl)-1-butanone

$C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses

-Obtained by butylation of 2,4-dihydroxybutyrophenone [1587].

-Also refer to: [2400].

b.p.$_8$ 200° [1587]; m.p. 30° [1587].

Oxime [161138-02-9] $C_{14}H_{21}NO_3$ mol. wt. 251.33

m.p. 106° [1587].

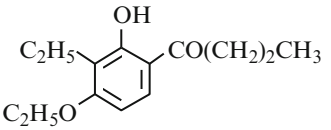
USE: Nickel (II) and copper (II) simultaneous detn. in synthetic mixts. and alloy samples using this oxime as an extractive spectrophotometric reagent [2400]; Spectrophotometric and gravimetric reagent for Cu (II) [3048].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_6$ mol. wt. 416.43

m.p. 187° [1587].

1-(4-Ethoxy-3-ethyl-2-hydroxyphenyl)-1-butanone

$C_{14}H_{20}O_3$ mol. wt. 236.31



Synthesis
-Obtained by ethylation of 2,4-dihydroxybutyrophenone [1587].
b.p.$_5$ 155° [1587]; m.p. 45° [1587].

Oxime $C_{14}H_{21}NO_3$ mol. wt. 251.33

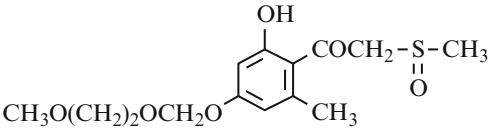
m.p. 141° [1587].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_6$ mol. wt. 416.43

m.p. 201° [1587].

1-[2-Hydroxy-4-(β-methoxyethoxymethoxy)-6-methylphenyl]-2-(methylsulfinyl)-1-ethanone

[104783-90-6] $C_{14}H_{20}O_6S$ mol. wt. 316.37

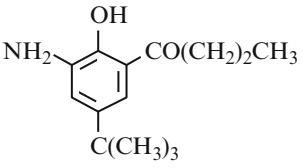


Synthesis
-A mixture of DMSO and sodium hydride (70 % in oil) in benzene was stirred at 80° for 1 h, then cooled to 35° and treated dropwise with ethyl 2-hydroxy-4-(β-methoxyethoxy)methoxy-6-methylbenzoate (86 %) [1157].

m.p. 106–107° [1157]. ^{1}H NMR [1157], IR [1157].

1-[3-Amino-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-butanone

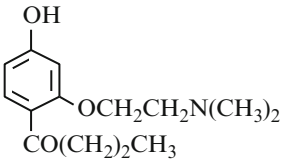
$C_{14}H_{21}NO_2$ mol. wt. 235.33



Synthesis
-Refer to: [2105].

1-[2-(N,N-Dimethylaminoethoxy)-4-hydroxyphenyl]-1-butanone

$C_{14}H_{21}NO_3$ mol. wt. 251.33



Synthesis
-Refer to: [787].

Methyl ether (hydrochloride)
$C_{15}H_{23}NO_3$, HCl mol. wt. 301.81

-Obtained by adding a solution of 2-hydroxy-4-methoxybutyrophenone and sodium ethoxide in ethanol to the N,N-dimethylaminoethyl chloride. Then, the mixture was refluxed for 3 h [787].

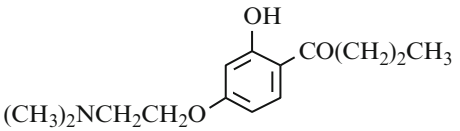
m.p. 101–102° [787].

BIOLOGICAL ACTIVITY: Local anaesthetic [787]; Antispasmodic [787]; Convulsions [787].

LD_{50} 130 [787].

1-[4-(N,N-Dimethylaminoethoxy)-2-hydroxyphenyl]-1-butanone

$C_{14}H_{21}NO_3$ mol. wt. 251.33



Synthesis
-Obtained by adding a solution of resbutyrophenone and sodium ethoxide in ethanol to the N, N-dimethylaminoethyl chloride. Then, the mixture was refluxed for 3 h [787].

Hydrochloride $C_{14}H_{21}NO_3$, HCl mol. wt. 287.79

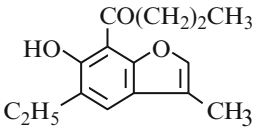
m.p. 154–156° [787].

BIOLOGICAL ACTIVITY: Local anaesthetic [787]; Antispasmodic [787]; Convulsions [787]; Transient decrease of arterial blood pressure [787]; Increase of resistance of isolated heart to anoxia [787].

LD_{50} 250 [787].

1-(5-Ethyl-6-hydroxy-3-methyl-7-benzofuranyl)-1-butanone

[101088-95-3] $C_{15}H_{18}O_3$ mol. wt. 246.31

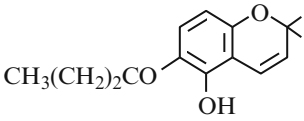


Synthesis
-Obtained by decarboxylation of 5-ethyl-6-hydroxy-3-methyl-7-(1-oxobutyl)-2-benzofurancarboxylic acid on heating for 10 min at 255° [2827].

m.p. 57° [2827].

1-(5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone
6-Butyryl-5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran

$C_{15}H_{18}O_3$ mol. wt. 246.31

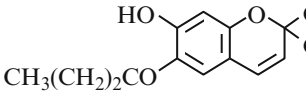


Synthesis
-Obtained by treatment of 6-butyryl-5-hydroxy-2,2-dimethyl-3,4-dihydro-2*H*-1-benzopyran with DDQ in refluxing benzene for 48 h (80 %) [58].

m.p. 65–66° [58]; ^{1}H NMR [58].

1-(7-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone
6-Butyryl-7-hydroxy-2,2-dimethyl-2*H*-1-benzopyran

$C_{15}H_{18}O_3$ mol. wt. 246.31

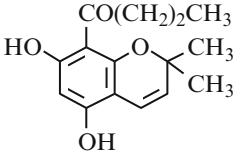


Synthesis
-Obtained by treatment of 6-butyryl-5-hydroxy-2,2-dimethyl-3,4-dihydro-2*H*-1-benzopyran with DDQ in refluxing benzene for 48 h (80 %) [58].

m.p. 53–54° [58]
^{1}H NMR [58].

1-(5,7-Dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-1-butanone

$C_{15}H_{18}O_4$ mol. wt. 262.31



Synthesis
-Refer to: [3203].
Dimethyl ether [924889-47-4]
$C_{17}H_{22}O_4$ mol. wt. 290.36

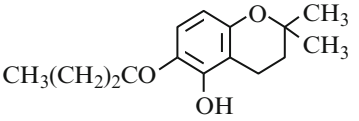
-Obtained by treatment of Malloapelta B with sodium borohydride in methanol, for 10 min at 10–15°, then 10 min at 60° (90 %) [3203].

white solid [3203]; m.p. 62.8° [3203];
^{1}H NMR [3203], IR [3203].

BIOLOGICAL ACTIVITY: Exploration of essential structure of malloapelta B for the inhibitory activity against TNF-induced NF-kB activation [3203]; Cytotoxicity [3203].

1-(3,4-Dihydro-5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone
6-Butyryl-5-hydroxy-2,2-dimethyl-3,4-dihydro-2*H*-1-benzopyran

[93970-91-3] $C_{15}H_{20}O_3$ mol. wt. 248.32



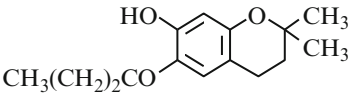
Syntheses
-Obtained by reaction of 2,4-dihydroxybutyrophenone with 2-methyl-1,3-butadiene in petrol in the presence of polyphosphoric acid at 30–35° for 18 h (45 %) [58].

-Also refer to: [59].

m.p. 53–54° [58]; ^{1}H NMR [58].

1-(3,4-Dihydro-7-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone
6-Butyryl-7-hydroxy-2,2-dimethyl-3,4-dihydro-2*H*-1-benzopyran

[93970-92-4] $C_{15}H_{20}O_3$ mol. wt. 248.32



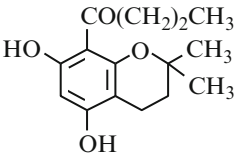
Syntheses
-Obtained by reaction of 2,4-dihydroxybutyrophenone with 2-methyl-1,3-butadiene in petrol in the presence of polyphosphoric acid at 30–35° for 18 h (40 %) [58].

-Also refer to: [59].

m.p. 95–96° [58]; ^{1}H NMR [58].

1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-1-butanone

[105306-66-9] $C_{15}H_{20}O_4$ mol. wt. 264.32



Syntheses
-Refer to: [708, 3192, 3203].
^{13}C NMR [840], IR [840], MS [3192].

Dimethyl ether [924889-46-3]
$C_{17}H_{24}O_4$ mol. wt. 292.30

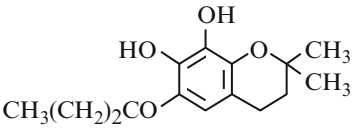
-Obtained by treatment of Malloapelta B in methanol with hydrogen in the presence of 10 % Pd/C at r.t. for overnight (80 %) [3203].

white solid [3203]; m.p. 48.8° [3203];
^{1}H NMR [3203], IR [3203]; TLC [3203].

1-(3,4-Dihydro-7,8-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone

6-Butyryl-7,8-dihydroxy-2,2-dimethyl-3,4-dihydro-2*H*-1-benzopyran

[93970-90-2] $C_{15}H_{20}O_4$ mol. wt. 264.32



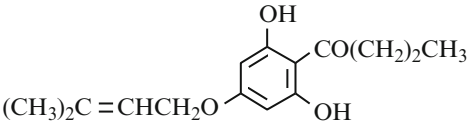
Synthesis

-Obtained by reaction of 2,3,4-trihydroxybutyrophenone with 2-methyl-1,3-butadiene in petrol in the presence of polyphosphoric acid at 30–35° for 18 h (80 %) [58].

m.p. 66–67° (page 360) and 82–83° (page 361) (?) [58];
^{1}H NMR [58].

1-[2,6-Dihydroxy-4-[(3-methyl-2-butenyl)oxy]phenyl]-1-butanone

[122585-49-3] $C_{15}H_{20}O_4$ mol. wt. 264.32



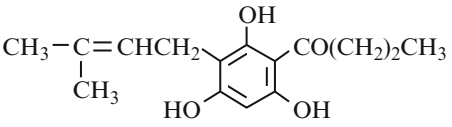
Isolation from natural sources

-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].

colourless crystals [1488]; m.p. 119° [1488];
^{1}H NMR [1488], IR [1488], MS [1488].

1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone

[69916-08-1] $C_{15}H_{20}O_4$ mol. wt. 264.32



Syntheses

-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and prenyl bromide to a solution of phlorobutyrophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

-Also prepared by adding prenyl bromide to a suspension of the sodium salt of phlorobutyrophenone in benzene, then the mixture obtained was refluxed for 3 h [1026].

-Also prepared by adding at 5° a solution of sodium methoxide in methanol, followed by isopentenyl bromide in ethyl ether to a solution of phlorobutyrophenone in benzene and ethyl ether; then the mixture was stirred at r.t. for 6 h (16 %) [2113].

-Also obtained by adding prenyl chloride to a two-phase mixture consisting of phlorobutyrophenone in diethyl ether and saturated aqueous sodium carbonate. A catalytic amount of CuCl was added and the mixture was stirred or shaken vigorously for 3 h at r.t. (70 %) [838].

Isolation from natural sources

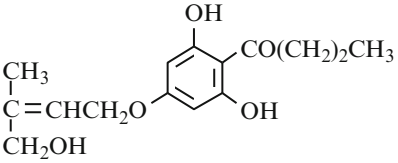
-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].

m.p. 147° [2113], 140–143° [838];
^{1}H NMR [1026, 1488], ^{13}C NMR [838, 1026],
IR [838, 1026, 1488], MS [838, 1488].

BIOLOGICAL ACTIVITY: Antifungal [2113].

1-[2,6-Dihydroxy-4-[(4-hydroxy-3-methyl-2-butenyl)oxy]phenyl]-1-butanone *(E)*

[122585-50-6] $C_{15}H_{20}O_5$ mol. wt. 280.32

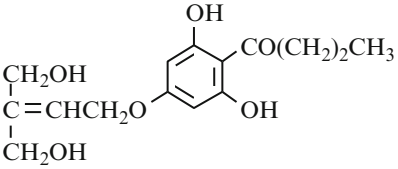


Isolation from natural sources
-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].

^{1}H NMR [1488], IR [1488], MS [1488].

1-[2,6-Dihydroxy-4-[[4-hydroxy-3-(hydroxymethyl)-2-butenyl]oxy]phenyl]-1-butanone

[122616-67-5] $C_{15}H_{20}O_6$ mol. wt. 296.32



Isolation from natural sources
-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].

Tetraacetate* [122585-96-0]
$C_{23}H_{28}O_{10}$ mol. wt. 464.47

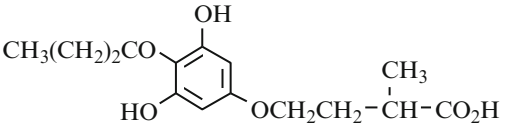
-Refer to: [1488].

^{1}H NMR [1488], IR [1488], MS [1488].

*1-[2,6-Bis(acetyloxy)-4-[[4-(acetyloxy)-3-[(acetyloxy)methyl]-2-butenyl]oxy]phenyl]-1-butanone

4-[3,5-Dihydroxy-4-(1-oxobutyl)phenoxy]-2-methyl-1-butanoic acid

[122585-56-2] $C_{15}H_{20}O_6$ mol. wt. 296.32

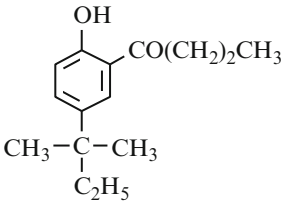


Isolation from natural sources
-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].

^{1}H NMR [1488], IR [1488], MS [1488].

1-]2-Hydroxy-5-(1,1-dimethylpropyl)phenyl]-1-butanone

[854867-25-7] $C_{15}H_{22}O_2$ mol. wt. 234.34



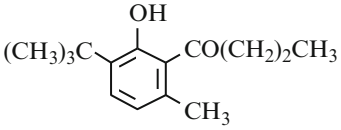
Synthesis
-Obtained by Fries rearrangement of p-tert-amylphenyl butyrate at 120° for 1 h (73 %) [2796].
b.p.$_{20}$ 165° [2796].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 186° [2796].

1-[2-Hydroxy-6-methyl-3-(1,1-dimethylethyl)phenyl]-1-butanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Obtained by Fries rearrangement of 2-tert-butyl-5-methylphenyl butyrate,
*in the presence of aluminium chloride (1.5 equiv.) in nitrobenzene at 25° for 6 h (80 %) [3118];
*in the presence of aluminium chloride (3 equiv.) without solvent at 110° for 2 h (78 %) [3118].

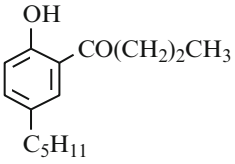
b.p.$_8$ 112° [3118].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 219° [3118].

1-(2-Hydroxy-5-pentylphenyl)-1-butanone

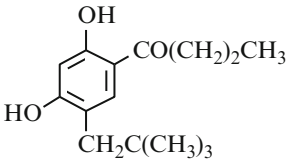
[101100-37-2] $C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis
-Preparation by reaction of butyric acid with n-pentylphenol in the presence of boron trifluoride at 140–150° (88 %) [142].
b.p.$_{16}$ 185–192° [142].
$n_D^{25} = 1.518$ [142].

1-[2,4-Dihydroxy-5-(2,2-dimethylpropyl)phenyl]-1-butanone

$C_{15}H_{22}O_3$ mol. wt. 250.34

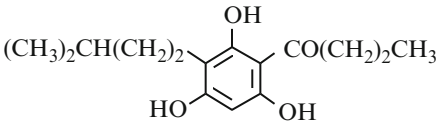


Synthesis
-Refer to: [2704] (Japanese patent).
m.p. 117° [2704].

USE: As colour developer [2704].

1-[2,4,6-Trihydroxy-3-(3-methylbutyl)phenyl]-1-butanone

[74477-97-7] $C_{15}H_{22}O_4$ mol. wt. 266.34



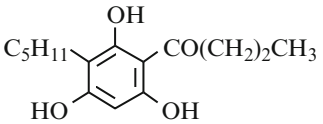
Synthesis
-Obtained by hydrogenation of 1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)-phenyl]-1-butanone in the presence of PtO_2 in methanol under a hydrogen atmosphere at r.t. for 1 h (81 %) [2113].

m.p. 188° [2113].

BIOLOGICAL ACTIVITY: Antifungal [2113].

1-(2,4,6-Trihydroxy-3-pentylphenyl)-1-butanone

[74477-96-6] $C_{15}H_{22}O_4$ mol. wt. 266.34



Syntheses
-Obtained by adding a solution of butanoyl chloride in nitrobenzene to a suspension, of 2,4,6-trihydroxypentyl-benzene and aluminium chloride in carbon disulfide at r.t., then stirring the mixture for 6 h at 30–35° (48 %) [2113].

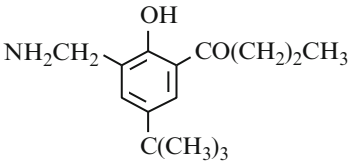
-Also refer to: [1026, 1501, 1502].

m.p. 150° [2113].

BIOLOGICAL ACTIVITY: Antimicrobial [1026, 1501, 1502]; Antifungal [2113].

1-[3-(Aminomethyl)-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-butanone

$C_{15}H_{23}NO_2$ mol. wt. 249.35



Synthesis
-Refer to: [1475].

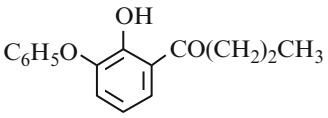
Hydrochloride [75060-71-8]
$C_{15}H_{23}NO_2$, HCl mol. wt. 285.81

-Obtained by treatment of 1-[3-(N-chloroacetylaminomethyl)-5-(1,1-dimethylethyl)-2-hydroxy-phenyl]-1-butanone with conc. hydrochloric acid in refluxing ethanol for 20 h (56 %) [1475].
-Also refer to: [1289].

white amorphous crystals [1475]; m.p. 197–200° [1289, 1475];
^{1}H NMR [1475]; TLC [1475].

1-(2-Hydroxy-3-phenoxyphenyl)-1-butanone

[479580-83-1] $C_{16}H_{16}O_3$ mol. wt. 256.30

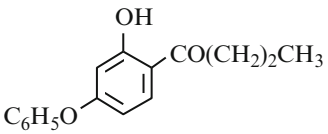


Syntheses
-Refer to: [1018–1022].

USE: Cosmetic compounds containing derivs of hydroxydiphenyl ether for inhibiting body odours [1018–1022].

1-(2-Hydroxy-4-phenoxyphenyl)-1-butanone

[307000-31-3] $C_{16}H_{16}O_3$ mol. wt. 256.30



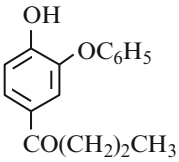
Syntheses
-Refer to: [1018–1022, 1345].

USE: Cosmetic compounds containing derivs of hydroxydiphenyl ether for inhibiting body odours [1018–1022].

BIOLOGICAL ACTIVITY: Antimicrobial [1345].

1-(4-Hydroxy-3-phenoxyphenyl)-1-butanone

[307000-52-8] $C_{16}H_{16}O_3$ mol. wt. 256.30



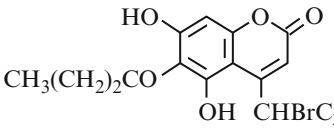
Syntheses
-Refer to: [1018–1022, 1345].

USE: Cosmetic compounds containing derivs of hydroxydiphenyl ether for inhibiting body odours [1018–1022].

BIOLOGICAL ACTIVITY: Antimicrobial [1345].

4-(1-Bromopropyl)-5,7-dihydroxy-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one

$C_{16}H_{17}BrO_5$ mol. wt. 368.21



Synthesis
-Refer to: [763].

Dimethyl ether [111249-73-1]
$C_{18}H_{21}BrO_5$ mol. wt. 397.27

-Preparation by refluxing a mixture of 6-butyryl-5,7-dimethoxy-4-propylcoumarin, N-bromo-succinimide and azobis(isobutyronitrile) in tetrachloromethane under nitrogen (quantitative yield) [766], (99 %) [763].

white solid [763]; m.p. 91–93° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

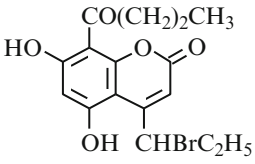
Diacetate [111249-88-8] $C_{20}H_{21}BrO_7$ mol. wt. 453.29

-Obtained by treatment of 5,7-diacetoxy-6-butyryl-4-propylcoumarin with N-bromosuccinimide [766] in tetrachloromethane. A trace of azobis(isobutyronitrile) was added and the mixture heated at reflux for 2 days (61 %) [763].

m.p. 84–85° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

4-(1-Bromopropyl)-5,7-dihydroxy-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

$C_{16}H_{17}BrO_5$ mol. wt. 368.21



Synthesis
-Refer to: [763].

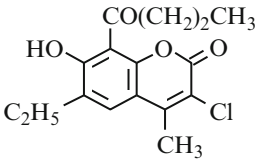
Dimethyl ether [111249-74-2]
$C_{18}H_{21}BrO_5$ mol. wt. 397.27

-Preparation by refluxing a mixture of 8-butyryl-5,7-dimethoxy-4-propylcoumarin, N-bromosuccinimide and azo-isobutyronitrile in tetrachloromethane under nitrogen (86 %) [763].

white solid [763]; m.p. 85–86° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

3-Chloro-6-ethyl-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

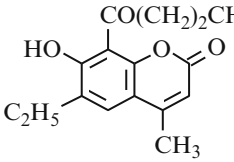
$C_{16}H_{17}ClO_4$ mol. wt. 308.76



Synthesis
-Obtained by Fries rearrangement of 7-butyryloxy-3-chloro-6-ethyl-4-methylcoumarin with aluminium chloride for 1.5 h at 155° [2827].

6-Ethyl-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[109473-68-9] $C_{16}H_{18}O_4$ mol. wt. 274.32



Syntheses
-Obtained by Pechmann condensation of 1-(2,6-dihydroxy-3-ethylphenyl)-1-butanone with ethyl acetoacetate in presence of 80 % sulfuric acid [2811].
-Also obtained by Fries rearrangement of 7-butyryloxy-6-ethyl-4-methylcoumarin (m.p. 125°) [2811].

yellow needles [2811]; m.p. 110° [2811].

Oxime $C_{16}H_{19}NO_4$ mol. wt. 289.33

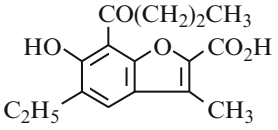
colourless needles [2811]; m.p. 167° (d) [2811].

Acetate [110055-35-1] $C_{18}H_{20}O_5$ mol. wt. 316.35

colourless needles [2811]; m.p. 114° [2811].

5-Ethyl-6-hydroxy-3-methyl-7-(1-oxobutyl)-2-benzofurancarboxylic acid

[109441-87-4] $C_{16}H_{18}O_5$ mol. wt. 290.32

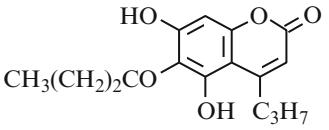


Synthesis
-Obtained by Fries rearrangement of 5-ethyl-6-butyryloxy-3-methylcoumarilic acid with aluminium chloride for 1 h at 150–160° [2827].

m.p. 223° [2827].

5,7-Dihydroxy-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

[98192-62-2] $C_{16}H_{18}O_5$ mol. wt. 290.32



Syntheses

-Obtained by reaction of ethyl 3-oxohexanoate with phlorobutyrophenone in the presence of acetic acid containing 5 % (v/v) sulfuric acid (38–42 %) [762].

-Also refer to: [763].

^{1}H NMR [762], IR [762], UV [762].

Dimethyl ether [98498-67-0] $C_{18}H_{22}O_5$ mol. wt. 318.37

-Preparation from a mixture of 6-butyryl-5,7-dihydroxy-4-propylcoumarin, dimethyl sulfate and potassium carbonate in refluxing acetone for 3 h (91 %) [763].

-Also refer to: [766].

white needles [763]; m.p. 66–68° [763];

^{1}H NMR [763], IR [763], UV [763], MS [763].

Diacetate [98498-64-7] $C_{20}H_{22}O_7$ mol. wt. 374.39

-Obtained by reaction of acetic anhydride with 5,7-dihydroxy-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of pyridine for 2 days at 20° (71 %) [763].

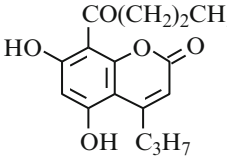
-Also refer to: [766].

white needles [763]; m.p. 125–127° [763];

^{1}H NMR [763], IR [763], UV [763], MS [763].

5,7-Dihydroxy-8-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

[98192-68-8] $C_{16}H_{18}O_5$ mol. wt. 290.32



Syntheses

-Obtained by reaction of ethyl 3-oxohexanoate with phlorobutyrophenone in the presence of acetic acid containing 5 % (v/v) sulfuric acid (25–28 %) [762].

-Also refer to: [763].

^{1}H NMR [762], IR [762], UV [762].

Dimethyl ether [111249-72-0] $C_{18}H_{22}O_5$ mol. wt. 318.37

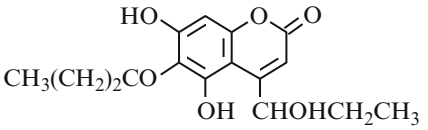
-Preparation from a mixture of 8-butyryl-5,7-dihydroxy-4-propylcoumarin, dimethyl sulfate and potassium carbonate in refluxing acetone for 3 h (95 %) [763].

white plates [763]; m.p. 93–95° [763];

^{1}H NMR [763], IR [763], UV [763], MS [763].

5,7-Dihydroxy-4-(1-hydroxypropyl)-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[111249-82-2] $C_{16}H_{18}O_6$ mol. wt. 306.32



Syntheses

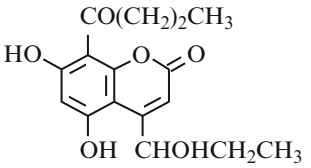
-Obtained by treatment of 5-acetoxy-4-(1-acetoxy-propyl)-6-butyryl-7-methoxycoumarin with boron tribromide in methylene chloride at −78° under nitrogen for 2 h (70 %) [763].

-Also obtained by treatment of 4-(1-acetoxypropyl)-6-butyryl-5,7-dihydroxycoumarin with 10 % aqueous potassium hydroxide at 0° for 1.5 h [763].

yellow needles [763]; m.p. 226–228° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763]; TLC [763].

5,7-Dihydroxy-4-(1-hydroxypropyl)-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[111249-85-5] $C_{16}H_{18}O_6$ mol. wt. 306.32



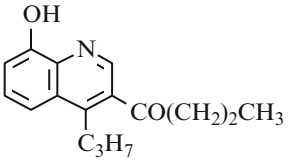
Synthesis

-Obtained by adding lithium tert-butyl sulfide in HMPA to a solution of 4-(1-acetoxypropyl)-8-butyryl-7-hydroxy-5-methoxycoumarin in HMPA and the mixture wad heated at 75° for 2 h under nitrogen (26 %) [763].

white solid [763]; m.p. 180–183° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

1-(8-Hydroxy-4-propyl-3-quinolinyl)-1-butanone

$C_{16}H_{19}NO_2$ mol. wt. 257.33



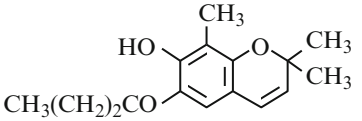
Synthesis

-Refer to: [170].

Methyl ether [189568-62-5]
$C_{17}H_{21}NO_2$ mol. wt. 271.36
-Refer to: [170].

1-(7-hydroxy-8-methyl-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone
6-Butyryl-7-hydroxy-2,2,8-trimethyl-2*H*-1-benzopyran

$C_{16}H_{20}O_3$ mol. wt. 260.33



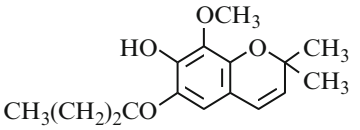
Synthesis

-Obtained by treatment of 6-butyryl-7-hydroxy-8-methyl-2,2-dimethyl-3,4-dihydro-2*H*-1-benzopyran with DDQ in refluxing benzene for 48 h (85 %) [58].

m.p. 71–72° [58]; ^{1}H NMR [58].

1-(7-hydroxy-8-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone
6-Butyryl-7-hydroxy-8-methoxy-2,2-dimethyl-2*H*-1-benzopyran

$C_{16}H_{20}O_4$ mol. wt. 276.33

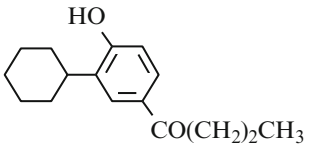


Synthesis
-Obtained by treatment of 6-butyryl-7-hydroxy-8-methoxy-2,2-dimethyl-3,4-dihydro-2*H*-1-benzopyran with DDQ in refluxing benzene for 48 h (70 %) [58].

m.p. 79–80° [58]; ^{1}H NMR [58].

1-(3-Cyclohexyl-4-hydroxyphenyl)-1-butanone

$C_{16}H_{22}O_2$ mol. wt. 246.35

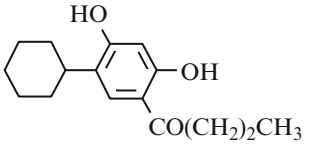


Synthesis
-Refer to: [2704] (Japanese patent).
m.p. 88° [2704].

USE: As colour developer [2704].

1-(5-Cyclohexyl-2,4-dihydroxyphenyl)-1-butanone

$C_{16}H_{22}O_3$ mol. wt. 262.35



Synthesis
-Obtained (**XVIII**) by reaction of butyric acid with 4-cyclohexylresorcinol in the presence of boron trifluoride etherate at 105–108° for 15 min, the hydrolysis of the BF_2-chelate (**VIII**) obtained [2382].

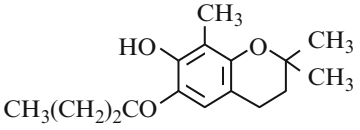
m.p. 124–125° [2382]; IR [2382], UV [2382].

BF_2-chelate (VIII) $C_{16}H_{21}BF_2O_3$ mol. wt. 310.15 (54 %) [2382].

m.p. 113–114° [2382]; IR [2382].

1-(3,4-Dihydro-7-hydroxy-2,2,8-trimethyl-2*H*-1-benzopyran-6-yl)-1-butanone
6-Butyryl-7-hydroxy-2,2,8-trimethyl-3,4-dihydro-2*H*-1-benzopyran

[93970-94-6] $C_{16}H_{22}O_3$ mol. wt. 262.35



Syntheses
-Obtained by reaction of 2,4-dihydroxy-3-methyl-butyrophenone with 2-methyl-1,3-butadiene in petrol in the presence of polyphosphoric acid at 30–35° for 18 h (85 %) [58].

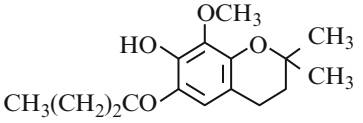
-Also refer to: [59].

m.p. 85–86° [58]; ^{1}H NMR [58].

1-(3,4-Dihydro-7-hydroxy-8-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone

6-Butyryl-7-hydroxy-8-methoxy-2,2-dimethyl-3,4-dihydro-2*H*-1-benzopyran

[93970-95-7] $C_{16}H_{22}O_4$ mol. wt. 278.35



Syntheses

-Obtained by treatment of 6-butyryl-7,8-dihydroxy-2,2-dimethyl-3,4-dihydro-2*H*-1-benzopyran with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 2.5 h (90 %) [58].

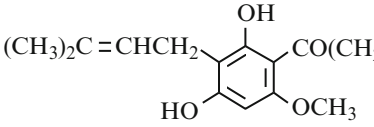
-Also refer to: [59].

m.p. 66–67° [58]; ^{1}H NMR [58].

1-[2,4-Dihydroxy-6-methoxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone

(HP57.4)

[933786-84-6] $C_{16}H_{22}O_4$ mol. wt. 278.35



Isolation from natural sources

-From *Helichrysum paronychioides* (Asteraceae, tribe Inuleae) [2201].

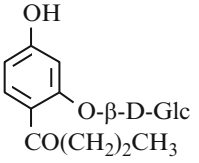
yellow gum [2201];

^{1}H NMR [2201], ^{13}C NMR [2201], IR [2201], UV [2201], MS [2201]; TLC [2201].

BIOLOGICAL ACTIVITY: Antioxidant [2201].

1-[2-(β-D-Glucopyranosyloxy)-4-hydroxyphenyl]-1-butanone

$C_{16}H_{22}O_8$ mol. wt. 342.35



Synthesis

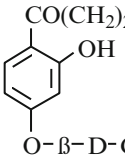
-Obtained by treatment of 4-acetyloxy-2-tetraacetyl-β-D-glucosyloxylbutyrophenone with sodium methoxide in boiling methanol for 3 min [3243].

Monohydrate $C_{16}H_{22}O_8$, H_2O mol. wt. 360.40

$(\alpha)_D^{30} = -73.2°$ (water) [3243].

1-[4-(β-D-Glucopyranosyloxy)-2-hydroxyphenyl]-1-butanone

$C_{16}H_{22}O_8$ mol. wt. 342.35



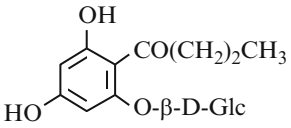
Synthesis
-Obtained by treatment of resbutyrophenone tetra-acetyl-β-D-glucoside with 0.2 M sodium methoxide in methanol (70–75 %) [3243].
m.p. 187–188° [3243].

Monohydrate $C_{16}H_{22}O_8, H_2O$ mol. wt. 360.40

m.p. 134–135° [3243]; $(\alpha)_D^{21} = -38.8°$ (dimethylformamide) [3243].

1-[2-(β-D-Glucopyranosyloxy)-4,6-dihydroxyphenyl]-1-butanone

[1067245-70-8] $C_{16}H_{22}O_9$ mol. wt. 358.35

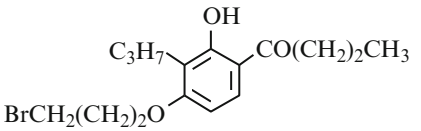


Isolation from natural sources
-From *Aster subulatus* Michx. [1709].

USE: Antioxidant [1709].

1-[4-(3-Bromopropoxy)-2-hydroxy-3-propylphenyl]-1-butanone

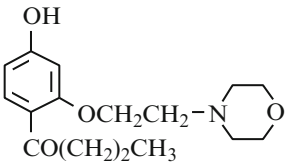
[194792-32-0] $C_{16}H_{23}BrO_3$ mol. wt. 343.26



Synthesis
-Refer to: [307].
^{1}H NMR [21].

1-[2-(N-Morpholinoethoxy)-4-hydroxyphenyl]-1-butanone

$C_{16}H_{23}NO_4$ mol. wt. 293.36



Synthesis
-Refer to: [787].

Methyl ether (Hydrochloride) [21092-65-9]
$C_{17}H_{25}NO_4$, HCl mol. wt. 343.85

-Obtained by adding a solution of 2-hydroxy-4-methoxybutyrophenone and sodium ethoxide in ethanol to the N-morpholinoethyl chloride. Then, the mixture was refluxed for 3 h [787].

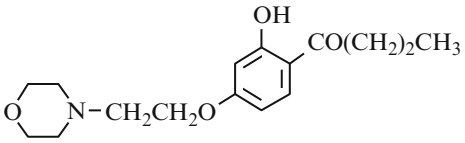
m.p. 152–153° [787].

BIOLOGICAL ACTIVITY: Local anaesthetic [787]; Antispasmodic [787]; Depression [787].

LD_{50} 180 [787].

1-[4-(N-Morpholinoethoxy)-2-hydroxyphenyl]-1-butanone

$C_{16}H_{23}NO_4$ mol. wt. 293.36



Synthesis
-Refer to: [787].
Hydrochloride [20800-12-8]
$C_{16}H_{23}NO_4$, HCl mol. wt. 329.82

-Obtained by adding a solution of resbutyrophenone and sodium ethoxide in ethanol to the N-morpholinoethyl chloride. Then, the mixture was refluxed for 3 h [787].

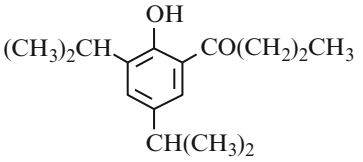
m.p. 180–182° [787].

BIOLOGICAL ACTIVITY: Local anaesthetic [787]; Antispasmodic [787]; Depression [787].

LD_{50} 700 [787].

1-[2-Hydroxy-3,5-bis(1-methylethyl)phenyl]-1-butanone

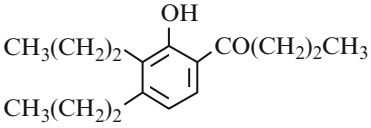
$C_{16}H_{24}O_2$ mol. wt. 248.37



Synthesis
-Refer to: [2940].
ESR [2940].

1-(2-Hydroxy-3,4-dipropylphenyl)-butanone

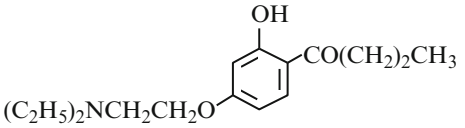
[936642-87-4] $C_{16}H_{24}O_2$ mol. wt. 248.37



Synthesis
-Obtained by reaction of 2,3-dipropylcyclobutenone with propyl vinyl ketone catalyzed by $[RhCl(C_2H_4)_2]_2$-P(cyclo-$C_6H_{11})_3$ in toluene at 130° for 12 h under argon atmosphere (65 %) [1731].

1-[4-(N,N-Diethylaminoethoxy)-2-hydroxyphenyl]-1-butanone

$C_{16}H_{25}NO_3$ mol. wt. 279.38



Synthesis
-Obtained by adding a solution of resbutyrophenone and sodium ethoxide in ethanol to the N, N-diethylaminoethyl chloride. Then, the mixture was refluxed for 3 h [787].

Hydrochloride $C_{16}H_{25}NO_3$, HCl mol. wt. 315.84

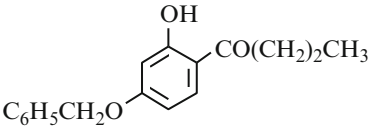
m.p. 155–157° [787].

BIOLOGICAL ACTIVITY: Local anaesthetic [787]; Antispasmodic [787]; Convulsions [787]; Transient decrease of arterial blood pressure [787]; Inhibition of formaldehyde paw edema [787]; Protection against $CaCl_2$ ventricular fibrillation [787].

LD_{50} 300 [787].

1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-butanone

[230976-82-6] $C_{17}H_{18}O_3$ mol. wt. 270.33



Syntheses

-Obtained by reaction of benzyl chloride with resbutyrophenone,

*in the presence of potassium hydroxide in methanol, first at r.t. overnight, then at reflux for 5 h [2181];

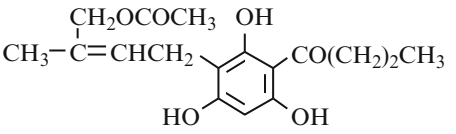
*in the presence of potassium carbonate in refluxing acetone for 8 h (50 %) [2181].

-Also refer to: [2411].

m.p. 85° [2181].

1-[3-[4-(Acetyloxy)-3-methyl-2-butenyl]-2,4,6-trihydroxyphenyl]-1-butanone *(E)*

[122585-61-9] $C_{17}H_{22}O_6$ mol. wt. 322.36



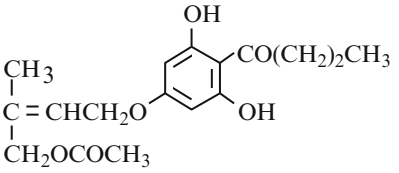
Isolation from natural sources

-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].

^{1}H NMR [1488], IR [1488], MS [1488].

1-[4-[[4-(Acetyloxy)-3-methyl-2-butenyl]oxy]-2,6-dihydroxyphenyl]-1-butanone *(E)*

[122585-51-7] $C_{17}H_{22}O_6$ mol. wt. 322.36



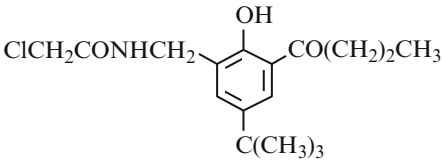
Isolation from natural sources

-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].

^{1}H NMR [1488], IR [1488], MS [1488].

1-[3-(N-Chloroacetylaminomethyl)-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-butanone

$C_{17}H_{24}ClNO_3$ mol. wt. 325.84

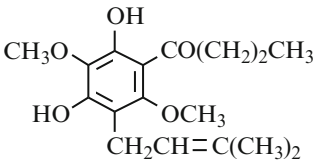


Synthesis
-Obtained by adding N-hydroxymethyl-chloroacetamide to 2-butyryl-4-tert-butylphenol dissolved in acetic acid and conc. sulfuric acid mixture at r.t. and stirred at 60° for 2 h (82 %) [1475].

^{1}H NMR [1475]; TLC [1475].

1-[2,4-Dihydroxy-3,6-dimethoxy-5-(3-methyl-2-butenyl)phenyl]-1-butanone

[70219-89-5] $C_{17}H_{24}O_5$ mol. wt. 308.38



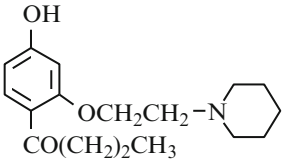
Isolation from natural sources
-From *Leontonyx spathulatus* Less. (Compositae) (**13**) [400].
colourless oil [400];
^{1}H NMR [400], IR [400], MS [400].

Diacetate [70219-90-8] $C_{21}H_{28}O_7$ mol. wt. 392.45 (**14**).

colourless oil [400]; ^{1}H NMR [400], IR [400].

1-[2-(N-Piperidinoethoxy)-4-hydroxyphenyl]-1-butanone

$C_{17}H_{25}NO_3$ mol. wt. 291.39



Synthesis
-Refer to: [787].

Methyl ether $C_{18}H_{27}NO_3$ mol. wt. 305.42
-Refer to: [787].

Hydrochloride of the methyl ether $C_{18}H_{27}NO_3$, HCl mol. wt. 341.88

-Obtained by adding a solution of 2-hydroxy-4-methoxybutyrophenone and sodium ethoxide in ethanol to the N-piperidinoethyl chloride. Then, the mixture was refluxed for 3 h [787].

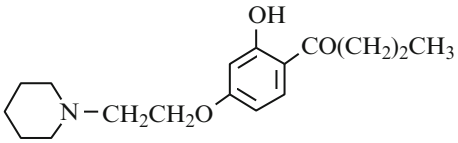
m.p. 178° [787].

BIOLOGICAL ACTIVITY: Local anaesthetic [787]; Antispasmodic [787]; Convulsions [787]; Inhibition of formaldehyde paw edema [787].

LD_{50} 130 [787].

1-[4-(N-Piperidinoethoxy)-2-hydroxyphenyl]-1-butanone

$C_{17}H_{25}NO_3$ mol. wt. 291.39



Synthesis

-Obtained by adding a solution of resbutyrophenone and sodium ethoxide in ethanol to the N-piperidinoethyl chloride. Then, the mixture was refluxed for 3 h [787].

Hydrochloride $C_{17}H_{25}NO_3$, HCl mol. wt. 327.85

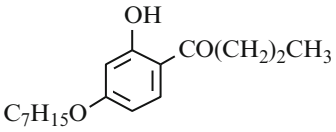
m.p. 145–147° [787].

BIOLOGICAL ACTIVITY: Local anaesthetic [787]; Antispasmodic [787]; Convulsions [787]; Transient decrease of arterial blood pressure [787]; Protection against $CaCl_2$ ventricular fibrillation [787].

LD_{50} 200 [787].

1-[4-(Heptyloxy)-2-hydroxyphenyl]-1-butanone

[22198-48-7] $C_{17}H_{26}O_3$ mol. wt. 278.39



Syntheses

-Obtained by reaction of butanoyl chloride with resorcinol diheptyl ether in the presence of aluminium chloride at 80° for 2 h (60 %) [3469].

-Also obtained by reaction of butanoyl chloride with m-diheptyloxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°. The temperature then raised to 80° and stirring was continued at that temperature for 5 h (60 %) [1194].

-Also refer to: [1861, 1862].

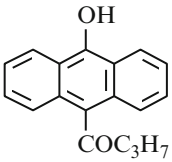
m.p. 41.5–42° [1194, 3469]; UV [1194, 3469].

USE: UV absorber [1194]; Light-stabilizer of polymeric materials [1194]; Substituted benzoimidazole compounds as transcription factor-modulating compounds useful as antiinfectives [1862].

BIOLOGICAL ACTIVITY: Antibacterial [1861].

9-Hydroxy-10-butyrylanthracene

$C_{18}H_{16}O_2$ mol. wt. 264.32

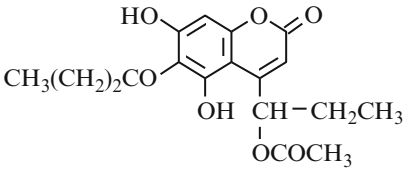


Synthesis

-Obtained by Fries rearrangement of 9-butyryloxyanthracene with various metal halides in benzene under reflux, but it is rapidly transformed into 10-butyrylanthrone [3052].

4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[111249-78-6] $C_{18}H_{20}O_7$ mol. wt. 348.35



Syntheses

-To a mixture of 4-(1-acetoxypropyl)-6-butyryl-5-hydroxy-7-methoxycoumarin and the 7-hydroxy-5-methoxy isomer and triethylamine in methylene chloride at 0° under nitrogen was added trimethylsilyl chloride.

The mixture was stirred for 30 min and the solvents were then evaporated under reduced pressure.

The residue was taken up in methylene chloride and the solution cooled to −78° under nitrogen.

Boron tribromide was added and the mixture stirred and allowed to warm to 0°. After stirring for 1 h the mixture was poured into dilute hydrochloric acid-ice (29 %) [763].

-Also obtained by treatment of 4-(1-acetoxypropyl)-6-butyryl-5,7-dimethoxycoumarin,

*in benzene with magnesium iodide-diethyl ether and refluxing for 2 h under nitrogen (3 %) [763];

*with boron tribromide (30 %) [766].

yellow needles [763]; m.p. 212–214° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

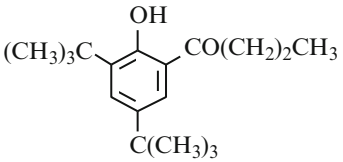
Dimethyl ether [111249-75-3] [98498-69-2] $C_{20}H_{24}O_7$ mol. wt. 376.41

-Preparation by reaction of tetramethylammonium acetate with 4-(1-bromopropyl)-6-butyryl-5,7-dimethoxycoumarin in acetone for 2–3 days at 20° (82 %) [763, 766].

white plates [763]; m.p. 120–122° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

1-[3,5-Bis(1,1-dimethylethyl)-2-hydroxyphenyl]-1-butanone

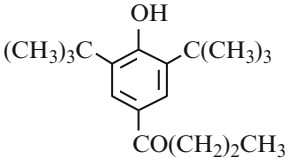
$C_{18}H_{28}O_2$ mol. wt. 276.42



Synthesis
-Refer to: [2940].
ESR [2940].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-butanone

[14035-35-9] $C_{18}H_{28}O_2$ mol. wt. 276.42



Syntheses
-Preparation by reaction of butyryl chloride with 2,6-di-tert-butylphenol in the presence of aluminium chloride,
*at −10° for 1–13 min (90 %) [2506];
*at 20° for 20 min, followed by hydrolysis of the keto ester obtained (**3c**) (87 %, m.p. 49.5–50.5°) [2971];
*in 1,1,2-trichloroethane at −10 to −20° [951].
-Preparation by reaction of butyryl chloride with 2,6-di-tert-butylphenol in the presence of titanium tetrachloride [1468].
-Also obtained by reaction of butyric anhydride with 2,6-di-tert-butylphenol in the presence of 5 drops 70 % perchloric acid, first at r.t. for 1 h and left overnight (90 %) [2136].
-Also refer to: [655, 2139].

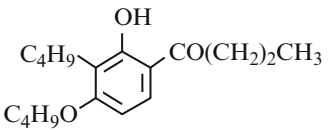
m.p. 91–93° [2139], 88–90° [2506], 88–89° [2136], 85.5–86.5° (**2c**) [2971];
^{1}H NMR [2136, 2971], IR [2136, 2971];
electrochemical characteristics [2136].

USE: Stabilize plastics, oils, and fats against heat, light, and oxidation [951].

BIOLOGICAL ACTIVITY: Inflammation inhibitor [2139].

1-(4-Butyloxy-3-butyl-2-hydroxyphenyl)-1-butanone

$C_{18}H_{28}O_3$ mol. wt. 292.42



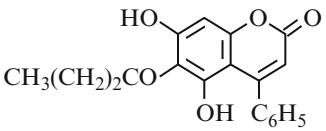
Synthesis
-Obtained by butylation of 2,4-dihydroxybutyrophenone [1587].
b.p.$_8$ 200–207° [1587].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_6$ mol. wt. 472.54

m.p. 140.5° [1587].

5,7-Dihydroxy-6-(1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
5-Butyryl-5,7-dihydroxy-4-phenylcoumarin

[80752-03-0] $C_{19}H_{16}O_5$ mol. wt. 324.33



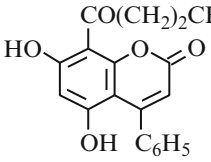
Syntheses
-Obtained by Pechman condensation of butyrylphloro-glucinol with ethyl benzoyl acetate in acetic acid in the presence of concentrated sulfuric acid at r.t. for 3 days (28 %) [3105].

-Also obtained by reaction of butyryl chloride with 5,7-dihydroxy-4-phenyl-2*H*-1-benzopyran-2-one in the presence of aluminium chloride in carbon disulfide, then in refluxing nitromethane [2146].

pale yellow needles [3105];
m.p. 228–229° [3105];
^{1}H NMR [3105], IR [3105].

5,7-Dihydroxy-8-(1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one

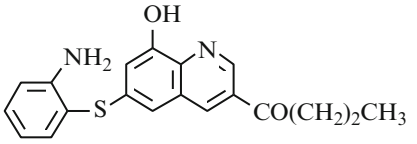
$C_{19}H_{16}O_5$ mol. wt. 324.33



Synthesis
-Obtained by reaction of butyryl chloride with 5,7-dihydroxy-4-phenyl-2*H*-1-benzopyran-2-one in the presence of aluminium chloride in carbon disulfide, then in refluxing nitromethane [2146].

1-[6-[2-(Aminophenyl)thio]-8-hydroxy-3-quinolinyl]-1-butanone

$C_{19}H_{18}N_2O_2S$ mol. wt. 338.43



Synthesis
-Refer to: [973].

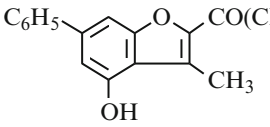
Methyl ether
$C_{20}H_{20}N_2O_2S$ mol. wt. 352.46

Hydrochloride of the methyl ether [209479-38-9] $C_{20}H_{20}N_2O_2S$, HCl mol. wt. 388.92

-Refer to: [973].

1-(4-Hydroxy-3-methyl-6-phenyl-2-benzofuranyl)-1-butanone

$C_{19}H_{18}O_3$ mol. wt. 294.35



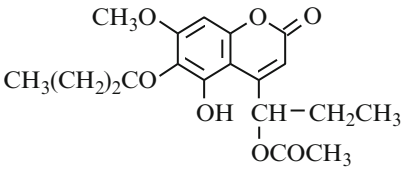
Synthesis
-Refer to: [1288].

Methoxymethyl ether [678184-68-4]
$C_{21}H_{22}O_4$ mol. wt. 338.40

-Refer to: [1288].

4-[1-(Acetyloxy)propyl]-5-hydroxy-7-methoxy-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[111249-77-5] $C_{19}H_{22}O_7$ mol. wt. 362.38



Syntheses
-Obtained by treatment of 4-(1-acetoxypropyl)-6-butyryl-5,7-dimethoxy-coumarin in benzene with magnesium iodide-diethyl ether and refluxing for 2 h under nitrogen (90 %) [763].

-Also obtained by adding boron tribromide to 4-(1-acetoxypropyl)-6-butyryl-5,7-dimethoxy-coumarin in methylene chloride at −78° under nitrogen. The solution was kept at −78° for 2 h then allowed to warm to 0° [766], (21 %) [763].

yellow solid [763]; m.p. 168–170° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

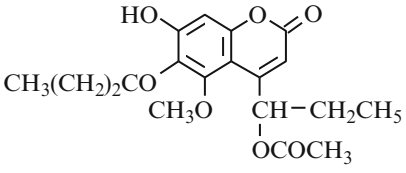
Acetate [111249-81-1] $C_{21}H_{24}O_8$ mol. wt. 404.42

-Preparation by treatment of 4-(1-acetoxypropyl)-6-butyryl-5-hydroxy-7-methoxy-coumarin with acetic anhydride in the presence of pyridine for 2 days (72 %) [763].

white needles [763]; m.p. 132–134° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

4-[1-(Acetyloxy)propyl]-7-hydroxy-5-methoxy-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[111249-80-0] $C_{19}H_{22}O_7$ mol. wt. 362.38

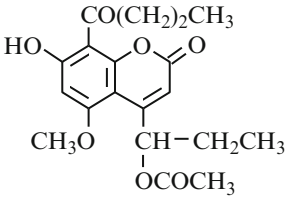


Syntheses
-Obtained by adding boron tribromide to 4-(1-acetoxypropyl)-6-butyryl-5,7-dimethoxy-coumarin in methylene chloride at −78° under nitrogen. The solution was kept at −78° for 2 h then allowed to warm to 0° [766], (42 %) [763].

white needles [763]; m.p. 129–131° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

4-[1-(Acetyloxy)propyl]-7-hydroxy-5-methoxy-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one

[111249-84-4] $C_{19}H_{22}O_7$ mol. wt. 362.38



Syntheses

-Obtained by adding boron tribromide to a solution of 4-(1-acetoxypropyl)-8-butyryl-5,7-dimethoxycoumarin in methylene chloride at −78° under nitrogen. Then, the mixture was allowed to warm to 0° (88 %) [763].

-Also refer to: [766].

white needles [763]; m.p. 136–138° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

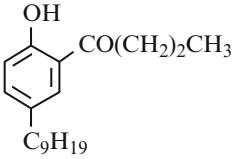
Methyl ether [111249-76-4] $C_{20}H_{24}O_7$ mol. wt. 376.41

-Obtained by reaction of tetramethylammonium acetate with 4-(1-bromopropyl)-8-butyryl-5,7-dimethoxycoumarin in acetone for 2–3 days at 20° (85 %) [763].

white solid [763]; m.p. 130–132° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

1-(2-Hydroxy-5-nonylphenyl)-1-butanone

$C_{19}H_{30}O_2$ mol. wt. 290.45



Synthesis

-Refer to: [1869].

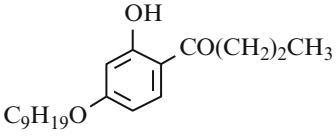
Oxime [758691-87-1]

$C_{19}H_{31}NO_2$ mol. wt. 305.46

USE: Extraction agent for copper [1869].

1-[4-(Nonyloxy)-2-hydroxyphenyl]-1-butanone

[22198-49-8] $C_{19}H_{30}O_3$ mol. wt. 306.45



Syntheses

-Obtained by reaction of butanoyl chloride with resorcinol dinonyl ether in the presence of aluminium chloride at 80° for 2 h (60 %) [3469].

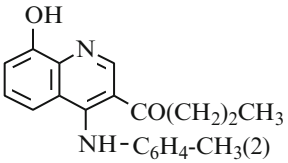
-Also obtained by reaction of butanoyl chloride with m-dinonyloxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°. The temperature was then raised to 80° and stirring was continued at that temperature for 5 h (60 %) [1194].

m.p. 38–38.5° [1194, 3469]; UV [1194, 3469].

USE: UV absorber [1194], Light-stabilizer of polymeric materials [1194].

1-[8-Hydroxy-4-[(2-methylphenyl)amino]-3-quinolinyl]-1-butanone

[125500-46-1] $C_{20}H_{20}N_2O_2$ mol. wt. 320.39



Syntheses
-Refer to: [170, 296, 1841, 1904].
m.p. 114–115° [1841].

BIOLOGICAL ACTIVITY: Refer to: [1841].

Methyl ether [115607-61-9] $C_{21}H_{22}N_2O_2$ mol. wt. 334.42

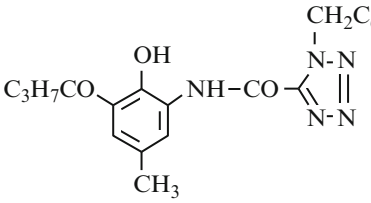
m.p. 112–114° [1420], 102° [1904]; ^{1}H NMR [1420].

-Refer to: [296, 370, 876, 1841].

BIOLOGICAL ACTIVITY: Antimicrobial agent [876]; Combinations of 5-HT_4 agonist or antagonist or 5-HT_3 antagonist and co-agent for treatment of gastrointestinal and abdominal visceral disorders [370].

N-(3-Butanoyl-2-hydroxy-5-methylphenyl)-1-phenylmethyltetrazole-5-carboxamide

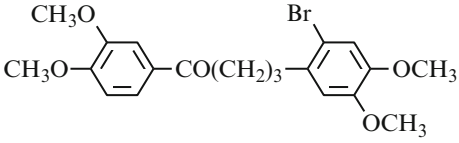
[70978-14-2] $C_{20}H_{21}N_5O_3$ mol. wt. 379.42



Synthesis
-Refer to: [1017 (78 %)].
m.p. 166–169° [1017].

4-(2-Bromo-4,5-dimethoxyphenyl)-1-(3,4-dimethoxyphenyl)-1-butanone

[111585-36-5] $C_{20}H_{23}BrO_5$ mol. wt. 423.30



Syntheses
-Obtained by reaction of 4-(2-bromo-4,5-dimethoxyphenyl)butyric chloride with veratrole in the presence of aluminium chloride in nitrobenzene for 24 h at r.t. (86 %) [1284].

-Also obtained by treatment of its semicarbazone with a saturated aqueous solution of oxalic acid at 100–110° for 2 h (91 %) [1284].
-Also refer to: [1284].

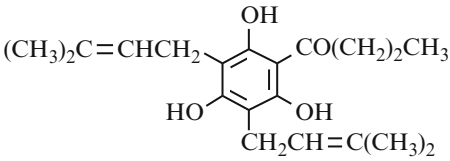
colourless prisms [1284]; m.p. 82–84° [1284].

Semicarbazone $C_{21}H_{26}BrN_3O_5$ mol. wt. 480.36

pale yellow needles [1284]; m.p. 172–173° [1284].

1-[2,4,6-Trihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-1-butanone

[50874-48-1] $C_{20}H_{28}O_4$ mol. wt. 332.44



Syntheses

-Obtained by reaction of resbutyrophenone with 1-bromo-3-methyl-2-buten (3 mol) in the presence of the weakly basic resin DeAcidite H-IP (OH^- form) in boiling benzene (12.6 %) [708].

N.B.: The yield was similar at this obtained by using 2-methyl-3-buten-2-ol but the isolation was simpler [708].

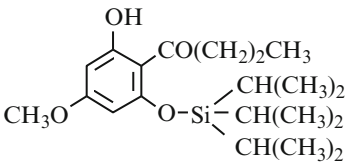
-Also obtained by reaction of phlorobutyrophenone with 1-chloro-3-methyl-2-butene (2 molar parts), magnesium oxide (0.5 equiv.) and potassium iodide (1 %) [3309].

-Also refer to: [707].

oil [708].

1-[2-Hydroxy-4-methoxy-6-[[tris(1-methylethyl)silyl]oxy]phenyl]-1-butanone

[326854-41-5] $C_{20}H_{34}O_4Si$ mol. wt. 366.57



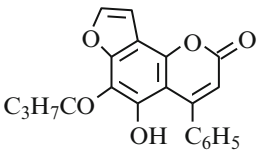
Syntheses

-Refer to: [1464, 3070].

5-Hydroxy-6-(1-butanoyl)-4-phenyl-2*H*-furo[2′,3′:5,6]benzo[1,2-b]pyran-2-one

(Furanoracemosone)

$C_{21}H_{16}O_5$ mol. wt. 348.36



Synthesis

-Obtained by heating a mixture of 5,7-dihydroxy-6-(1-butanoyl)-4-phenyl-2*H*-1-benzopyran-2-one and 4-chloro-1,3-dioxolan-2-one first at 150° for 4 h, then at 165° for 30 min (10 %) [2146].

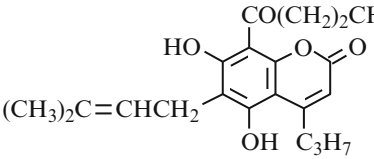
Isolation from natural sources

-From the leaves of *Mesua racemosa* (Clusiaceae) [2146].

white amorphous solid [2146];
^{1}H NMR [2146], ^{13}C NMR [2146], IR [2146], UV [2146], MS [2146].

5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one
(Normammein, Mammea B/BC)

[5085-54-1] $C_{21}H_{26}O_5$ mol. wt. 358.43



Syntheses

-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-8-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of 10 % aqueous potassium hydroxide at 0° (30–45 %) [765], (32 %) [762].

Isolation from natural sources

-From kernels of the fruit of *Mammea americana* L. and *Mammea africana* (Guttiferae) [765, 1006].
-From the seeds of *Mammea americana* L. [753, 758, 759, 1082].
-From the bark of *Mammea africana* G. Don (Guttiferae) [553].

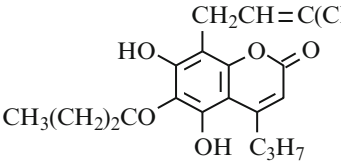
needles [753]; white needles [762];
m.p. 132–134° [762], 132–133° [753], 130–132° [1006];
^{1}H NMR [753, 762], IR [753, 762], UV [753, 762],
MS [753, 762]; GC-MS [1082].

USE: Insecticide [753, 758, 759, 765].

BIOLOGICAL ACTIVITY: Antitumor [1006].

5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one
(Mammea B/AC)

[38537-84-7] $C_{21}H_{26}O_5$ mol. wt. 358.43



Syntheses

-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of 10 % aqueous potassium hydroxide at 0° (30–45 %) [765], (25 %) [762].

-Also obtained by isomerization of 5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one (mammea B/BC) by treatment with methanolic 5 % potassium hydroxide at 20° overnight [757].

Isolation from natural sources

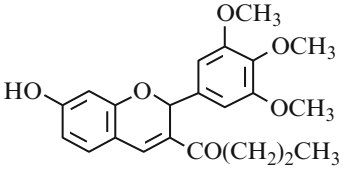
-From kernels of the fruit of *Mammea americana* L. [757] and *Mammea africana* (Guttiferae) [765].

yellow needles [757, 762];
m.p. 127–128.5° [757], 127–128° [762];
^{1}H NMR [757, 762], IR [757, 762], UV [757, 762],
MS [757, 762]; TLC [757].

USE: Insecticide [757, 765].

1-[7-Hydroxy-2-(3,4,5-trimethoxy)-2*H*-1-benzopyran-3-yl]-1-butanone

$C_{22}H_{24}O_6$ mol. wt. 384.43



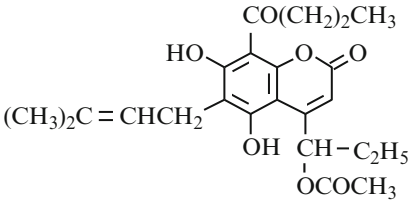
Synthesis
-Refer to: [634].

Methyl ether [364039-57-6]
$C_{23}H_{26}O_6$ mol. wt. 398.46
-Refer to: [633, 634].

BIOLOGICAL ACTIVITY: As TNF-α-inhibitor [634].

4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one
(Mammea E/BC)

$C_{23}H_{28}O_7$ mol. wt. 416.47



Isolation from natural sources
-From *mammea americana* L. (Guttifferae) (Clusiaceae) [756, 758, 3381].
-Also refer to: [762].
m.p. 50–53° [756];
^{1}H NMR [756, 758, 3381],
^{13}C NMR [3381], IR [756], UV [756, 3381], MS [756];
$(\alpha)_D^{25} = -28°$ (methanol) [3381].

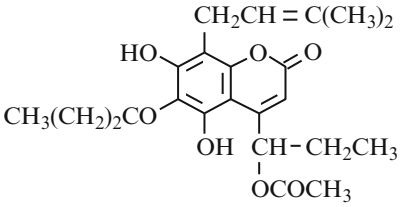
USE: Insecticide [758].

BIOLOGICAL ACTIVITY: Apoptosis induction of human colon cancer SW-480 cells [3381]; Cytotoxicity [3381].

4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one

(Mammea E/AC)

[111249-83-3] $C_{23}H_{28}O_7$ mol. wt. 416.47



Syntheses

-Obtained by reaction of 3-methyl-2-butenyl bromide with 4-(1-acetoxypropyl)-6-butyryl-5,7-dihydroxycoumarin in 5 % aqueous potassium hydroxide at 0° under nitrogen for 1.5 h (21 %) [763].

-Also obtained by prenylation of 4-[1-(acetyloxy)propyl]-5,7-dihydroxy-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one using prenyl bromide in the presence of 2 equiv. of aqueous 5 % potassium hydroxide at 0° (21 %) [766].

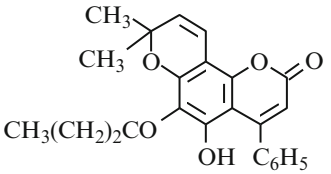
yellow needles [763]; m.p. 139–141° [763];
^{1}H NMR [763], IR [763], UV [763], MS [763].

5-Hydroxy-8,8-dimethyl-6-(1-oxobutyl)-4-phenyl-2*H*,8*H*-benzo[1,2-b:5,6-b′]dipyran-2-one

(Mammea A/AC)

6-Butyryl-5-hydroxy-4-phenylseselin

[42290-21-1] $C_{24}H_{22}O_5$ mol. wt. 390.44



Syntheses

-Obtained by treatment of 5-butyryl-5,7-dihydroxy-4-phenylcoumarin with 3-methyl-2-butenal in pyridine first at r.t., then at 110° for 10 h (80 %) [3105].

-Also obtained by oxidative cyclization of 5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one with DDQ in benzene at r.t. overnight (76 %) [3105].

Isolation from natural sources

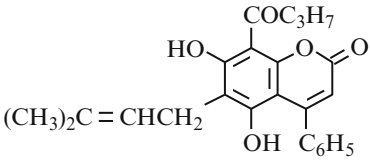
-From *Ochrocarpus siamensis* (Guttiferae) [3105].
-From flowers of *Kayea assamica* [3315].
-From seeds (Fruit and Spice Park) of *Mammea americana* L. (Clusiaceae) [3381].

yellow needles [3105]; m.p. 138–139° [3105];
^{1}H NMR [3105], IR [3105], UV [3105], MS [3105].

BIOLOGICAL ACTIVITY: Pancreatic cancer PANC-1 cells of human [3315]; Human colon cancer HCT-116 cells [3381]; Human colon cancer HT-29 cells [3381]; Human colon cancer SW-480 cells [3381]; Cytotoxicity [3381].

5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
(Mammea A/BC)

$C_{24}H_{24}O_5$ mol. wt. 392.45



Synthesis
-Obtained by reaction of 3-methyl-2-butenyl bromide with 5,7-dihydroxy-8-(1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one in the presence of 10 % KOH at 0° for 1.5 h (15 %) [2146].

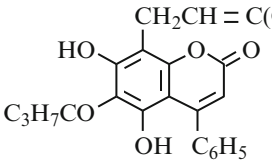
Isolation from natural sources

-From the leaves of *Mesua racemosa* (Clusiaceae) [2146].

m.p. 123–124° [2146];
^{1}H NMR [2146], ^{13}C NMR [2146], IR [2146], UV [2146], MS [2146].

5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
(Mammea A/AC)

$C_{24}H_{24}O_5$ mol. wt. 392.45



Syntheses
-Obtained by alkylation of 6-butyryl-5,7-dihydroxy-4-phenylcoumarin with 2-methyl-3-buten-2-ol in the presence of boron trifluoride etherate in dioxan at 50° for 90 min (10 %) [3105].
-Also refer to: [762].

Isolation from natural sources

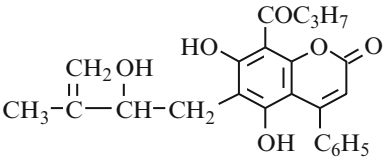
-From flowers of *Kayea assamica* [2222].
-From *Ochrocarpus siamensis* (Guttiferae) [3105].

pale yellow needles [3105]; m.p. 116–117° [3105];
^{1}H NMR [3105], IR [3105], UV [3105], MS [3105].

BIOLOGICAL ACTIVITY: Cytotoxicity [2222].

5,7-dihydroxy-6-(2-hydroxy-3-methyl-3-butenyl)-8-(1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
(Isoracemosol)

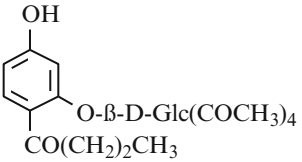
$C_{24}H_{24}O_6$ mol. wt. 408.45



Isolation from natural sources
-From the leaves of *Mesua racemosa* (Clusiaceae) [2146].
yellow amorphous solid [2146];
^{1}H NMR [2146], ^{13}C NMR [2146], IR [2146], UV [2146], MS [2146].

1-[2-(Tetraacetyl-β-D-glucopyranosyloxy)-4-hydroxyphenyl]-1-butanone
(Resbutyrophenon-4-tetraacetyl-β-D-glucoside)

$C_{24}H_{30}O_{12}$ mol. wt. 510.50

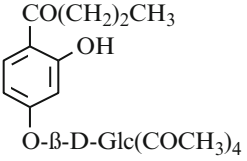


Synthesis
-Refer to: [3243].
Acetate $C_{26}H_{32}O_{13}$ mol. wt. 552.50
-Obtained by reaction of α-acetobromoglucose (α-ABG) with 4-acetoxyresbutyrophenone in the presence of silver oxide in quinoline for 30 min (16 %) [3243].

m.p. 182–184° [3243]; $(\alpha)_D^{21} = -46.2°$ (water) [3243].

1-[4-(Tetraacetyl-β-D-glucopyranosyloxy)-2-hydroxyphenyl]-1-butanone
(Resbutyrophenon-4-tetraacetyl-β-D-glucoside)

$C_{24}H_{30}O_{12}$ mol. wt. 510.50

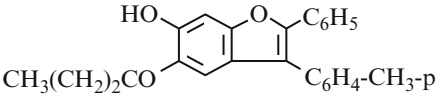


Synthesis
-Obtained by reaction of α-acetobromoglucose (α-ABG) with resbutyrophenone in the presence of silver oxide in quinoline for 2 h [3243].

m.p. 125–126° [3243]; $(\alpha)_D^{20} = -21.9°$ (chloroform) [3243].

1-(6-Hydroxy-3-(4-methylphenyl)-2-phenyl-5-benzofuranyl)-1-butanone

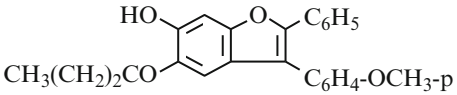
[438490-69-8] $C_{25}H_{22}O_3$ mol. wt. 370.45



Synthesis
-Refer to: [2930].

1-(6-Hydroxy-3-(4-methoxyphenyl)-2-phenyl-5-benzofuranyl)-1-butanone

[438490-66-5] $C_{25}H_{22}O_4$ mol. wt. 386.44



Syntheses
-Refer to: [2930, 2931].

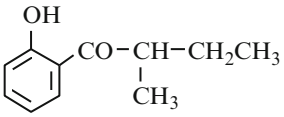
2 Aromatic Hydroxyketones Derived from Various Alkyl-1-Butanoic Acids

2.1 From 2-Methyl-1-Butanoic Acid

2.1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-2-methyl-1-butanone

[344408-25-9] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses
-Obtained by photo-Fries rearrangement of (S) (+) phenyl 2-methylbutanoate [1002].
-Also refer to: [369 (2 %), 2104].

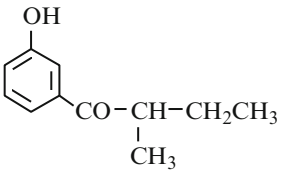
IR [1002], UV [1002].

Methyl ether [1196852-29-5] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Refer to: [1084].

1-(3-Hydroxyphenyl)-2-methyl-1-butanone

[195393-39-6] $C_{11}H_{14}O_2$ mol. wt. 178.23



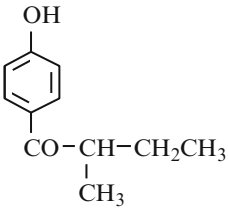
Synthesis
-Also obtained (**10**) by reaction of 1-acetoxy-5-sec-pentanoyl-1,3-cyclohexadiene tricarbonyl iron complex (**8**) with triethylamine N-oxide in DMA at r.t. for 1 h (53 %) [246].

Acetate [195393-36-3] $C_{13}H_{16}O_3$ mol. wt. 220.27

-Obtained in the same reaction that the phenol above (14 %) [246].

1-(4-Hydroxyphenyl)-2-methyl-1-butanone
(S)-4-(1-oxo-2-methylbutyl)phenol

[120836-88-2]
[120836-99-9] (2*S*)
[123020-88-2] (+) $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses
-Obtained by Friedel-Crafts acylation of anisole with (S)-(+)-2-methylbutyryl chloride in the presence of aluminium chloride in ethylene dichloride [1721].
-Also refer to: [1352 (+), 1416 (S), 1417, 1511 (+), 1645, 1715 (S), 3025 (S), 3098].

^{1}H NMR [1352, 1715], IR [1352, 1715];
$(\alpha)_D = +40.9°$ (chloroform) [1715].

N.B.: Metabolite of T-018 in the urine of female rats [1511].

Methyl ether [90269-46-8] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Obtained by treatment of anisole with 2-methylbutyric anhydride or 2-methylbutyryl chloride in the presence of sulfated zirconia [867].
-Also obtained by reaction of 2-methylbutanoyl chloride with anisole in the presence of aluminium chloride in carbon disulfide first at 0° for 15 min, then at r.t. for 1 h (54 %) [79].
-Also obtained from 4-methoxybenzaldehyde (52 %) [3024].
-Also refer to: [179, 1136, 1736, 1781, 2510].

b.p.$_{0.5}$ 99–100° [79], b.p.$_{0.4}$ 105° [1736], b.p.$_{12}$ 145–150° [1781],
b.p.$_{10}$ 152° [2510], b.p.$_{1}$ 152–153° [1136];
$(\alpha)_D = +25.3°$ [2510]; $n_D^{17.5} = 1.534$ [2510];
^{1}H NMR [79, 3024], IR [79], UV [1736].

2,4-Dinitrophenylhydrazone of the methyl ether

[14248-30-7] $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 97–100° [1781], 101.5–102.2° [2368].

Methyl ether (2*S*) [27763-55-9] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Obtained by reaction of 2-methylbutanoyl chloride with anisole (70 %) [179].
-Also refer to: [850, 867, 2069].

b.p.$_{0.3}$ 155° [179], b.p.$_{15–20}$ 160° [850];
$(\alpha)_D = +3.2°$ neat (no solvent) [850], $(\alpha)_D = +25°$ (dioxane) [179];
$n_D^{35} = 1.518$ [850];
Circular dichroism spectra [1736].

Methyl ether *(R)* [77942-74-6] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Refer to: [1107].

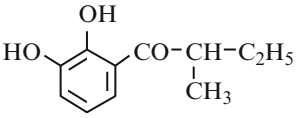
Phenyl ether [90269-45-7] $C_{17}H_{18}O_2$ mol. wt. 254.33

-Obtained by reaction of 2-methylbutanoyl chloride with diphenyl oxide in the presence of aluminium chloride in carbon disulfide first at 0° for 15 min, then at r.t. for 1 h (66 %) [79].

b.p.$_{0.18}$ 129–131° [79]; ^{1}H NMR [79], IR [79].

1-(2,3-Dihydroxyphenyl)-2-methyl-1-butanone

$C_{11}H_{14}O_3$ mol. wt. 194.23



Synthesis

-Refer to: [2747].

Dimethyl ether [15121-99-0]

$C_{13}H_{18}O_3$ mol. wt. 222.28

-Obtained by oxidation of 1-(2,3-dimethoxyphenyl)-1-(2-methylpropyl) carbinol with sodium dichromate in dilute sulfuric acid (75–80 %) [2747].

pale yellow viscous oil [2747]; b.p.$_{0.2}$ 90–92° [2747].

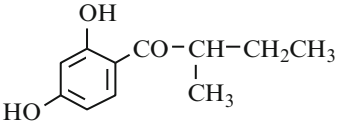
2,4-Dinitrophenylhydrazone of the methyl ether

[15116-04-8] $C_{19}H_{22}N_4O_6$ mol. wt. 402.41

m.p. 224.5–225.5° [2747].

1-(2,4-Dihydroxyphenyl)-2-methyl-1-butanone

[15116-15-1]
[123020-85-9] (2S) $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses

-Obtained by Friedel-Crafts acylation of resorcinol dimethyl ether with (S)-(+)-2-methylbutyryl chloride in the presence of aluminium chloride in ethylene dichloride [1721].

-Also obtained by reaction of sec-valeric acid with resorcinol in the presence of zinc chloride (55–75 %) [2747], for 2 h at 150° (55 %) [2829].

-Also obtained by enzymatic enantioselective deacetylation of its 2,4-diacetyl ester [2829].

-Also refer to: [1719, 3025].

yellow viscous oil [2747]; oil [2829]; b.p.$_1$ 143–148° [2747];
^{1}H NMR [2829], ^{13}C NMR [2829], IR [2829], UV [2829],
MS [2829]; TLC [2829].

Diacetates $C_{15}H_{18}O_5$ mol. wt. 278.30

-Refer to: [2829].

*racemic [406174-67-2].

-Obtained by reaction of acetic anhydride with 1-(2,4-dihydroxyphenyl)-2-methyl-1-butanone in the presence of catalytic amount of N,N-dimethylaminopyridine at 22–25° (90 %) [2829].

oil [2829];
^{1}H NMR [2829], ^{13}C NMR [2829], IR [2829], UV [2829], MS [2829]; TLC [2829].

*levogyre (−) [406174-79-6].

-Obtained by chemical acetylation of monoacetate [2829].

$(\alpha)_D^{25} = -23.9°$ (chloroform) [2829].

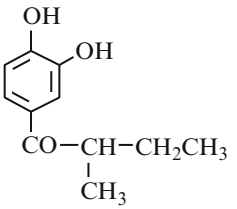
*dextrogyre (+) [406174-75-2].

-Obtained by treatment of racemic ketone with PPL pre-incubated in THF at 40–42° for 12 h in the presence of butanol (81 %) [2829].

$(\alpha)_D^{25} = +32.5°$ (chloroform) [2829].

1-(3,4-Dihydroxyphenyl)-2-methyl-1-butanone

[67049-69-8] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Obtained by heating 1-(3,4-dimethoxyphenyl)-2-methyl-1-butanone with pyridinium chloride at 200–220° for 1 h under nitrogen (89 %) [2127].
-Also refer to: [899].
yellow viscous oil [2127];
b.p.$_{0.02}$ 157° [2127].

BIOLOGICAL ACTIVITY: Central nervous system depressant [2127]; Antimelanoma and skin depigmentation by, *in vitro* method for screening [612].

Dimethyl ether [67049-70-1] $C_{13}H_{18}O_3$ mol. wt. 222.28

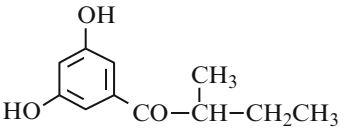
-Obtained by reaction of 2-methylbutyryl chloride with veratrole in the presence of aluminium chloride in refluxing benzene for 30 min (66 %) [2127].
-Also obtained by metallation of veratric acid with s-BuLi/TMEDA (2.2 equiv.) at −30° [66], (22 %) [617].

colourless liquid [2127]; b.p.$_{0.025}$ 101° [2127]; $n_D^{25} = 1.5409$ [2127].

BIOLOGICAL ACTIVITY: Central nervous system depressant [2127].

1-(3,5-Dihydroxyphenyl)-2-methyl-1-butanone

$C_{11}H_{14}O_3$ mol. wt. 194.23



Synthesis
-Refer to: [31].

Dimethyl ether
$C_{13}H_{18}O_3$ mol. wt. 222.28

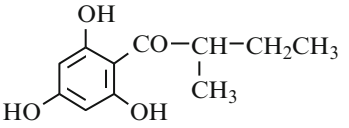
-Preparation from 3,5-dimethoxybenzamide (76 %) [31].

b.p.$_{0.5}$ 124–128° [31]; $n_D^{20} = 1.5266$ [31].

2-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone
(Multifidol)

[39652-80-7]
[125074-06-8]

$C_{11}H_{14}O_4$ mol. wt. 210.23



Syntheses
-Obtained by reaction of 2-methylbutanoic acid with phloroglucinol in the presence of boron trifluoride etherate [3019].

-Also obtained by adding phloroglucinol to a solution of phosphorous oxychloride plus aluminium chloride and stirred under nitrogen. 2-Methyl-butanoic acid was added and the reaction stirred under nitrogen at 0° for 8 h, then at 6° for 40 h (40–54 %) [3201].
-Also obtained by acid hydrolysis of 2-(2-methylbutyryl)phloroglucinol 1-*O*-(6″-*O*-β-D-apiofuranosyl)-β-D-glucopyranoside [3455].
-Also refer to: [762, 763, 765, 766, 1373, 1401, 1731, 1866, 2621, 3202, 3310].

Isolation from the natural sources

-From the latex of *Jatropha multifada* (Euphorbiaceae) [337, 1737].

m.p. 116–118° [1737], 62–64° [1401], 62–63° [1866], 61–64° [2621], 61–63° [1373].
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [762, 1737, 3019, 3455], ^{13}C NMR [1737, 3019],
IR [762, 1737, 3019], UV [1737, 3019], MS [1737].

BIOLOGICAL ACTIVITY: Antiprotozoal and antimicrobial [337]; Antimicrobial for *Staphylococcus aureus* [3372]; Antagonist both thromboxane A_2 and Leukotriene D_4 [3019]; Antifungal [3202]; Cytotoxicity [3202].

N.B.: Three CAS Registry Numbers attributed at this ketone:

[39652-80-7], [125074-06-8] and [98498-56-7] (racemic).

(S)-(+) isomer [111556-27-5] $C_{11}H_{14}O_4$ mol. wt. 210.23

Synthesis

-Obtained by reaction of S-(*) 2-methylbutanoyl chloride with phloroglucinol in the presence,
*of boron trifluoride etherate at 40° for 2 h (30.5 %) [2434];
*of aluminium chloride in nitrobenzene/carbon disulfide mixture (84 %) [286].
-Also refer to: [1115, 1737, 3455].

Isolation from the natural sources

-From the latex collected from the leaf-stalks of *Jatropha multidisa* (Euphorbiaceae) [1737].

m.p. 116–118° [1737], 76–78° [2434].
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [286, 1737, 3455], ^{13}C NMR [1737], IR [1737],
UV [1737, 2434], MS [1737].
$(\alpha)_D^{18} = +26.1$ (chloroform) [2434], $(\alpha)_D^{25} = +17.23$ (ethanol) [286];
circular dichroism [1737];

2-β-D-Glucoside $C_{17}H_{24}O_9$ mol. wt. 372.37

Isolation from the natural sources

-From the latex of *Jatropha multifada* (Euphorbiaceae) [1737].

m.p. 139–140° [1737];
^{1}H NMR [1737], ^{13}C NMR [1737], IR [1737], UV [1737], MS [1737].

Trimethyl ether (S) [124598-12-5] $C_{14}H_{20}O_4$ mol. wt. 252.31

-Preparation by reaction of S-2-methylbutanoyl chloride with phloroglucinol trimethyl ether in the presence of aluminium chloride (18 %) [2434].

^{1}H NMR [2434], UV [2434];
$(\alpha)_D^{21} = +4.54°$ (acetone) [2434].

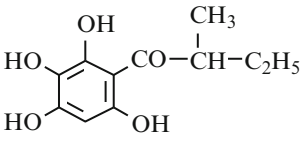
Triacetate (S) [124598-16-9] $C_{17}H_{20}O_7$ mol. wt. 336.34

-Obtained by reaction of acetic anhydride with S-2-methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone in the presence of pyridine (58 %) [2434].

^{1}H NMR [2434];
$(\alpha)_D^{21} = +9.41°$ (acetone) [2434].

2-Methyl-1-(2,3,4,6-tetrahydroxyphenyl)-1-butanone

[209122-44-1] $C_{11}H_{14}O_5$ mol. wt. 226.23

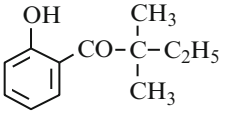


Synthesis
-Obtained by reaction of 2-methylbutanoic acid with 1,2,3,5-tetrahydroxybenzene (benzenetetrol) in the presence of boron trifluoride etherate and powdered molecular sieves 4 Å at 80° for 1 h under argon (77.5 %) [2721].

pale brown oil [2721];
^{1}H NMR [2721], IR [2721], MS [2721].

1-(2-Hydroxyphenyl)-2,2-dimethyl-1-butanone

[106141-14-4] $C_{12}H_{16}O_2$ mol. wt. 192.26



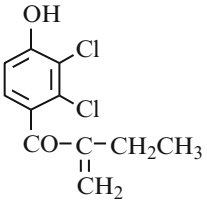
Synthesis
-Obtained by treatment of o-bromophenyl 2,2-dimethylbutyrate with 1.1 equiv. sec-butyllithium (0.25 M in THF/ether/hexane) at −95° and stirred for 30 min. After an additional 30 min at −78°, the mixture was hydrolyzed with saturated NH_4Cl (85 %) [2076].

^{1}H NMR [2076], IR [2076], UV [2076], MS [2076].

2.1.2 Substituted Hydroxyketones

1-(2,3-Dichloro-4-hydroxyphenyl)-2-methylene-1-butanone

[4115-00-8] $C_{11}H_{10}Cl_2O_2$ mol. wt. 245.10



Syntheses
-Refer to: [1517, 2054, 2055, 2058–2061].
m.p. 84–85° [2054, 2055, 2058–2061].

Methyl ether [59043-82-2] $C_{12}H_{12}Cl_2O_2$ mol. wt. 259.13

-Obtained by adding dropwise acetic anhydride to a suspension of the 4-methoxybutyrophenone in N,N,N′,N′-tetramethylmethanediamine. The reaction temperature was maintained at 90° (86 %) [833].
-Also refer to: [742 (94 %), 1517, 3333].

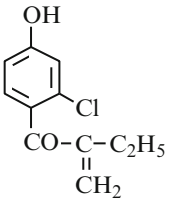
liquid [742];
m.p. 46–48° [833, 3333]; ^{1}H NMR [742].

2-Hydroxyethyl ether [327023-36-9] $C_{13}H_{14}Cl_2O_3$ mol. wt. 289.16

-Refer to: [863].

1-(2 Chloro-4-hydroxyphenyl)-2-methylene-1-butanone

[4115-02-0] $C_{11}H_{11}ClO_2$ mol. wt. 210.66



Syntheses

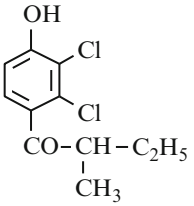
-Obtained from 2-dimethylaminoethyl-2′-chloro-4′-hydroxybutyrophenone (m.p. 89–92°) which was dissolved in aqueous saturated $NaHCO_3$, left 24 h at r.t.; and worked up to give the title ketone [2765].

-Also refer to: [2047, 2054, 2055, 2058, 2060, 2061].

b.p.$_{0.2}$ 165° [2047], b.p.$_{0.02}$ 165° [2054, 2061], b.p.$_{0.4}$ 173° [2058], b.p.$_{0.04}$ 173° [2055, 2060];
m.p. 47–49° [2047, 2055, 2060, 2765].

1-(2,3-Dichloro-4-hydroxyphenyl)-2-methyl-1-butanone

$C_{11}H_{12}Cl_2O_2$ mol. wt. 247.12



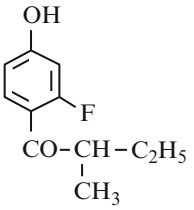
Synthesis

-Refer to: [863].

m.p. 85–86° [2057].

1-(2-Fluoro-4-hydroxyphenyl)-2-methyl-1-butanone (2S)

[505084-77-5] $C_{11}H_{13}FO_2$ mol. wt. 196.22



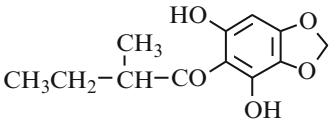
Synthesis

-Refer to: [3025].

USE: In preparation of polymeric ferroelectric liquid crystals [3025].

1-(4,6-Dihydroxy-1,3-benzodioxol-5-yl)-2-methyl-1-butanone

$C_{12}H_{14}O_5$ mol. wt. 238.24



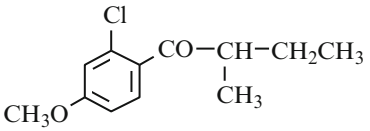
Synthesis
-Refer to: [411].
Dimethyl ether [73213-21-5]
$C_{14}H_{18}O_5$ mol. wt. 266.29

Isolation from natural sources
-From *Helichrysum chrysargyrum* [411].

colourless oil [411]; ^{1}H NMR [411], IR [411], MS [411].

1-(2-Chloro-4-methoxyphenyl)-2-methyl-1-butanone

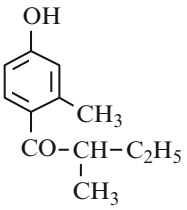
$C_{12}H_{15}ClO_2$ mol. wt. 226.70



Synthesis
-Refer to: [1736].
UV [1736].

1-(4-Hydroxy-2-methylphenyl)-2-methyl-1-butanone (2S)

[505084-75-3] $C_{12}H_{16}O_2$ mol. wt. 192.26

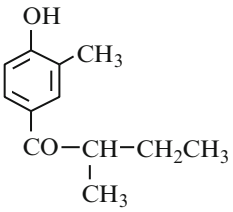


Synthesis
-Refer to: [3025].
^{1}H NMR [1352], IR [1352].

USE: In preparation of polymeric ferroelectric liquid crystals [3025].

1-(4-Hydroxy-3-methylphenyl)-2-methyl-1-butanone

$C_{12}H_{16}O_2$ mol. wt. 192.26



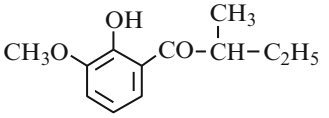
Synthesis
-Refer to: [218].
Methyl ether [927911-91-9]
$C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of 2-methylbutanoic acid with 2-methylanisole in the presence of $HSiMe_2Cl$ and $InCl_3$ in 1,2-dichloroethane, first 1 h at r.t., then heated at 80° for 4 h (81 %) [218].

^{1}H NMR [218], ^{13}C NMR [218], IR [218], MS [218].

1-(2-Hydroxy-3-methoxyphenyl)-2-methyl-1-butanone

[15116-07-1] $C_{12}H_{16}O_3$ mol. wt. 208.26

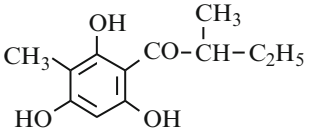


Synthesis
-Obtained by partial demethylation of its methyl ether with aluminium chloride in toluene (50–70 %) [2747].

oil [2747]; b.p.$_{0.4}$ 89–94° [2747].

2-Methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-butanone (S)

[124598-11-4] $C_{12}H_{16}O_4$ mol. wt. 224.26



Synthesis
-Obtained by reaction of S-2-methylbutanoyl chloride with 2-methylphloroglucinol in the presence of aluminium chloride (68.3 %) [2434].

m.p. 132–135° [2434]; UV [2434]; $(\alpha)_D^{18} = +31°$ (acetone) [2434].

Trimethyl ether (S) [124598-14-7] $C_{15}H_{22}O_4$ mol. wt. 266.34

-Obtained by reaction of S-2-methyl-1-butanoyl chloride with 2-methylphloroglucinol trimethyl ether in the presence of aluminium chloride (21 %) [2434].

^{1}H NMR [2434], UV [2434]; $(\alpha)_D^{21} = +10.6°$ (acetone) [2434].

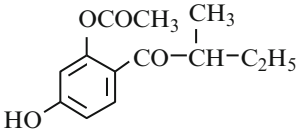
Triacetate (S) [124598-18-1] $C_{18}H_{22}O_7$ mol. wt. 350.37

-Obtained by reaction of acetic anhydride with S-2-methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-butanone in the presence of pyridine (77 %) [2434].

^{1}H NMR [2434];
$(\alpha)_D^{21} = +21.9°$ (acetone) [2434].

1-[2-(Acetyloxy)-4-hydroxyphenyl]-2-methyl-1-butanone (−)

[406174-71-8] $C_{13}H_{16}O_4$ mol. wt. 236.27

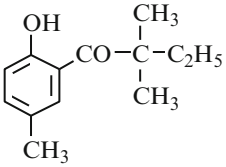


Synthesis
-Obtained by enzymatic enantioselective deacetylation of diester in the presence of PPL (72 %) [2829].

oil [2829];
^{1}H NMR [2829], ^{13}C NMR [2829], IR [2829], UV [2829],
MS [2829]; TLC [2829]; $(\alpha)_D^{25} = -41.4°$ (chloroform) [2829].

1-(2-Hydroxy-5-methylphenyl)-2,2-dimethyl-1-butanone

[106141-15-5] $C_{13}H_{18}O_2$ mol. wt. 206.28

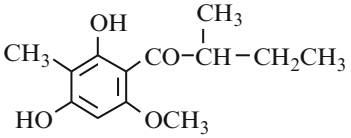


Synthesis
-Obtained by treatment of 2-bromo-5-methylphenyl 2,2-dimethylbutyrate with 1.1 equiv. sec-butyllithium (0.25 M in THF/ether/hexane) at −95° and stirred for 30 min. After an additional 30 min at −78°, the mixture was hydrolyzed with saturated NH_4Cl (76 %) [2076].

^{1}H NMR [2076], IR [2076], UV [2076], MS [2076].

1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-2-methyl-1-butanone

[918896-70-5] $C_{13}H_{18}O_4$ mol. wt. 238.28



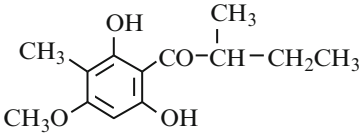
Isolation from natural sources
-From the aerial parts of *Hypericum beanii* (Guttiferae) [2496].
pale yellow oil [2496];

^{1}H NMR [2496], ^{13}C NMR [2496], IR [2496], UV [2496], MS [2496].

BIOLOGICAL ACTIVITY: Antistaphylococcal [2496].

1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-2-methyl-1-butanone
(Pulverulentone B)

[89647-61-0] $C_{13}H_{18}O_4$ mol. wt. 238.28

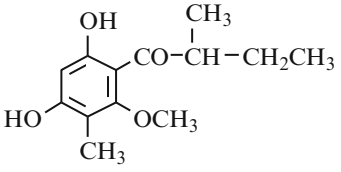


Isolation from natural sources
-From *Eucalyptus pulverulenta* [420, 421].
-From *Eucalyptus pulverulenta* Sims (Myrtaceae) [1106].

MS [420]; HPLC [420]; GC/MS [420].

1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-2-methyl-1-butanone
(Pseudoaspidinol 2-MeB)

[55382-32-6] $C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses
-Obtained by reductive alkaline cleavage,
*of kosotoxin (**II**) and protokosin (**III**) from female flowers of *Hagenia abyssinica* (Bruce) Gmelin [1916] (**IVc**);
*of "kosin" (**IV**), from *Flos koso* "Siegfried" by treatment with 15 % potassium hydroxide in the presence of zinc powder on a water bath for 24 h [1915] (**VIIIc**).

m.p. 59–61° [1915]; ^{1}H NMR [2744].

N.B.: "Kosin" (**IV**), others names: Methylene-bis-pseudo-aspidinol; pseudo-aspidin.

m.p. 148–150° [1915];
^{1}H NMR [1915], ^{13}C NMR [1912], IR [1915], UV [1915], MS [1915]; GLC [2531].

(S)-(+) [124598-08-9].

-Obtained by reaction of S-2-methylbutanoyl chloride (4 mol) with methyl 2,6-dihydroxy-4-methoxy-3-methylbenzoate (4 mol) in the presence of aluminium chloride (12 mol) in carbon disulfide for 1.5 h (7 %) [2434].

m.p. 39–40° [2434]; ^{1}H NMR [2434], UV [2434];
$(\alpha)_D^{23} = +18.6°$ (acetone) [2434].

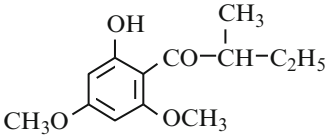
Diacetate (S)-(+) [124598-17-0] $C_{17}H_{22}O_6$ mol. wt. 322.36

-Obtained by reaction of acetic anhydride with S-1-(4,6-dihydroxy-2-methoxy-3-methylphenyl)-2-methyl-1-butanone in the presence of pyridine (84 %) [2434].

^{1}H NMR [2434]; $(\alpha)_D^{21} = +10.3°$ (acetone) [2434].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-2-methyl-1-butanone (S)

[124598-07-8] $C_{13}H_{18}O_4$ mol. wt. 238.28

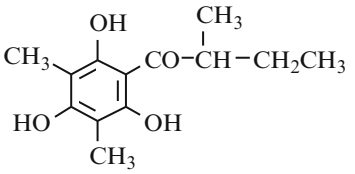


Synthesis
-Preparation by reaction of diazomethane with S-2-methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone in ethyl ether (78 %) [2434].

^{1}H NMR [2434], UV [2434]; $(\alpha)_D^{18} = +16.2°$ (chloroform) [2434].

2-Methyl-1-(2,4,6-trihydroxy-3,5-dimethylphenyl)-1-butanone

[87035-85-6] $C_{13}H_{18}O_4$ mol. wt. 238.28
[65792-31-6]



Synthesis
-Obtained by reductive alkaline cleavage of kosotoxin (**II**) and protokosin (**III**) from female flowers of *Hagenia abyssinica* (Bruce) Gmelin [1916] (**XIXc**).
m.p. 105–106° [2858].

Trimethyl ether [245063-60-9] $C_{16}H_{24}O_4$ mol. wt. 280.36
(Isotorquatone)

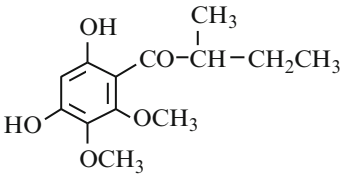
Isolation from natural sources

-From the leaf oils of the *genus Xanthostemon* (Myrtaceae) in Australia [462].
-From essential oil of *Eucalyptus apodophylla* (Myrtaceae) [2046].
-From volatile leaf oils of some southwestern and southern Australian species of the genus *Eucalyptus* [353–356, 359, 366].
-Compound of leaf essential oils of *Eucalyptus chartaboma* (chemotype II) (3.1 %) and *Eucalyptus miniata* (1.3 %) (Myrtaceae) [1453].

^{1}H NMR [1453, 2046], ^{13}C NMR [1453, 2046], MS [1453, 2046]; GC-MS [462].

1-(4,6-Dihydroxy-2,3-dimethoxyphenyl)-2-methyl-1-butanone

[73694-18-5] $C_{13}H_{18}O_5$ mol. wt. 254.28



Isolation from natural sources
-From *Helichrysum nanum* (Compositae) (**15**) [401].
^{1}H NMR [401], IR [401], MS [401].

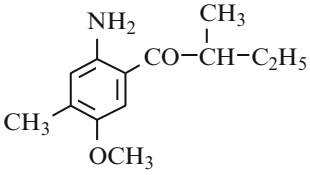
Diacetate [73694-27-6] $C_{17}H_{22}O_7$ mol. wt. 338.36 (**16**).

Synthesis
-Obtained by heating a mixture of acetic anhydride, 1-(4,6-dihydroxy-2,3-dimethoxyphenyl)-2-methyl-1-butanone and 4-pyrrolidinopyridine for 1 h at 70° (7 %) [401].

oil [401]; ^{1}H NMR [401], MS [401]; TLC [401].

1-(2-Amino-5-methoxy-4-methylphenyl)-2-methyl-1-butanone

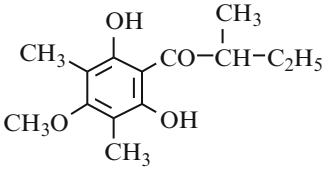
[959137-60-1] $C_{13}H_{19}NO_2$ mol. wt. 221.30



Synthesis
-Refer to: [2027].
^{1}H NMR [2027].

1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-2-methyl-1-butanone

[138690-39-8] $C_{14}H_{20}O_4$ mol. wt. 252.31



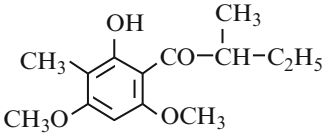
Isolation from natural sources
-From *Hagenia Abyssinica* (Rosaceae) [2744].
-From *Eucalyptus robusta* Smith (Myrtaceae) [637, 1106].
-Also refer to: [727, 2533].

pale yellow [2744]; m.p. 47–49° [2744];
^{1}H NMR [637, 2744], ^{13}C NMR [637, 1106, 2744],
IR [637, 2744], UV [637], MS [637, 2744];
$(\alpha)_D = +17°$ (chloroform) [2744]; TLC [2744].

BIOLOGICAL ACTIVITY: Refer to: [637].

1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-2-methyl-1-butanone (S)

[124598-13-6] $C_{14}H_{20}O_4$ mol. wt. 252.31



Synthesis
-Obtained by reaction of S-2-methyl-1-butanoyl chloride with 3,5-dimethoxy-2-methylphenol in the presence of aluminium chloride (8 %) [2434].

^{1}H NMR [2434], UV [2434]; $(\alpha)_D^{21} = +21.2°$ (acetone) [2434].

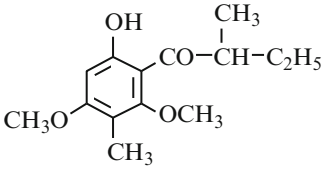
Acetate [124598-19-2] $C_{16}H_{22}O_5$ mol. wt. 294.35

-Obtained by reaction of acetic anhydride with S-1-(2-hydroxy-4,6-dimethoxy-3-methylphenyl)-2-methyl-1-butanone in the presence of pyridine (91 %) [2434].

^{1}H NMR [2434], UV [2434];
$(\alpha)_D^{21} = +14.4°$ (acetone) [2434].

1-(6-Hydroxy-2,4-dimethoxy-3-methylphenyl)-2-methyl-1-butanone
(Homoisobaeckeol)

[808751-13-5] $C_{14}H_{20}O_4$ mol. wt. 252.31



Isolation from natural sources
-Compound of leaf essential oils of *Eucalyptus chartaboma* (chemotype I) (27.5 %), *Eucalyptus chartaboma* (chemotype II) (8 %) and *Eucalyptus miniata* (6.3 %) (Myrtaceae) [1453].

^{1}H NMR [1453], ^{13}C NMR [1453], MS [1453].

Methyl ether [808749-86-2] $C_{15}H_{22}O_4$ mol. wt. 266.34
(Homobaeckeol methyl ether)

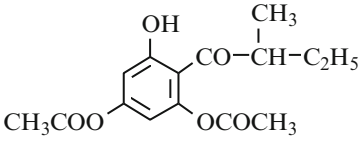
Isolation from natural sources

-Compound of leaf essential oils of *Eucalyptus chartaboma* (chemotype II) (4.7 %) and *Eucalyptus miniata* (7.3 %) (Myrtaceae) [1453].

^{1}H NMR [1453], ^{13}C NMR [1453], MS [1453].

1-[2,4-Bis(acetyloxy)-6-hydroxyphenyl]-2-methyl-1-butanone (S)

[124598-15-8] $C_{15}H_{18}O_6$ mol. wt. 294.30



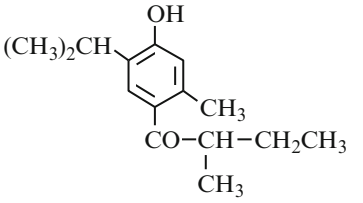
Synthesis

-Obtained by reaction of acetic anhydride with S-2-methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone in the presence of pyridine (54 %) [2434].

^{1}H NMR [2434];
$(\alpha)_D^{21} = +7.94°$ (acetone) [2434].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-2-methyl-1-butanone

[80356-13-4] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses

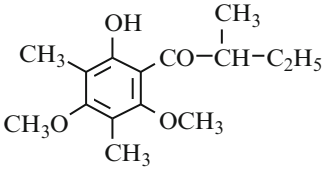
-Obtained by photo-Fries rearrangement of thymyl 2-methylbutanoate in methanol for 6 h at 25° under nitrogen (16 %) (**2c**) [2421].

-Also refer to: [2421].

m.p. 126° [2421];
^{1}H NMR [2421], IR [2421].

1-(2-Hydroxy-4,6-dimethoxy-3,5-dimethylphenyl)-2-methyl-1-butanone
(Chartabomone)

[808751-11-3] $C_{15}H_{22}O_4$ mol. wt. 266.34



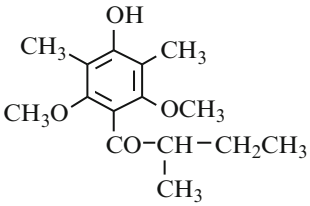
Isolation from natural sources

-Compound of leaf essential oils of *Eucalyptus chartaboma* (chemotype II) (0.5 %) and *Eucalyptus miniata* (0.3 %) (Myrtaceae) [1453].

^{1}H NMR [1453], ^{13}C NMR [1453], MS [1453].

1-(4-Hydroxy-2,6-dimethoxy-3,5-dimethylphenyl)-2-methyl-1-butanone

[87035-88-9] $C_{15}H_{22}O_4$ mol. wt. 266.34



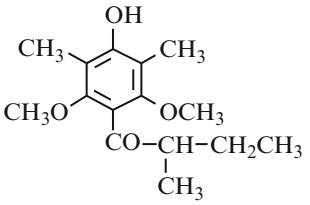
Syntheses
-Obtained by deprotection of 1-[4-(tert-butyldimethylsilyl)-oxy-2,6-dimethoxy-3,5-dimethylphenyl]-2-methyl-1-butanone with tetra-n-butylammonium fluoride in THF for 1 h (82 %) [475].
-Also refer to: [2512].

m.p. 58.5–59° [475];
^{1}H NMR [2512], ^{13}C NMR [2512], IR [2512], UV [475], MS [2512].

USE: Asym. synthesis of wasabidienones B_1 an B *via* SIBX-mediated hydroxylative phenol dearomatization [2512].

1-(4-Hydroxy-2,6-dimethoxy-3,5-dimethylphenyl)-2-methyl-1-butanone (2*R*)

[1080023-65-9] $C_{15}H_{22}O_4$ mol. wt. 266.34

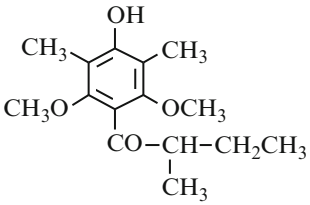


Synthesis
-Refer to: [2512].
^{1}H NMR [2512], ^{13}C NMR [2512], IR [2512], MS [2512].
$(\alpha)_D^{20} = -4.1°$ [2512].

USE: Asym. synthesis of wasabidienones B_1 an B *via* SIBX-mediated hydroxylative phenol dearomatization [2512].

1-(4-Hydroxy-2,6-dimethoxy-3,5-dimethylphenyl)-2-methyl-1-butanone (2S)

[1080023-64-8] $C_{15}H_{22}O_4$ mol. wt. 266.34

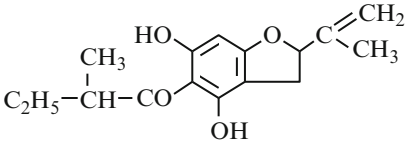


Synthesis
-Refer to: [2512].
^{1}H NMR [2512], ^{13}C NMR [2512], IR [2512], MS [2512];
$(\alpha)_D^{20} = +5°$ [2512].

USE: Asym. synthesis of wasabidienones B_1 an B *via* SIBX-mediated hydroxylative phenol dearomatization [2512].

1-[2,3-Dihydro-4,6-dihydroxy-2-(1-methylethenyl)-5-benzofuranyl]-2-methyl-1-butanone

[103771-75-1] $C_{16}H_{20}O_4$ mol. wt. 276.33

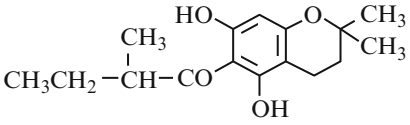


Isolation from natural sources

-From *Helichrysum cephaloideum* and *Helichrysum mixtum* (Compositae) [1487].

1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-2-methyl-1-butanone

[39652-88-5] $C_{16}H_{22}O_4$ mol. wt. 278.35



Synthesis

-Obtained by heating of 2-methyl-1-[2,4,6-tri-hydroxy-3-(3-methyl-2-butenyl) phenyl]-1-butanone in benzene with sulfuric acid in the presence of acetic anhydride [398].

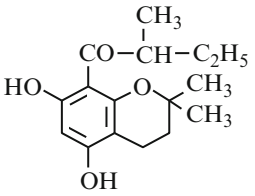
Isolation from natural sources

-From the aerial parts of *Helichrysum platypterum* DC (Compositae) [1487].
-From *Helichrysum gymnoconum* (Compositae) [398].

^{1}H NMR [398], IR [398], MS [398].

1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-2-methyl-1-butanone

[39652-87-4] $C_{16}H_{22}O_4$ mol. wt. 278.35



Syntheses

-Obtained by heating of 2-methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone in benzene with sulfuric acid in the presence of acetic anhydride [398].
-Also refer to: [708].

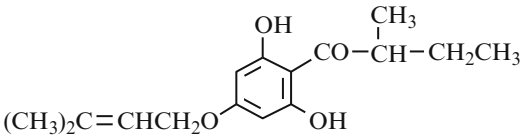
Isolation from natural sources

-From *Helichrysum platypterum* (Compositae) [1487].
-From *Helichrysum gymnoconum* (Compositae) [398].

^{1}H NMR [398, 1487], IR [398], MS [398, 1487].

1-[2,6-Dihydroxy-4-[(3-methyl-2-butenyl)oxy]phenyl]-2-methyl-1-butanone

[70219-82-8] $C_{16}H_{22}O_4$ mol. wt. 278.35



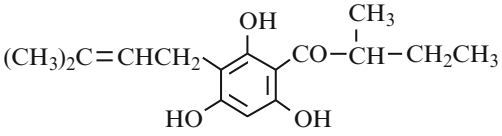
Isolation from natural sources
-From *Helichrysum crispum* (Compositae) (**30**) [401].
-From *Helichrysum squarrosus* DC (Compositae) (**6**) [400].

-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].

colourless oil [400]; ^{1}H NMR [400], IR [400], MS [400].

2-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone
(HP34.12)

[71539-60-1] $C_{16}H_{22}O_4$ mol. wt. 278.35



Isolation from natural sources
-From *Helichrysum infaustum* (Compositae) [401].
-From *Helichrysum paronychioides* (Asteraceae, tribe Inuleae) [2201].

-From *Helichrysum platypterum* DC (Compositae) [404, 1487].
-From *Helichrysum gymmnoconum* (Compositae) [398].
-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].
-From *Helichrysum indicum* (L.) Grieson (86/248, near Clanwilliam) [1488].
-From *Helichrysum moeserianum* Thell. (86/249, near Clanwilliam) [1488].
-From *Helichrysum odoratissimum* (Compositae) [1238].

colourless oil [398];
^{1}H NMR [398, 2201], ^{13}C NMR [2201], IR [398, 2201],
UV [2201], MS [2201]; TLC [2201].

BIOLOGICAL ACTIVITY: Antioxidant [2201].

Triacetate [71539-61-2] $C_{22}H_{28}O_7$ mol. wt. 404.46

-Obtained by heating 2-methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl) phenyl]-1-butanone with acetic anhydride and sodium acetate [398].

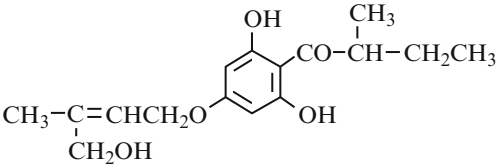
colourless oil [398]; ^{1}H NMR [398], IR [398], MS [398].

Trimethyl ether [1175530-97-8] $C_{19}H_{28}O_4$ mol. wt. 320.43

^{1}H NMR [3334], ^{13}C NMR [3334], IR [398], MS [3334].

1-[2,6-Dihydroxy-4-[(4-hydroxy-3-methyl-2-butenyl)oxy]phenyl]-2-methyl-1-butanone (*E*)

[122585-54-0] $C_{16}H_{22}O_5$ mol. wt. 294.35

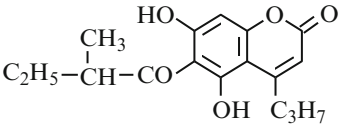


Isolation from natural sources
-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].

^{1}H NMR [1488], IR [1488], MS [1488].

5,7-Dihydroxy-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one *(MAB 2)*

[5022-22-0] $C_{17}H_{20}O_5$ mol. wt. 304.34



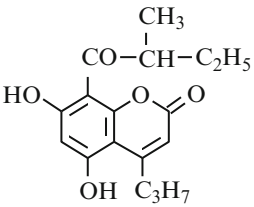
Syntheses
-Obtained by condensation of 2-(2-methylbutyryl)-phloroglucinol with ethyl 4-bromo-3-oxohexanoate [763].

-Also obtained by reaction of ethyl 3-oxohexanoate with 1-(2,4,6-trihydroxyphenyl)-2-methyl-1-butanone in the presence of concentrated sulfuric acid in acetic acid at r.t. for 3 days [753].
-Also refer to: [553, 762].

crystals [753]; m.p. 209–211° [762], 207–208° [753];
^{1}H NMR [553, 753, 762], IR [753, 762],
UV [553, 753, 762], MS [753].

5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

[5022-23-1] $C_{17}H_{20}O_5$ mol. wt. 304.34



Syntheses
-Obtained by condensation of 2-(2-methylbutyryl)-phloroglucinol with ethyl 4-bromo-3-oxohexanoate (3 %) [763].
-Also obtained by reaction of ethyl 3-oxohexanoate with 1-(2,4,6-trihydroxyphenyl)-2-methyl-1-butanone in the presence of concentrated sulfuric acid in acetic acid at r.t. for 3 days (34 %) [753].

-Also refer to: [553, 762].

crystals [753];
m.p. 248–250° for racemic material [286], 235–236° [753];
^{1}H NMR [286, 753], IR [753], UV [553, 753],
MS [753].

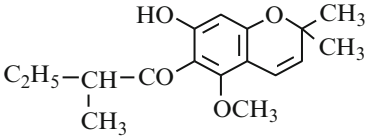
(S)-(−) isomer

-Obtained by adding ethyl 3-oxohexanoate followed by concentrated sulfuric acid to (S)-(+)-(2-methylbutyryl)phloroglucinol in glacial acetic acid. The mixture was allowed to stand for 4 days (27 %) [286].

m.p. 254–256° [286]; ^{1}H NMR [286]; $(\alpha)_D^{25} = -5.4°$ (ethanol) [286].

1-(7-Hydroxy-5-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-2-methyl-1-butanone
(Rhynchonin B) (−)

[163734-38-1] $C_{17}H_{22}O_4$ mol. wt. 290.36

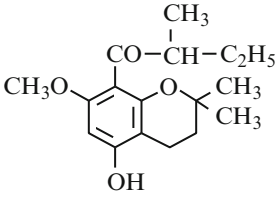


Synthesis
-Refer to: [493].

BIOLOGICAL ACTIVITY: Bioactive chromenes from *Rhyncholacis penicillata* [493].

1-(3,4-Dihydro-5-hydroxy-7-methoxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-2-methyl-1-butanone

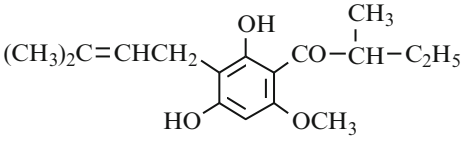
$C_{17}H_{24}O_4$ mol. wt. 292.37



Isolation from natural sources
-From *Helichrysum platypterum* (Compositae) [1487].
^{1}H NMR [1487], MS [1487].

1-[2,4-Dihydroxy-6-methoxy-3-(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone

[71539-62-3] $C_{17}H_{24}O_4$ mol. wt. 292.37



Isolation from natural sources
-From the aerial parts of *Helichrysum cephaloideum* (Compositae) [1487].
-From *Helichrysum gymmnoconum* (Compositae) [398].

^{1}H NMR [398], IR [398], MS [398].

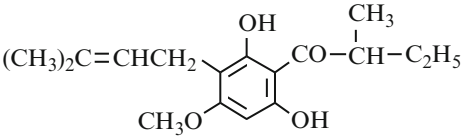
Diacetate [71539-64-5] $C_{21}H_{28}O_6$ mol. wt. 376.45

-Obtained by reaction of acetic anhydride with 1-[2,4-dihydroxy-6-methoxy-3-(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone in the presence of sodium acetate for 12 h at 70° [398].

^{1}H NMR [398], IR [398], MS [398].

1-[2,6-Dihydroxy-4-methoxy-3-(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone

[103771-69-3] $C_{17}H_{24}O_4$ mol. wt. 292.37

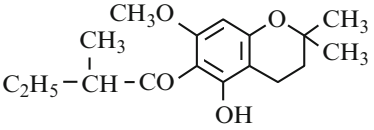


Isolation from natural sources
-From the aerial parts of *Helichrysum platypterum* (Compositae) [1487].

^{1}H NMR [1487], MS [1487].

1-(3,4-Dihydro-5-hydroxy-7-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-2-methyl-1-butanone

[71539-70-3] $C_{17}H_{24}O_4$ mol. wt. 292.37



Synthesis
-Obtained by heating of 1-[2,4-dihydroxy-6-methoxy-3-(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone in benzene with sulfuric acid in the presence of acetic anhydride [398].

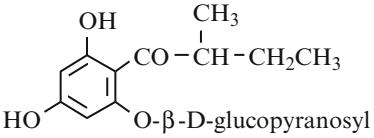
Isolation from natural sources

-From *Helichrysum platypterum* (Compositae) [1487].
-From *Helichrysum gymmnoconum* (Compositae) [398].

^{1}H NMR [398, 1487], IR [398, 1487], MS [398, 1487].

1-[2-(β-D-Glucopyranosyloxy)-4,6-dihydroxyphenyl]-2-methyl-1-butanone

[124960-73-2] $C_{17}H_{24}O_9$ mol. wt. 372.37



Isolation from natural sources
-From flowering twigs of *Emblica officinalis* Gaertn. (syn. *Phyllanthus emblica*) commonly known as *Amla* (Indian goose berry) (Euphorbiaceae) [2839].

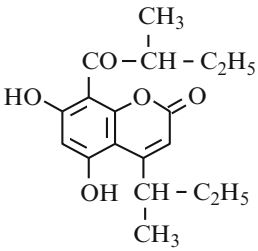
-From hops [277].
-From the latex of *Jatropha multifada* [337, 1737].
-From the leaves and branches of *Phyllanthus emblica* (Euphorbiaceae) [3455].

m.p. 139–140° [1737];
^{1}H NMR [1737, 3455], ^{13}C NMR [1737, 3455], IR [1737], UV [1737], MS [1737].

BIOLOGICAL ACTIVITY: Antiinflammatory agent [277]; Antiprotozoal and antimicrobial [337].

5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-(1-methylpropyl)-2*H*-1-benzopyran-2-one

[98192-74-6] $C_{18}H_{22}O_5$ mol. wt. 318.37

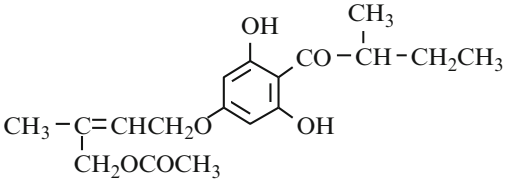


Syntheses
-Obtained by reaction of 2-methylbutanoyl chloride with 5,7-dihydroxy-4-(1-methylpropyl)-2*H*-1-benzopyran-2-one in the presence of aluminium chloride in nitrobenzene for 6 days at 20° (43 %) [765].
-Also refer to: [764].
m.p. 182–184° [764];

^{1}H NMR [764], IR [764], UV [764], MS [764].

1-[4-[[(4-Acetyloxy)-3-methyl-2-butenyl]oxy]-2,6-dihydroxyphenyl]-2-methyl-1-butanone *(E)*

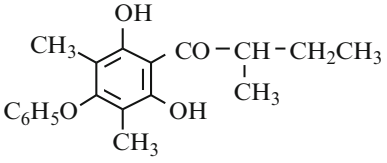
[122585-55-1] $C_{18}H_{24}O_6$ mol. wt. 336.38



Isolation from natural sources
-From *Helichrysum asperum* (Thunb.) Hilliard et Burtt. var. *albidulum* (DC) Hilliard [1488].
^{1}H NMR [1488].

1-[2,6-Dihydroxy-3,5-dimethyl-4-(phenyloxy)phenyl]-2-methyl-1-butanone

$C_{19}H_{22}O_4$ mol. wt. 314.38

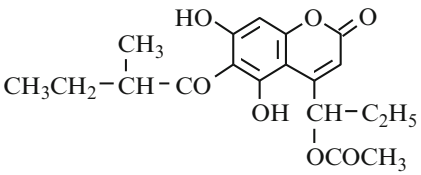


Synthesis
-Refer to: [2512].
Dimethyl ether (2S) [1080023-63-7]
$C_{21}H_{26}O_4$ mol. wt. 342.44
-Refer to: [2512].

USE: Asym. synthesis of wasabidienones B_1 an B *via* SIBX-mediated hydroxylative phenol dearomatization [2512].

4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-6-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

$C_{19}H_{22}O_7$ mol. wt. 362.38

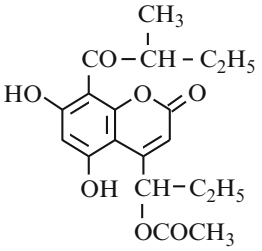


Synthesis

-Obtained by condensation of ethyl 3-oxo-4-acetoxyhexanoate with (2-methylbutyroyl)-phloroglucinol in the presence of 5 % sulfuric acid in acetic acid (traces) [766].

4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

[98498-77-2] $C_{19}H_{22}O_7$ mol. wt. 362.38



Syntheses

-Obtained by condensation of ethyl 3-oxo-4-acetoxyhexanoate with (2-methylbutyroyl)phloroglucinol in the presence of 5 % sulfuric acid in acetic acid (traces) [766].

-Also obtained by reaction of 2-methylbutyryl chloride with 4-[1-(acetyloxy)propyl]-5,7-dihydroxy-2*H*-1-benzopyran-2-one in the presence of aluminium chloride in carbon disulfide/nitrobenzene for 4 days at 20° (41 %) [766].

-Also refer to: [764].

m.p. 182–184° [764];
^{1}H NMR [764], IR [764], UV [764], MS [764].

Stereoisomer (1′RS,2″S) $C_{19}H_{22}O_7$ mol. wt. 362.38

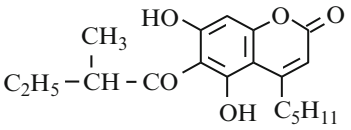
[98498-79-4] [98498-80-7] [98574-78-8] [98574-81-3].

-Refer to: [286].

$(\alpha)_D^{25} = +16.83°$ (chloroform) [286].

5,7-Dihydroxy-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one

[98192-60-0] $C_{19}H_{24}O_5$ mol. wt. 332.40



Syntheses

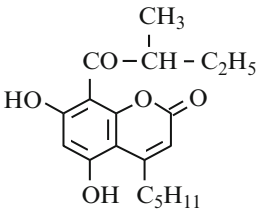
-Obtained by Fries rearrangement of 5-hydroxy-7-(2-methylbutanoyloxy)-4-pentyl-2*H*-1-benzopyran-2-one [765].

-Also obtained by reaction of ethyl 3-oxooctanoate with (2-methylbutyryl) phloroglucinol in the presence of acetic acid containing 5 % (v/v) sulfuric acid (38–42 %) [762].

m.p. 196–197° [762];
^{1}H NMR [762], IR [762], UV [762].

5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one

[36478-56-5] *(Mammea C/OB)* $C_{19}H_{24}O_5$ mol. wt. 332.40
[111821-07-9] *(Unusual mammea C/O)*



Syntheses

-Obtained by Fries rearrangement of 5-hydroxy-7-(2-methylbutanoyloxy)-4-pentyl-2*H*-1-benzopyran-2-one (40 %) [765].

-Also obtained by reaction of ethyl 3-oxooctanoate with (2-methylbutyryl)phloroglucinol in the presence of acetic acid containing 5 % (v/v) sulfuric acid (25–28 %) [762].

Isolation from natural sources

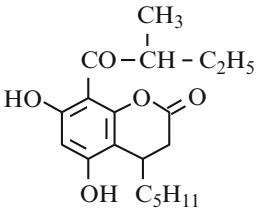
-From the bark of *Mammea africana* G. Don (Guttiferrae) [553, 751].
-Also refer to: [827].

needles [553]; m.p. 218–220° [553], 218° [762, 2591];
^{1}H NMR [553, 751, 2591], IR [553, 762, 2591], UV [553, 762, 2591], MS [553, 751, 2591].

3,4-Dihydro-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one

(Dihydromammea C/OB)

[70233-75-9] $C_{19}H_{26}O_5$ mol. wt. 334.41
[111321-15-4]



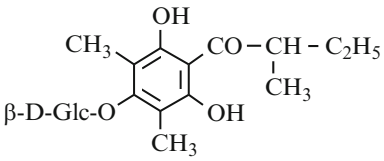
Synthesis
-Refer to: [751].
Isolation from natural sources
-From only seed of *Mammea africana* (Guttiferae) [751].

needles [751]; m.p. 132–134° [764], 125° [751];
^{1}H NMR [751, 764], ^{13}C NMR [751], IR [751, 764],
UV [751, 764], MS [751, 764].
$(\alpha)_D^{24} = +127°$ (chloroform) [751].

USE: Insecticide [751].

1-[4-(β-D-Glucopyranosyloxy)-2,6-dihydroxy-3,5-dimethylphenyl]-2-methyl-1-butanone

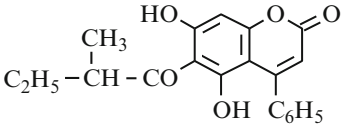
[241133-23-3] $C_{19}H_{29}O_9$ mol. wt. 401.43



Isolation from natural sources
-From *Hypericum japonicum* [3342].

5,7-Dihydroxy-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one

[98192-58-6] $C_{20}H_{18}O_5$ mol. wt. 338.36



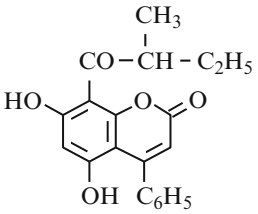
Syntheses
-Preparation as a mixture (70 %) from (2-methylbutyryl)-phloroglucinol and ethyl benzoylacetate [762] in acetic acid/concentrated sulfuric acid for 7 days at 20° [754].

-Also refer to: [765, 2380, 2381, 2556].

yellow needles [762]; yellow crystals [754];
m.p. 207–209° [762], 201–202° [754];
^{1}H NMR [754, 762], IR [754, 762], UV [754, 762],
MS [754, 762].

5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one

[98192-65-5] $C_{20}H_{18}O_5$ mol. wt. 338.36

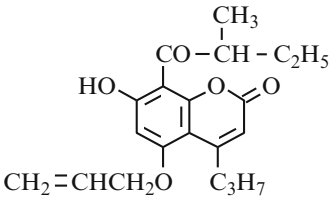


Syntheses
-Preparation as a mixture (70 %) from (2-methylbutyryl)-phloroglucinol and ethyl benzoylacetate [762] in acetic acid/concentrated sulfuric acid for 7 days at 20° [754].
-Also refer to: [765, 2380, 2381].

white plates [762];
m.p. 222–224° [762], 210–211° [754];
^{1}H NMR [754, 762], IR [754, 762], UV [754, 762], MS [754, 762].

7-Hydroxy-8-(2-methyl-1-oxobutyl)-5-(2-propenyloxy)-4-propyl-2*H*-1-benzopyran-2-one

[111761-38-7] $C_{20}H_{24}O_5$ mol. wt. 344.41

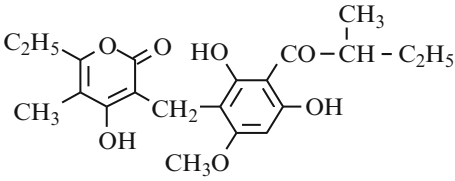


Synthesis
-Obtained by treatment of 5,7-dihydroxy-8-(2-methyl-butyryl)-4-propylcoumarin with allyl bromide in the presence of potassium carbonate and potassium iodide in refluxing acetone overnight [762].
white needles [762]; m.p. 95–96° [762];

^{1}H NMR [762], IR [762], UV [762], MS [762].

3-[[2,4-Dihydroxy-6-methoxy-3-(2-methyl-1-oxobutyl)phenyl]methyl]-6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one
(Methyl-nor-auricepyrone)

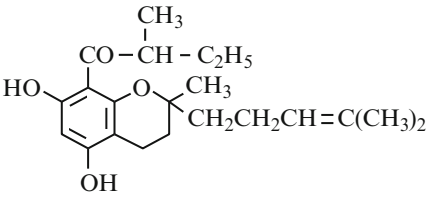
[103766-18-3] $C_{21}H_{26}O_7$ mol. wt. 390.43



Isolation from natural sources
-From *Helichrysum cephaloideum* [1487].
yellow oil [1487];
^{1}H NMR [1487], IR [1487], MS [1487].

1-[3,4-Dihydro-5,7-dihydroxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran-8-yl]-2-methyl-1-butanone

[658702-63-7] (+) $C_{21}H_{30}O_4$ mol. wt. 346.47



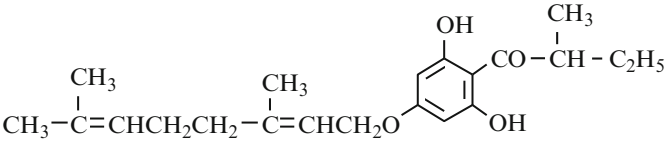
Isolation from natural source
-From the aerial parts of *Hypericum amblycalyx* (Guttiferae) [3316].
yellow oil [3316];
$(\alpha)_D^{22} = +14°$ (methanol) [3316];

^{1}H NMR [3316], ^{13}C NMR [3316], UV [3316], MS [3316].

BIOLOGICAL ACTIVITY: Antibacterial [3316]; Cytotoxicity against KB cancer cells [3316].

1-[4-[(3,7-Dimethyl-2,6-octadienyl)oxy]-2,6-dihydroxyphenyl]-2-methyl-1-butanone (*E*)

[71539-67-8] $C_{21}H_{30}O_4$ mol. wt. 346.47



Isolation from natural sources
-From *Helichrysum gymnoconum* (Compositae) [398].

^{1}H NMR [398], IR [398], MS [398].

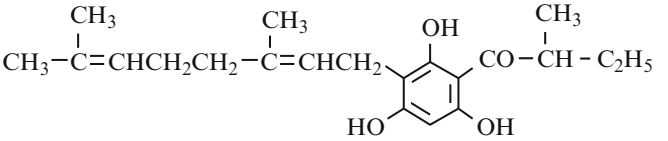
Diacetate (*E*) [71539-68-9] $C_{25}H_{34}O_6$ mol. wt. 430.54

-Obtained by reaction of acetic anhydride with 1-[3-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone in the presence of sodium acetate for 12 h at 70° [398].

^{1}H NMR [398], IR [398], MS [398].

1-[3-(3,7-Dimethyl-2,6-octadienyl)-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone (*E*)

[72008-04-9] $C_{21}H_{30}O_4$ mol. wt. 346.47



Isolation from natural sources
-From the aerial part *Helichrysum stenopterum* (Compositae) [1487].

-From *Helichrysum natalitium* DC (Compositae) [404].
-From the aerial parts of *Achyrocline alata* (HBK) DC (Compositae) [406].
-From *Helichrysum krookii* Moeser (Compositae) [412].
-From *Helichrysum monticola* [1488].
-From *Esenbeckia nesiotica* Stand. (Rutaceae) [2625].

colourless oil [404];
^{1}H NMR [404, 2625], ^{13}C NMR [2625], IR [404], MS [404].

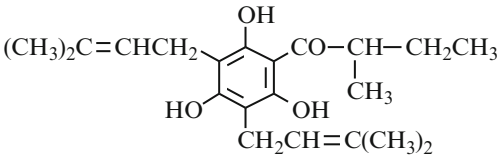
Triacetate [72008-09-4] $C_{27}H_{36}O_7$ mol. wt. 472.58

-Obtained by reaction of acetic anhydride with 1-[3-(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone in chloroform in the presence of pyrrolidinopyridine at 70° for 1 h [404].
-Also refer to: [2625].

colourless oil [404];
^{1}H NMR [404, 2625], IR [404], MS [404].

1-[2,4,6-Trihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone
(Deoxyadhumulone)

[4374-92-9] $C_{21}H_{30}O_4$ mol. wt. 346.47



Syntheses
-Obtained by reaction of 2-methyl-3-buten-2-ol with 2,4,6-trihydroxy-phenyl sec-butyl ketone with boron trifluoride complex dioxane at 20° [705], (21 %) [704], (13 %) [702].
-Also obtained by reaction of Z-methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone with 1-bromo-3-methyl-2-buten (3 mol) in the presence of the weakly basic resin DeAcidite H-IP (OH-form) in boiling benzene (14 %) [708]. **N.B.**: The yield was similar at this obtained by using 2-methyl-3-buten-2-ol but the isolation was simpler [708].
-Also obtained by reaction of 2-methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone with 1-chloro-3-methyl-2-butene (2 molar parts), magnesium oxide (0.5 equiv.) and potassium iodide [3310].
-Also refer to: [907, 1397].

oil [702]; m.p. 82° [708]; UV [702].

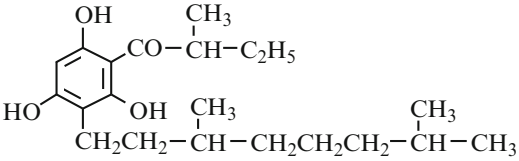
Tribenzoate [39652-89-6] $C_{42}H_{42}O_7$ mol. wt. 658.79

-Refer to: [704, 1397].

m.p. 127° [704], 126–127° [1397].

2-Methyl-1-[3-(3,7-dimethyloctyl)-2,4,6-trihydroxyphenyl]-1-butanone

$C_{21}H_{34}O_4$ mol. wt. 350.50



Synthesis

-Refer to: [404].

Triacetate

$C_{27}H_{40}O_7$ mol. wt. 476.28

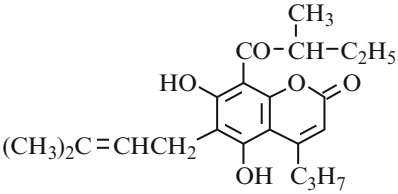
-Obtained by hydrogenation of 1-[2,4,6-tris(acetoxy)-3-(3,7-dimethyl-2,6-octadienyl)phenyl]-2-methyl-1-butanone in ethyl ether in the presence of 5 % palladium/barium sulfate.

colourless oil [404]; ^{1}H NMR [404], IR [404], MS [404].

5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

(Neomammein, Mammea B/BB)

[5022-20-8] racemic [37975-64-7] $C_{22}H_{28}O_5$ mol. wt. 372.46



Syntheses

-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of 10 % aqueous potassium hydroxide at 0° (30–45 %) [765], (29 %) [762].

-Also obtained by treatment of its dipotassium salt with trifluoroethanol [765].

Isolation from natural sources

-From kernels of the fruit of *Mammea americana* L. and *Mammea africana* (Guttiferae) [765, 1006].

-From only seed of *Mammea africana* (Guttiferae) [751].

-From the seed of *Mammea americana* L. (Guttiferae) [753, 758, 759].

-From the bark of *Mammea africana* G. Don (Guttiferae) [553, 1082].

pale yellow needles [751]; white needles [762];

m.p. 122–123° [1006], 122° [553, 753], 121–122° [762], 117–118° [755], 72–74° [751];

^{1}H NMR [553, 751, 753, 762], ^{13}C NMR [751], IR [553, 751, 753, 755, 762], UV [553, 751, 753, 755, 762, 1150], MS [553, 751, 753, 755, 762]; GC-MS [1082].

USE: Insecticide [753, 758, 759, 765].

BIOLOGICAL ACTIVITY: Antitumor [1006].

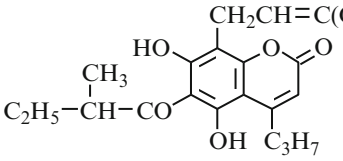
(S) isomer [98244-57-6]

-(S) – (−) – isomer was obtained by prenylation of 5,7-dihydroxy-8-(2-methylbutanoyl)-4-propylcoumarin. Natural mammea B/BB has the (S) – configuration [765].

m.p. 121–122° [765];
^{1}H NMR [2591], ^{13}C NMR [2591], IR [2591];
$(\alpha)_D = -2.78°$ [765].

5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one
(Mammea B/A)

[30390-12-6] $C_{22}H_{28}O_5$ mol. wt. 372.46



Syntheses

-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of 10 % aqueous potassium hydroxide at 0° (30–45 %) [765], (22 %) [762].

-Also obtained by treatment of its dipotassium salt with trifluoroethanol [765].
-Also obtained by isomerization of 5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one (mammea B/BB) by treatment with methanolic 5 % potassium hydroxide at 20° overnight [757].
-Also obtained by treatment of 5,7-dihydroxy-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one with 2-methyl-3-buten-2-ol in the presence of boron trifluoride-ether complex [757] in dioxane solution at r.t. for 24 h (2 %) [1081].

Isolation from natural sources

-From kernels of the fruit of *Mammea americana* L. [757] and *Mammea africana* (Guttiferae) [765].
-From the bark of *Mammea africana* G. Don (Guttiferae) [1082].

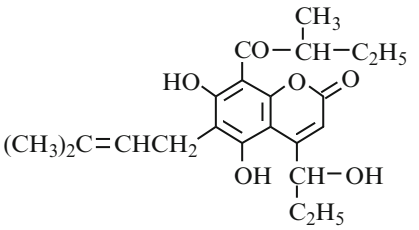
yellow needles [757, 762];
m.p. 118–120° [1081], 115–116° [552, 553], 114° [760], 98–100° [757], 97–100° [762];

^{1}H NMR [553, 756, 757, 760, 762], IR [553, 756, 757, 760, 762], UV [552, 553, 756, 757, 760, 762], MS [552, 757, 762]; GC-MS [1082]; TLC [757].

USE: Insecticide [757, 765].

5,7-Dihydroxy-4-[1-(hydroxy)propyl]-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one
(Assamene)

$C_{22}H_{28}O_6$ mol. wt. 388.46

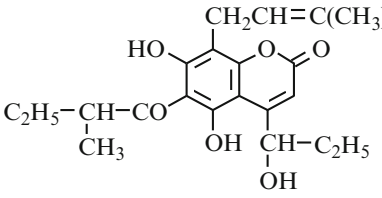


Isolation from natural sources
-From *Kayea assamica* (Guttiferae) [428].
yellow plates [428];
m.p. 135° [428];
^{1}H NMR [428], ^{13}C NMR [428], IR [428], UV [428], MS [428].

BIOLOGICAL ACTIVITY: Inhibition of cell growth [2264].

5,7-Dihydroxy-4-(1-hydroxypropyl)-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

[38534-77-9] $C_{22}H_{28}O_6$ mol. wt. 388.46



Synthesis
-The 4-[1-(acetyloxy)propyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one was isomerised and deacylated when treated with methanolic 5 % potassium hydroxide at 20° overnight [758].

IR [756, 758], UV [756, 758], MS [756, 758].

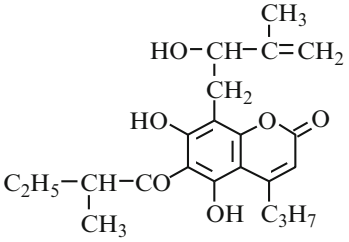
Triacetate [38534-70-2] $C_{28}H_{34}O_9$ mol. wt. 514.57

-Obtained by treatment of the titled compound with pyridine-acetic anhydride mixture [758].

IR [756, 758], UV [756, 758], MS [756, 758].

5,7-Dihydroxy-8-(2-hydroxy-3-methylbut-3-enyl)-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one
(Disparpropylinol B)

$C_{22}H_{28}O_6$ mol. wt. 388.46



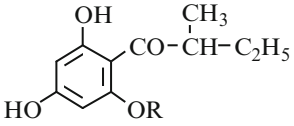
Isolation from natural sources
-From the fruits and the stem bark of *Calophyllum dispar* (Clusiaceae) [1178].
-Also refer to: [2544].
yellow crystals [1178];
m.p. 111–112° [1178];
^{1}H NMR [1178], ^{13}C NMR [1178], IR [1178], UV [1178], MS [1178];

$(\alpha)_D^{25} = 0°$ (chloroform) [1178].

BIOLOGICAL ACTIVITY: Human erythroleukemic K562/R7 MDR cells [2544]; Cytotoxicity [1178].

1-[2-[(6-*O*-D-Apio-β-D-furanosyl-β-D-glucopyranosyl)oxy]-4,6-dihydroxyphenyl]-2-methyl-1-butanone (2*S*)

[467437-62-3] $C_{22}H_{33}O_{13}$ mol. wt. 505.50



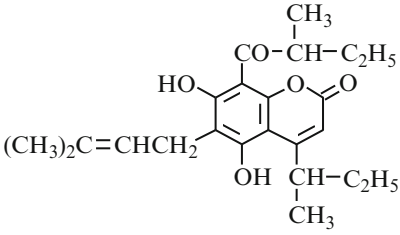
Isolation from natural sources
-From the leaves and branches of *Phyllanthus emblica* (Euphorbiaceae) [3455].

OR = (6-O-D-apio-β-D-furanosyl-β-D-glucopyranosyl)oxy

yellow amorphous powder [3455];
^{1}H NMR [3455], ^{13}C NMR [3455], UV [3455], circular dichroism [3455], MS [3455];
$(\alpha)_D^{18} = -60.3°$ (methanol) [3455].

5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-(1-methylpropyl)-2*H*-1-benzopyran-2-one
(Ferruol A, Mammea D/BB)

[92844-55-4] (*R*,*R*)
[98244-56-6] (*R*,*S*) $C_{23}H_{30}O_5$ mol. wt. 386.49
[16117-33-2]



Syntheses
-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-(1-methylpropyl)-2*H*-1-benzopyran-2-one (22 %) [765].
-Also refer to: [553, 762].

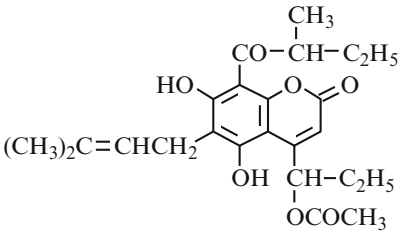
Isolation from natural sources

-From the trunk bark of *Mesuua ferrea* L. [753, 765, 1150].

m.p. 126.5° [1150], 126–127° [753];
^{1}H NMR [753, 764, 765, 1150], IR [753, 764, 1150],
UV [753, 764, 1150], MS [753, 764, 1150].

4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one
(1‴-Acetoxy-mammea E/BB)

[26477-65-6] $C_{24}H_{30}O_7$ mol. wt. 430.50
[111321-12-1]
[188817-91-6]



Syntheses

-Obtained by reaction of prenyl bromide with 4-[1-(acetyloxy)propyl]-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one in the presence of aqueous potassium hydroxide at 0° (40 %) [766].

-Also obtained by acetylation of *Assamene* with acetic anhydride in the presence of pyridine at r.t. overnight (80 %) [428].

-Also refer to: [373, 762, 764, 765, 912, 3381].

Isolation from natural sources

-From *Mammea americana* [756, 758, 759, 766, 912].
-From the Bark of *Mammea africana* G. Don (Guttiferae) [553, 759].
-From *Mammea siamensis* seeds [1828].
-From twigs of *Mammea suriga* [2554].

semi-solid [2554];
m.p. 114–116° [764], 50–53° [756], 50–51° [758];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [428, 756, 758, 759, 764, 912, 1828, 2554], ^{13}C NMR [1828, 2554],
IR [428, 756, 758, 759, 764], UV [756, 758, 759, 764],
MS [428, 756, 758, 759, 764, 2554];
TLC [2554]; HPLC [912, 2554]; $(\alpha)_D^{25} = -28°$ (ethanol) [428];

BIOLOGICAL ACTIVITY: Insecticidal [553, 758, 759, 766]; Inhibitor of IKBα kinase [2554]; Toxicity [759].

-Also refer to: [912].

Isomers of Mammea E/BB $C_{24}H_{30}O_7$ mol. wt. 430.50

(N° 1) Isolation from seeds (Fruit and Spice Park) *Mammea americana* L (Clusiaceae) [3381].

^{13}C NMR [3381]; $(\alpha)_D^{25} = -62°$ (methanol) [3381].

BIOLOGICAL ACTIVITY: Cytotoxicity [3381].

(N°2) [1263908-96-8]; Isolation from stem bark of *Mammea americana* [912].

BIOLOGICAL ACTIVITY: Refer to: [912].

Diacetate $C_{28}H_{34}O_9$ mol. wt. 514.57

-Obtained by treatment of the titled ketone with pyridine-acetic anhydride at 100° temperature overnight [758].

m.p. 20–22° [758]; IR [758], UV [758], MS [758].

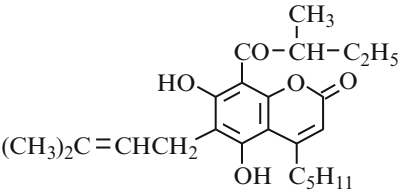
Dimethyl ether [26477-66-7] $C_{26}H_{34}O_7$ mol. wt. 458.55

-Refer to: [758, 759].

m.p. 88–90° [758, 759]; IR [758], UV [758], MS [758].

5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one
(Mammea C/BB)

[5085-55-2] $C_{24}H_{32}O_5$ mol. wt. 400.52



Synthesis
-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one in the presence of 10 % aqueous potassium hydroxide at 0° (19 %) [762].

Isolation from natural sources

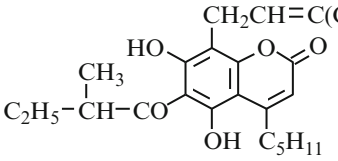
-From kernels of the fruit of *Mammea americana* L. and *Mammea africana* [765] (Guttiferae).
-From only seed of *Mammea africana* (Guttiferae) [751].
-From the seeds of *Mammea americana* L. [753, 758, 759].
-From *Mammea africana* G. Don (Guttiferae) [1082].

needles [751, 753];
m.p. 100–101° [753], 85–86° [762], 81–83° [751];
^1H NMR [751, 753, 762], IR [751, 753, 762],
UV [751, 753, 762, 1150], MS [751, 753, 762];
GC-MS [1082].

USE: Insecticide [751, 753, 758, 759, 765].

5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one
(Mammea C/AB)

[98192-70-2] $C_{24}H_{32}O_5$ mol. wt. 400.52



Synthesis
-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one in the presence of 10 % aqueous potassium hydroxide at 0° (19 %) [762].

Isolation from natural sources

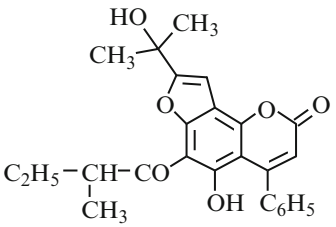
-From kernels of the fruit of *Mammea americana* L. and *Mammea africana* (Guttiferae) [765].

yellow crystals [762]; m.p. 78–80° [762];
^{1}H NMR [762], IR [762], UV [762], MS [762].

USE: Insecticide [765].

5-Hydroxy-8-(1-hydroxy-1-methylethyl)-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2′,3′:5,6]benzo[1,2-b]pyran-2-one
(Ochrocarpin A)

$C_{25}H_{24}O_6$ mol. wt. 420.46

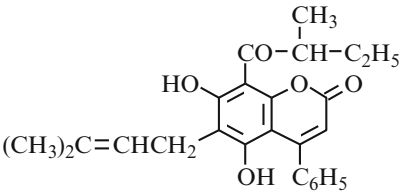


Isolation from natural sources
-From the bark of *Ochrocarpos punctatus* H. Perrier (Clusiaceae = Guttiferae) [616].
viscous liquid [616];
^{1}H NMR [616], ^{13}C NMR [616],
IR [616], UV [616];
$(\alpha)_D^{20} = -0.28°$ (chloroform) [616].

BIOLOGICAL ACTIVITY: Against ovarian cancer cells [616, 1884]; Cytotoxicity [616].

5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
(Mammea A/BB)

[6916-62-7] $C_{25}H_{26}O_5$ mol. wt. 406.48
[870084-45-0]



Synthesis
-Obtained by reaction of 3-methyl-2-butenyl bromide with 5,7-dihydroxy-8-(2-methylbutyryl)-4-phenylcoumarin in the presence of 10 % potassium hydroxide at 0° under nitrogen over 1.5 h (21 %) [762].

Isolation from natural sources

-From kernels of the fruit of *Mammea americana* L. [754, 758, 759] and *Mammea africana* (Guttiferae) [765].
-From the leaves of *Mesua ferrea* [2554].

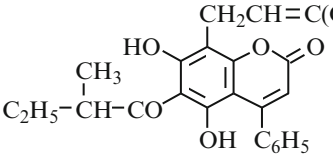
white needles [762]; colourless needles [754]; white solid [2554];
m.p. 124–125° [754, 2554], 111–112° [762];
^{1}H NMR [754, 762, 2554], ^{13}C NMR [2554],
IR [754, 762], UV [754, 762], MS [754, 762, 2554];
TLC [2554]; HPLC [2554].

USE: Insecticide [758, 759, 765].

BIOLOGICAL ACTIVITY: Inhibitor of IKBα kinase [2554].

5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
(Mammea A/AB, MAB 1)

[7058-70-0] $C_{25}H_{26}O_5$ mol. wt. 406.48



Synthesis
-Obtained by reaction of 3-methyl-2-butenyl bromide with 5,7-dihydroxy-6-(2-methylbutyryl)-4-phenylcoumarin in the presence of 10 % potassium hydroxide at 0° under nitrogen over 1.5 h (21 %) [762].

Isolation from natural sources

-From kernels of the fruit of *Mammea americana* L. [754, 758, 759] and *Mammea africana* (Guttiferae) [765].

-From the bark of *Mammea africana* G. Don (Guttiferae) [553, 1082].
-From the fruits of *Mammea suriga* [2554].

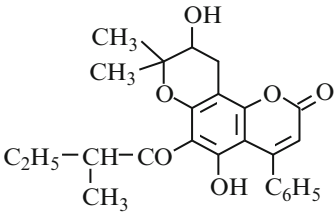
yellow needles [754]; yellow crystalline solid [2554];
m.p. 109–110° [762], 107–108° [754], 106–107° [2554], 105–106° [553];
^{1}H NMR [553, 754, 762, 2554], ^{13}C NMR [2554],
IR [553, 754, 762], UV [553, 754, 762],
MS [553, 754, 762, 2554];
GC-MS [1082]; TLC [2554]; HPLC [2554].

USE: Insecticide [758, 759].

BIOLOGICAL ACTIVITY: Inhibitor of IKBα kinase [2554].

9,10-Dihydro-5,9-dihydroxy-8,8-dimethyl-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*,8*H*-benzo[1,2-b:5,6-b′]dipyran-2-one
(Mammea A/AB cyclo E)

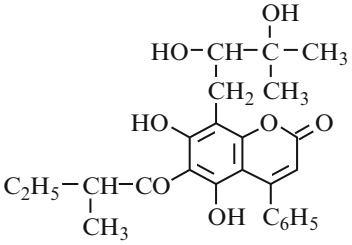
$C_{25}H_{26}O_6$ mol. wt. 422.48



Isolation from natural sources
-From the fruits and the stem bark of *Calophyllum dispar* (Clusiaceae) [1178].
^{1}H NMR [1178], ^{13}C NMR [1178],
IR [1178], UV [1178], MS [1178];
$(\alpha)_D^{25} = 0°$ (chloroform) [1178].

5,7-Dihydroxy-8-(2,3-dihydroxy-3-methylbutyl)-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
(Dispardiol B)

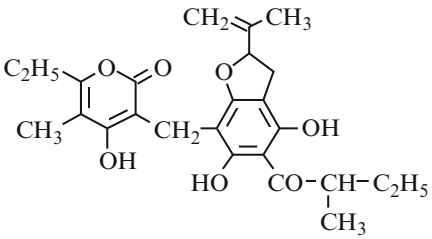
$C_{25}H_{28}O_7$ mol. wt. 440.49



Isolation from natural sources
-From the fruits and the stem bark of *Calophyllum dispar* (Clusiaceae) [1178].
^{1}H NMR [1178], ^{13}C NMR [1178],
IR [1178], UV [1178], MS [1178];
$(\alpha)_D^{25} = 0°$ (chloroform) [1178].

3-[[2,3-Dihydro-4,6-dihydroxy-2-(1-methylethenyl)-5-(2-methyl-1-oxobutyl)-7-benzo-furanyl]methyl]-6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one

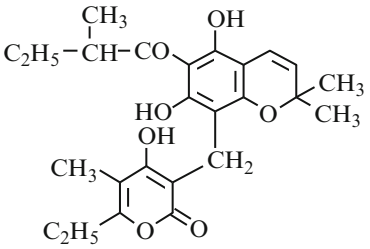
[103834-39-5] $C_{25}H_{30}O_7$ mol. wt. 442.51



Isolation from natural sources
-From *Helichrysum cephaloudeum* and *Helichrysum mixtum* (Compositae) [1487].

3-[[5,7-Dihydroxy-2,2-dimethyl-6-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-8-yl]methyl]-6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one

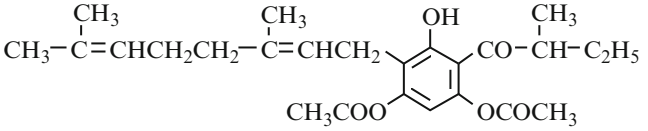
[103771-76-2] $C_{25}H_{30}O_7$ mol. wt. 442.51



Isolation from natural sources
-From *Helichrysum mixtum* (Compositae) [1487].
yellow oil [1487];
^{1}H NMR [1487], IR [1487], MS [1487].

1-[4,6-(Diacetyloxy)-2-hydroxy-3-(3,7-dimethyl-2,6-octanediene)phenyl]-2-Methyl-1-butanone

[144785-81-9] $C_{25}H_{34}O_6$ mol. wt. 430.54

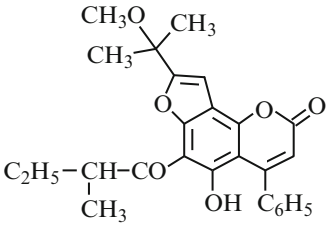


Isolation from natural sources
-Refer to: [2625].

^{1}H NMR [2625].

5-Hydroxy-8-(1-methoxy-1-methylethyl)-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2′,3′:5,6]benzo[1,2-b]pyran-2-one
(Ochrocarpin D)

$C_{26}H_{26}O_6$ mol. wt. 434.49

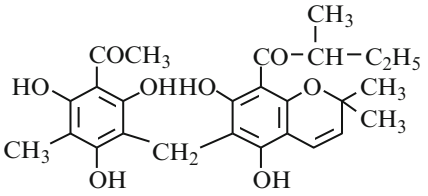


Isolation from natural sources
-From the bark of *Ochrocarpos punctatus* H. Perrier (Clusiaceae = Guttiferae) [616].
viscous liquid [616];
^{1}H NMR [616], ^{13}C NMR [616],
IR [616], UV [616];
$(\alpha)_D^{20} = -0.48°$ (chloroform) [616].

BIOLOGICAL ACTIVITY: Against ovarian cancer cells [616, 1884]; Cytotoxicity [616].

1-[6-[(3-Acetyl-2,4,6-trihydroxy-5-methylphenyl)methyl]-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-2-methyl-1-butanone
(Mallotophilippen B)

[500109-65-9] $C_{26}H_{30}O_8$ mol. wt. 470.52



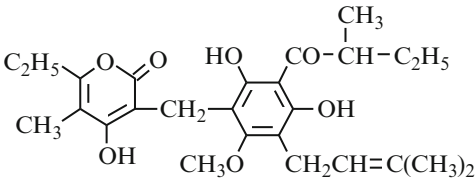
Isolation from natural sources
-From *mallotus philippinensis* pericarp (Euphorbiaceae) [793, 1697].
yellow powder [793];

^{1}H NMR [793], ^{13}C NMR [793], IR [793], UV [793], MS [793]; $(\alpha)_D^{23} = 0°$ (methanol) [793].

BIOLOGICAL ACTIVITY: Antiallergic agent [793]; Antiallergic agent for the treatment of asthma, atopic dermatitis, allergic rhinitis, and hay fever [1697].

3-[[2,4-Dihydroxy-6-methoxy-5-(3-methyl-2-butenyl)-3-(2-methyl-1-oxobutyl) phenyl]-methyl]-6-ethyl-4-hydroxy-5-methyl-2H-pyran-2-one

[103771-71-7] $C_{26}H_{34}O_7$ mol. wt. 458.55



Isolation from natural sources
-From *Helichrysum cephaloideum* (Compositae) [405, 1487].
-From *Helichrysum auriceps* (Compositae) [405].

^{1}H NMR [405], IR [405], MS [405].

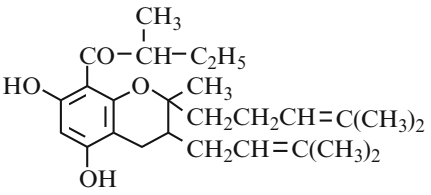
Triacetate $C_{32}H_{40}O_{10}$ mol. wt. 584.66

-Obtained by reaction of acetic anhydride with the title ketone in chloroform in the presence of 4-pyrrolidinopyridine [405].

colourless oil [405]; ^{1}H NMR [405], MS [405].

1-[(2*R*,3*S*)-3,4-Dihydro-5,7-dihydroxy-2-methyl-3-(3-methyl-2-butenyl)-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran-8-yl]-2-methyl-1-butanone
(Hypercalyxone B)

[658702-61-5] (−) $C_{26}H_{38}O_4$ mol. wt. 414.58



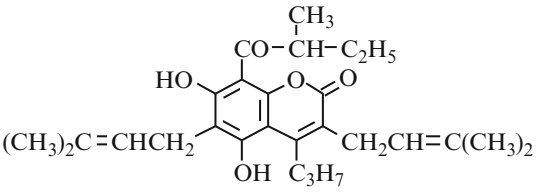
Isolation from natural source
-From the aerial parts of *Hypericum amblycalyx* (Guttiferae) [3316].
yellow oil [3316];

^{1}H NMR [3316], ^{13}C NMR [3316], UV [3316], MS [3316];
$(\alpha)_D^{22} = -1°$ (methanol) [3316].

BIOLOGICAL ACTIVITY: Antibacterial [3316]; Cytotoxicity against KB cancer cells [3316].

5,7-Dihydroxy-3,6-bis(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

[111761-40-1] $C_{27}H_{36}O_5$ mol. wt. 440.58



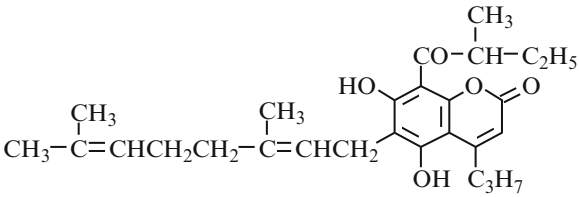
Syntheses
-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of 10 % aqueous potassium hydroxide at 0° (1 %) [762, 765].

^{1}H NMR [762], IR [762], UV [762], MS [762].

6-(3,7-Dimethyl-2,6-octadienyl)-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

(Surangin A) (E)

[98244-54-3] $C_{27}H_{36}O_5$ mol. wt. 440.58



Syntheses

-Obtained by reaction of geranyl chloride with 5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of 10 % potassium hydroxide for 24 h at 40–50° (7 %) [762, 765].

Isolation from natural sources

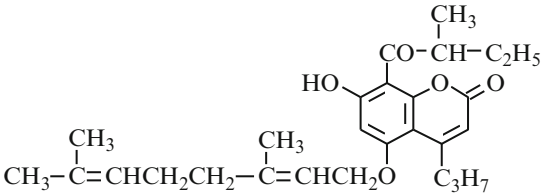
-From *Mammea longifolia* (Wight) Planch and Triana (Syn.) *Ochrocarpus longifolius* (Wt.) Benth and Hook. f. ex T. Anders. (Guttiferae) [765, 1548].

colourless needles [1548]; white solid [762];
m.p. 83–85° [1548], 81–82° [762];
^{1}H NMR [762, 1548], IR [762, 1548], UV [762, 1548], MS [762, 1548];
$(\alpha)_D^{26} = -1.6°$ (chloroform) [1548].

BIOLOGICAL ACTIVITY: High *in vitro* antibacterial [1548].

5-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7-hydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

[98193-78-3] $C_{27}H_{36}O_5$ mol. wt. 440.58



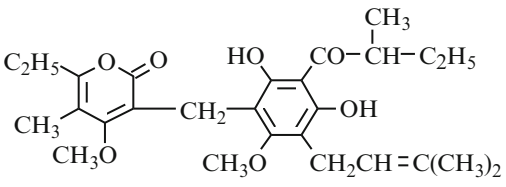
Syntheses

-Obtained by reaction of geranyl chloride with 5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of 10 % potassium hydroxide for 24 h at 40–50° (6 %) [762, 765].

white needles [762]; m.p. 54–55° [762];
^{1}H NMR [762], IR [762], UV [762], MS [762].

3-[[2,4-Dihydroxy-6-methoxy-5-(3-methyl-2-butenyl)-3-(2-methyl-1-oxobutyl) phenyl]-methyl]-6-ethyl-4-methoxy-5-methyl-2*H*-pyran-2-one

$C_{27}H_{36}O_7$ mol. wt. 472.58



Synthesis
-Obtained by reaction of diazomethane with 3-[[2,4-dihydroxy-6-methoxy-5-(3-methyl-2-butenyl)-3-(2-methyl-1-oxobutyl)-phenyl] methyl]-6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one in ethyl ether at r.t. for 1 h [405].

colourless oil [405];
^{1}H NMR [405], ^{13}C NMR [405], IR [405], MS [405].

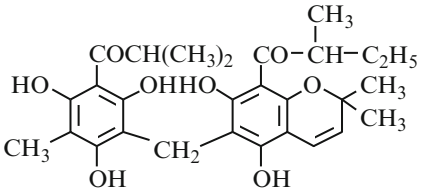
Diacetate $C_{31}H_{40}O_9$ mol. wt. 556.65

-Obtained by reaction of acetic anhydride with the title ketone in chloroform in the presence of 4-pyrrolidinopyridine for 3 h [405].

colourless oil [405];
^{1}H NMR [405], ^{13}C NMR [405], IR [405], MS [405].

1-[5,7-Dihydroxy-2,2-dimethyl-6-[[2,4,6-trihydroxy-3-methyl-5-(2-methyl-1-oxopropyl) phenyl]methyl]-2*H*-1-benzopyran-8-yl]-2-methyl-1-butanone
(Mallotophilippen A)

[500109-64-8] $C_{28}H_{34}O_8$ mol. wt. 498.57



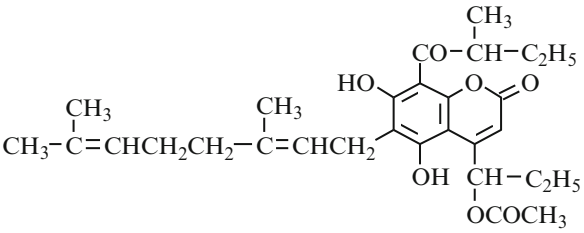
Isolation from natural sources
-From *mallotus philippinensis* pericarp (Euphorbiaceae) [793, 1697].
yellow powder [793];
^{1}H NMR [793],

^{13}C NMR [793], IR [793], UV [793], MS [793];
$(\alpha)_D^{23} = 0°$ (methanol) [793].

BIOLOGICAL ACTIVITY: Antiallergic agent [793]; Antiallergic agent for the treatment of asthma, atopic dermatitis, allergic rhinitis, and hay fever [1697].

4-[1-(Acetyloxy)propyl]-6-(3,7-dimethyl-2,6-octadienyl)-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one
(Surangin B)

[28319-38-2] $C_{29}H_{38}O_7$ mol. wt. 498.62
[98574-77-7] R,R
[98574-79-9] R-R,S
[98574-80-2] S-R,R
[98575-56-5] R,S



Isolation from natural sources
-From *Mammea longifolia* (Wight) Planch and Triana (Syn.) *Ochrocarpus longifolius* (Wt.) Benth and Hook. f. ex T. Anders. (Guttiferae) [758, 759, 766, 1548].

-Also refer to: [373, 762, 1150].

m.p. 98–100° [1548];
^{1}H NMR [1548], IR [1548], UV [1548], MS [1548];
$(\alpha)_D^{24} = -30°$ [1548].

BIOLOGICAL ACTIVITY: Insecticidal [758, 759, 766]; High *in vitro* antibacterial [758, 759, 1548]; Toxic to mosquito larvae [759].

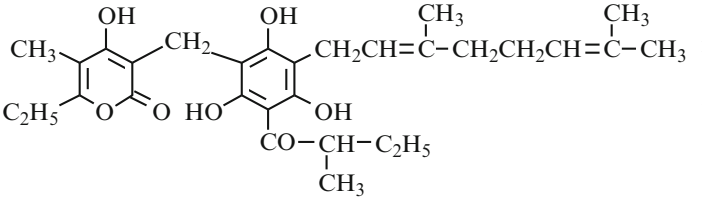
Dimethyl ether $C_{31}H_{42}O_7$ mol. wt. 526.27

-Obtained by reaction of dimethyl sulfate with *Surangin B* in the presence of potassium carbonate in refluxing acetone overnight (71 %) [1548].

gummy solid [1548]; IR [1548], UV [1548], MS [1548].

3″-Mergtlachyroclinopyrone

$C_{30}H_{40}O_7$ mol. wt. 512.64



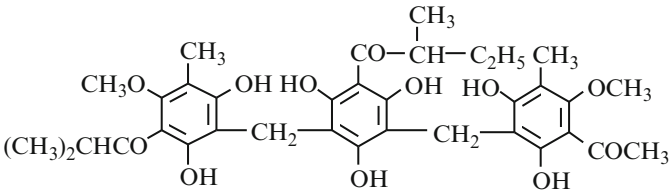
Isolation from natural sources
Isolated as its tetraacetate [406].

Tetraacetate $C_{38}H_{48}O_{11}$ mol. wt. 680.79

colourless gum [406]; ^{1}H NMR [406], MS [406].

1-[3-[(3-Acetyl-2,6-dihydroxy-4-methoxy-5-methylphenyl)methyl]-5-[[2,6-dihydroxy-4-methoxy-3-methyl-5-(2-methyl-1-oxopropyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone
(Agrimol D)

[55576-64-2] $C_{35}H_{42}O_{12}$ mol. wt. 654.71



Synthesis
-Refer to: [1866] (Chinese paper).

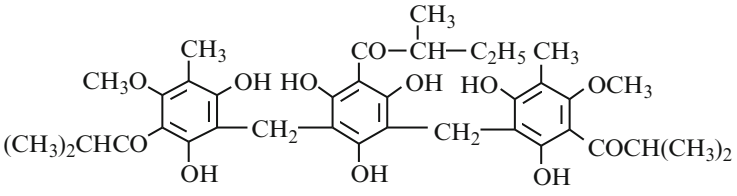
Isolation from natural sources

-From the whole plant *Agrimol pilosa*, ledeb [2860] (Chinese paper).
-From the Chinese herb medicine *Agrimonia pilosa* [632] (Chinese paper).

m.p. 147–149° [2860];
^{1}H NMR [632], IR [632], UV [632], MS [632].

1-[3,5-Bis[[2,6-dihydroxy-4-methoxy-3-methyl-5-(2-methyl-1-oxopropyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone
(Agrimol A)

[55576-65-3] $C_{37}H_{46}O_{12}$ mol. wt. 682.77



Synthesis
-Refer to: [1866] (Chinese paper).

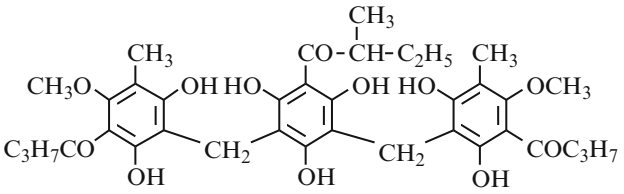
Isolation from natural sources

-From the whole plant *Agrimol pilosa*, ledeb [2860] (Chinese paper).
-From the Chinese herb medicine *Agrimonia pilosa* [632] (Chinese paper).

m.p. 176–178° [2860];
^{1}H NMR [632], IR [632], UV [632], MS [632].

1-[3,5-Bis[[2,6-dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone
(Agrimol B)

[55576-66-4] (2*S*) $C_{37}H_{46}O_{12}$ mol. wt. 682.77
[125292-98-0]



Syntheses
-Preparation from 1-butyryl-2,4-dihydroxy-6-methoxy-5-methyl-benzene and 1,3,5-trihydroxy-2-(1-methylbutyryl)-benzene [3017].

-Also refer to: [1866] (Chinese paper).

Isolation from natural sources
-From the Chinese herb medicine *Agrimonia pilosa* [632, 2860] (Chinese papers).

m.p. 167–169° [2860], 166–168° [1866];
^{1}H NMR [632], IR [632, 1866], UV [632], MS [632].

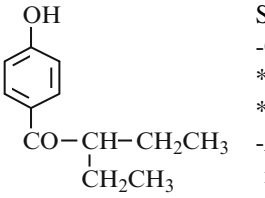
BIOLOGICAL ACTIVITY: Inhibited melanin formation in mouse melanoma cells [3017].

2.2 From 2-Ethyl-1-Butanoic Acid

2.2.1 Unsubstituted Hydroxyketones

2-Ethyl-1-(4-hydroxyphenyl)-1-butanone

[100256-47-1] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses
-Obtained by treatment of p-(2′-ethylbutyroyl)anisole,
*with boiling pyridinium chloride [508], (68 %) [2087];
*with hydrobromic acid in acetic acid [508].
-Also obtained by reaction of diethylacetic acid with phenol in the presence of boron trifluoride (82 %) [2087].

-Also refer to: [509].

colourless and microcrystalline substance [2087];
b.p.$_1$ 175° [2087], b.p.$_{10}$ 204–205° [508, 509];
m.p. 70° [2087]; UV [2087];
$n_D^{23} = 1.5585$ [509].

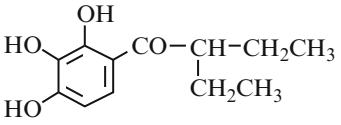
Methyl ether [84836-32-8] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Preparation of aryl ketones *via* modified Friedel-Crafts acylation catalyzed by rare metal triflates that generates reduced amounts of toxic by-products [3258].
-Also obtained by Friedel-Crafts reaction of anisole with diethylacetic acid (82 %) [2583].
-Also obtained by reaction of diethylacetyl chloride with anisole in the presence of aluminium chloride in carbon disulfide (70 %) [2087].
-Also obtained by methylation of 2-ethyl-1-(4-hydroxyphenyl)-1-butanone (74 %) [2087].
-Also obtained by ruthenium-catalyzed cross-coupling diethylacetaldehyde with 4-methoxy-phenylboronic acid (84 %) [1864].
-Also refer to: [508, 509, 1606, 3178].

colourless oil [2583]; Pleasantly smelling pale yellow oil [2087];
b.p.$_{11}$ 154° [2583], b.p.$_{12}$ 156° [508, 509],
b.p.$_{14}$ 168–170° [3178], b.p.$_{16}$ 172° [2087];
^{1}H NMR [1864, 2583], ^{13}C NMR [1864], IR [1864, 2583],
UV [2087], MS [1864];
$n_D^{24} = 1.528$ [2087].

2-Ethyl-1-(2,3,4-trihydroxyphenyl)-1-butanone

$C_{12}H_{16}O_4$ mol. wt. 224.26

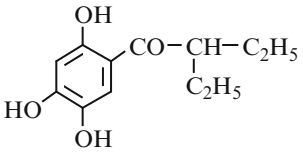


Syntheses
-Preparation by reaction of diethylacetic acid with pyrogallol in the presence of boron trifluoride in ethyl ether at 0° (71 %) [540, 2822].

m.p. 111° [540, 2822], UV [540].

2-Ethyl-1-(2,4,5-trihydroxyphenyl)-1-butanone

[100257-71-4] $C_{12}H_{16}O_4$ mol. wt. 224.26



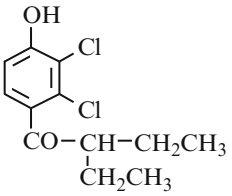
Synthesis
-Preparation by reaction of diethylacetic acid chloride with 1,3,4-trihydroxybenzene in the presence of aluminium chloride in nitrobenzene [292].
m.p. 123–124° [292].

USE: Antioxidant for fats, oils and paraffin waxes [292].

2.2.2 Substituted Hydroxyketones

1-(2,3-Dichloro-4-hydroxyphenyl)-2-ethyl-1-butanone

[1539-14-6] $C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15



Syntheses

-Obtained by reaction of diethylacetyl chloride with 2,3-dichloroanisole in the presence of aluminium chloride in carbon disulfide at r.t. for 22 h and at 55° for 90 min. Then, after carbon disulfide elimination, addition of heptane and to heat on a water bath for 3 h (44 %) [2929].

-Also obtained by treatment of its methyl ether with aluminium chloride (2 equiv.) in refluxing heptane [2060].

-Also refer to: [2047, 2050, 2054–2056, 2058, 2059, 2061, 2767 (44 %), 2768, 3294].

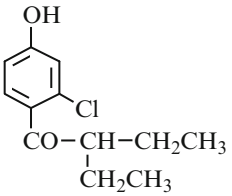
b.p.$_{0.5}$ 140–142° [2054, 2767, 2929];
m.p. 85–86° [2047, 2054–2056, 2058–2061, 2767, 2768, 2929, 3294],
84–86° [2050].

Methyl ether $C_{13}H_{16}Cl_2O_2$ mol. wt. 275.17

-Preparation by reaction of 2-ethylbutyryl chloride with 2,3-dichloroanisole [2768] (m.p. 32–33°) in petroleum ether at r.t. [2060].

1-(2-Chloro-4-hydroxyphenyl)-2-ethyl-1-butanone

[4804-56-2] $C_{12}H_{15}ClO_2$ mol. wt. 226.70



Syntheses

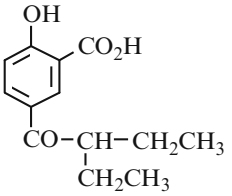
-To diethylacetyl chloride, 3-chloroanisole and carbon disulfide was added in small portions at 25°, aluminium chloride; the mixture stirred 1 h at r.t. and 45 min at 55°; pentane and aluminium chloride added, heated 3 h at 80° [2056].

-Also refer to: [2047, 2057, 2767].

b.p.$_{0.3}$ 148–181° [2047, 2057, 2767].

5-(2-Ethylbutyryl)-2-hydroxybenzoic acid
5-Diethylacetylsalicylic acid

[106393-54-8] $C_{13}H_{16}O_4$ mol. wt. 236.27



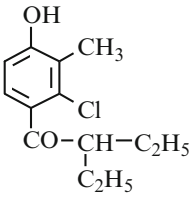
Synthesis

-Obtained by alkaline hydrolysis of 5-diethylacetylsalicylamide [1158].

m.p. 140° [1158].

1-(2-Chloro-4-hydroxy-3-methylphenyl)-2-ethyl-1-butanone

[92019-26-6] $C_{13}H_{17}ClO_2$ mol. wt. 240.73



Syntheses

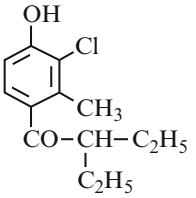
-To diethylacetyl chloride, 3-chloro-2-methylanisole and carbon disulfide was added in small portions at 25°, aluminium chloride; the mixture stirred 1 h at r.t. and 45 min at 55°; pentane and aluminium chloride added, heated 3 h at 80° [2056].

-Also refer to: [2046].

m.p. 87–89° [2046, 2056].

1-(3-Chloro-4-hydroxy-2-methylphenyl)-2-ethyl-1-butanone

[4798-10-1] $C_{13}H_{17}ClO_2$ mol. wt. 240.73



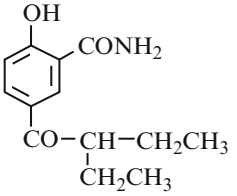
Synthesis

-Refer to: [2767 (44 %)].

m.p. 87–89° [2767].

2-Hydroxy-5-(2-ethylbutyryl)benzamide

$C_{13}H_{17}NO_3$ mol. wt. 235.28



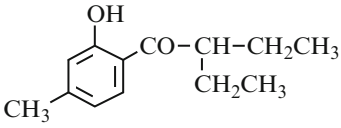
Synthesis

-Obtained by Fries rearrangement of salicylamide diethylacetate in the presence of aluminium chloride in nitrobenzene for 3 h at 20° [1158].

m.p. 231° [1158].

2-Ethyl-1-(2-hydroxy-4-methylphenyl)-1-butanone

$C_{13}H_{18}O_2$ mol. wt. 206.28



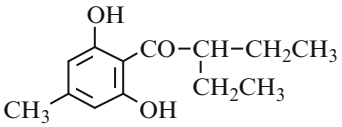
Synthesis

-Obtained by reaction of $[Ru_2(p\text{-cymene})_2Cl_2]_2$ with bis(acetoxy)iodobenzenze in trifluoroacetic acid and trifluoroacetic anhydride at 50° for 12 h in a sealed tube (13 %) [2830].

^{1}H NMR [2830], ^{13}C NMR [2830]; MS [2830].

1-(2,6-Dihydroxy-4-methylphenyl)-2-ethyl-1-butanone

$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Obtained by reaction of $[Ru_2(p\text{-cymene})_2Cl_2]_2$ with bis(acetoxy)iodobenzene in trifluoroacetic acid and trifluoroacetic anhydride at 50° for 12 h in a sealed tube (65 %) [2830].

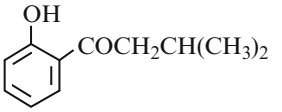
^{1}H NMR [2830], ^{13}C NMR [2830]; MS [2830].

2.3 From 3-Methyl-1-Butanoic Acid

2.3.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-3-methyl-1-butanone

[19019-21-7] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses
-Obtained by Fries rearrangement of phenyl isovalerate in the presence of aluminium chloride,
*in nitrobenzene for 18 h at 50° (24 %) [776];
*without solvent for 4 h at 130–140° [186].

-Also obtained by reaction of isovaleric acid with phenol in the presence of aluminium chloride,
*in petroleum ether, first at r.t. for 12–14 h, then on a water bath for 3–5 h (25 %) [3478];
*in benzene [3477].
-Also obtained by treatment of 1-(2-hydroxyphenyl)-3-methyl-1-butanol with manganese dioxide in methylene chloride for 7 h at r.t. (33 %) [77].
-Also obtained from 2,2-dimethyl-4-chromanone, also named 2,2-dimethyl-4-oxo-4*H*-1-benzopyran (13 %) [118].

oil [118], colourless oil [77];
b.p.$_{0.1}$ 76–77° [776], b.p.$_{20}$ 138–140° [186], b.p. 248–250° [3477, 3478];
^{1}H NMR [77, 118], ^{13}C NMR [77], IR [77, 118], MS [77];
$n_D^{20} = 1.5295$ [118].

BIOLOGICAL ACTIVITY: Antifeedant against storage pests and aphids [1076].

Semicarbazone $C_{12}H_{17}N_3O_2$ mol. wt. 235.29

m.p. 195° [812], 173° [3477].

p-Nitrophenylhydrazone $C_{17}H_{19}N_3O_3$ mol. wt. 313.36

m.p. 121–122° [186].

Methyl ether [857803-59-9] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Refer to: [186, 1084].

$b.p._{12}$ 142–144° [186];
^{1}H NMR [1231], ^{13}C NMR [1231], IR [1231], MS [1231].

Acetate $C_{13}H_{16}O_3$ mol. wt. 220.27

$b.p._{20}$ 164–166° [186].

2,4-Dinitrophenylhydrazone [93650-62-5] $C_{17}H_{18}N_4O_5$ mol. wt. 358.35

m.p. 187–189° [423], 181° [1523].

1-(3-Hydroxyphenyl)-3-methyl-1-butanone

$C_{11}H_{14}O_2$ mol. wt. 178.23

Synthesis
-Obtained by action of bis(4-methylbutyl)cadmium with m-acetoxybenzoyl chloride (70 %), then saponification of the keto ester obtained (60 %) [2586].

$b.p._{.2}$ 136–138° [2586]; m.p. 83° [2586].

Acetate $C_{13}H_{16}O_3$ mol. wt. 220.27

$b.p._{2.5}$ 76–77° [2586].

Methyl ether [1183770-52-6] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Refer to: [624].

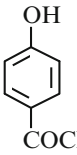
^{1}H NMR [624, 1231], ^{13}C NMR [624, 1231], IR [624, 1231], MS [624, 1231].

2,4-Dinitrophenylhydrazone $C_{17}H_{18}N_4O_5$ mol. wt. 358.35

m.p. 171° [2586].

1-(4-Hydroxyphenyl)-3-methyl-1-butanone

[34887-83-7] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses

-Preparation by Fries rearrangement of phenyl isovalerate in the presence of aluminium chloride,

*in nitrobenzene for 18 h at 50° (68 %) [776];

*without solvent at 130–140° for 4 h [186].

-Also obtained by Fries rearrangement of phenylisovalerate in the presence of BF_3-H_2O in a closed pressure tube at 80° for 1 h (87 %) [2514].

-Also obtained by reaction of isovaleric acid with phenol,

*in the presence of boron trifluoride for 2 h at 70° (52 %) [1685];

*in the presence of aluminium chloride in petroleum ether, first at r.t. for 12–14 h, then on a water bath for 3–5 h (38 %) [3478].

-Also obtained by dealkylation of its ethyl ether with aluminium chloride in carbon disulfide for 8 h at 60–70° [191].

-Also obtained by treatment of its methyl ether with pyridinium chloride at 190° [627].

-Also obtained by reaction of 4-iodophenol with iso-Bu_3In in the presence of $(PPPh_3)_4$ in THF at 66° under atmospheric pressure of CO gas (61 %) [1851].

-Also refer to: [884, 1414, 3477 (63 %)].

b.p.$_{0.1}$ 145–147° [812], b.p.$_3$ 201–202° [1685];
m.p. 97–98° [191], 96–97° [3477, 3478], 95.5–96.5° [186], 95–96° [776, 1685];
^{1}H NMR [881, 2514], ^{13}C NMR [2514], MS [2514].

Methyl ether [82938-20-3] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Obtained by reaction of isovaleric acid/isovaleric anhydride mixture with anisole in the presence of perchloric acid (73 %) [1781].

-Also obtained by reaction of isovaleric acid with anisole in the presence of PPA at 80° (76–100 %) [627].

-Also obtained by reaction of isovaleric chloride with anisole in the presence of aluminium chloride,

*in methylene chloride at 0° (76–100 %) [627];

*in 1,2-dichloroethane first at 0°, then at r.t. for 8–15 h (84 %) [2942].

-Also obtained by direct acylation of 4-bromoanisole with isovaleraldehyde by palladium catalysis (75 %) [2668].

-Also obtained by reaction of 1,3-dimethyl-1-phenyl-3-buten-1-ol with 4-methoxybenzaldehyde in the presence of Ru/CeO_2 as catalyst in mesitylene at 170° for 24 h under argon atmosphere (93 %) [2101].

-Synthesis and *Rhizopus oryzae* mediated enantioselective hydrolysis of α-acetoxy derivative [846].

-Also obtained from 4-methoxybenzaldehyde (77 %) [3024].

-Also refer to: [698 (55 %), 1114].

pale yellow oil [2942]; b.p.$_{12}$ 145–159° (bath temp.) [1781].
b.p.$_{12}$ 158.5–159.5° [3178], b.p.$_{25}$ 167° [251];
^{1}H NMR [698, 2942, 3024], ^{13}C NMR [698, 2942],
IR [698], MS [698, 2942].

Ethyl ether [92035-99-9] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of isovaleryl chloride with phenetole in the presence of,
*aluminium chloride in carbon disulfide at 60–70° for 8 h [191];
*of zinc chloride for 4 h at 70° (68 %) [1780].
-Also obtained by reaction of isovaleric acid with phenetole in the presence of aluminium chloride, in petroleum ether, first at r.t. for 12–14 h, then on a water bath for 3–5 h (82 %) [3477, 3478].
-Also refer to: [964].

b.p.$_{18}$ 133–137° [3477, 3478], b.p.$_{20}$ 136–138° [1780];
$n_D^{15} = 1.5332$ [3478], $n_D^{20} = 1.5338$ [1780].

Semicarbazone of the ethyl ether $C_{14}H_{21}N_3O_2$ mol. wt. 263.34

m.p. 191–192° [3477].

Oxime of the ethyl ether $C_{13}H_{19}NO_2$ mol. wt. 221.30

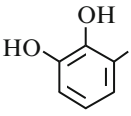
m.p. 118–119° [3477].

Benzoate $C_{18}H_{18}O_3$ mol. wt. 282.34

m.p. 75–76° [3477, 3478].

1-(2,3-Dihydroxyphenyl)-3-methyl-1-butanone

[104216-24-2] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Obtained by treatment of guaiacol isovalerate with aluminium chloride in carbon disulfide at 90° for 50 min, then at 135–140° for 2 h after solvent elimination [2075].

-Also obtained by treatment of its dimethyl ether below with hydriodic acid (d = 1.71) in refluxing acetic acid for 6 h (88 %) [198].

m.p. 93–95° [2075], 48° [198];
N.B.: One of the reported melting point is obviously wrong.
IR [198].

Dimethyl ether [15121-98-9] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Preparation by action of isobutylmagnesium iodide with 2,3-dimethoxybenzaldehyde (73 %) [198].
-Also obtained by treatment of 1-(2,3-dimethoxyphenyl)-3-methyl-1-butanol with potassium dichromate in dilute sulfuric acid (59 %) [198].
-Obtained by oxidation of 1-(2,3-dimethoxyphenyl)-1-(3-methylpropyl) carbinol with sodium dichromate in dilute sulfuric acid (75–80 %) [2747].
-Also refer to: [198, 2747].

pale yellow oil [198, 2747];
b.p.$_{0.2}$ 103–105° [2747], b.p.$_{0.5}$ 118–120° [198], b.p.$_3$ 130° [198];
^{1}H NMR [1231], ^{13}C NMR [1231], IR [198, 1231], MS [1231].

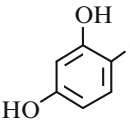
2,4-Dinitrophenylhydrazone of the dimethyl ether

[15116-03-7] $C_{19}H_{22}N_4O_6$ mol. wt. 402.41

m.p. 225–226° [2747].

1-(2,4-Dihydroxyphenyl)-3-methyl-1-butanone

[15116-14-0] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Obtained by reaction of isovaleric acid with resorcinol,
*in the presence of boron trifluoride for 2 h at 70° (77 %) [2312];

*in the presence of zinc chloride at 150° [2517], (70–78 %) [2747], (68–78 %) [2501], for 2 h at 125–136° [893].
-Also obtained by reaction of iso-amyl chloride with resorcinol at 85–90° for 20–30 min (85.3 %) [731].
-Also refer to: [773, 1300, 2685].

yellow viscous oil [2747];
b.p.$_1$ 145–152° [2747], b.p.$_{6–7}$ 183–185° [893];
m.p. 108–110° [893, 2245], 73° [2312]; ^{1}H NMR [829].

BIOLOGICAL ACTIVITY: Antitumor [1300]; For the prevention and treatment of bone and cartilage diseases [2685].

USE: Spectrophotometric determination of uranium [3213].

Oxime [159457-03-1] $C_{11}H_{15}NO_3$ mol. wt. 209.25

-For preparation of transition metal complexes [1506].

m.p. 203–205° [3375], 205–207° [2267].

Diacetate [251463-54-4] $C_{15}H_{18}O_5$ mol. wt. 278.30

-Obtained by reaction of acetic anhydride with the title ketone in the presence of pyridine (>80 %) [2517].

oil [2517];
^{1}H NMR [2517], ^{13}C NMR [2517], IR [2517], UV [2517], MS [2517].

Dimethyl ether [54874-25-8] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Obtained by reaction of dimethyl sulfate with 2,4-dihydroxyisovalerophenone in the presence of potassium carbonate in refluxing acetone for 4 h [1788].
-Also obtained by hydrogenation of 2′,4′-dimethoxydehydroisovalerophenone (b.p.$_{3–4}$ 152–153°) in the presence of 10 % Pd/C in ethanol in an hydrogen atmosphere (96 %) [1613].
-Also obtained by reaction of isovaleric acid with 1,3-dimethoxyphenyl in the presence of a mixture of phosphorous pentoxide and orthophosphoric acid at 90° for 1 h (73 %) [1613].

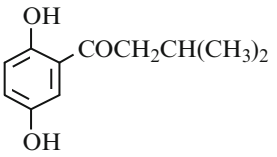
b.p.$_2$ 120–125° [1613]; ^{1}H NMR [1613], IR [1613].

2,4-Dinitrophenylhydrazone [94711-66-7] $C_{17}H_{18}N_4O_6$ mol. wt. 374.35

m.p. 234° [2245].

1-(2,5-Dihydroxyphenyl)-3-methyl-1-butanone
(2-Isovaleroylhydroquinone)

[124557-52-4] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Obtained by reaction of isovaleric acid with hydroquinone in the presence of boron trifluoride for 2 h at 125° (71 %) [2312].
-Also obtained by reaction of isovaleryl chloride with hydroquinone in the presence of aluminium chloride in nitrobenzene for 3 h in a water bath [1442].

-Also obtained by Fries rearrangement of hydroquinone diisovalerate in the presence of hydroquinone and aluminium chloride at 150–160° for 1 h (77 %) [770].
-Also obtained by Fries rearrangement of hydroquinone diisovalerate in the presence of aluminium chloride at 150–155° (oil bath) and maintained at that temperature till no more hydrogen chloride was evolved (1 h) (50 %) [613].
-Also obtained by hydrogenation of 1-(2,5-dihydroxyphenyl)-3-methyl-2-buten-1-one in the presence of 10 % Pd/C in ethanol at r.t. [2540].
-Also obtained by Fries rearrangement of 4-methoxyphenyl isovalerate with aluminium chloride (5 part)/sodium chloride (2 part) mixture at 180–200° (30 %) [1796].

-Also refer to: [1629, 1703, 1794, 2882].

yellow plates [613];
m.p. 115° [1703], 114–115° [1442], 111° [2312],
110° [770, 1796, 2540], 106–108° [613];
^{1}H NMR [613], IR [613, 2540],
UV [613, 2540, 2882].

USE: As antioxidant for vitamin A [1629].

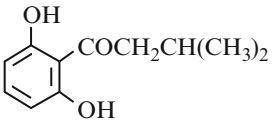
Dimethyl ether [124557-51-3] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Obtained by treatment of 2-hydroxy-5-methoxyisovalerophenone with dimethyl sulfate in the presence of 10 % aqueous sodium hydroxide in refluxing acetone for 20 min [770].
-Also obtained by Friedel-Crafts reaction of isovaleryl chloride with hydroquinone dimethyl ether [2540].

colourless oil [770]; b.p.$_1$ 124–126° [770].

1-(2,6-Dihydroxyphenyl)-3-methyl-1-butanone

[13936-90-8] $C_{11}H_{14}O_3$ mol. wt. 194.23



Synthesis
-Refer to: [1858].
m.p. 75–76° [862], 67–68° [2631].

Dimethyl ether [52856-20-9] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Obtained by condensation of 2,6-dimethoxyphenyllithium with ethyl isovalerate (42 %) [1858].

b.p.$_{0.5}$ 116° [1858].

2,4-Dinitrophenylhydrazone of the dimethyl ether

[52856-31-2] $C_{19}H_{22}N_4O_6$ mol. wt. 402.41

m.p. 147.2–148° [1858].

1-(3,4-Dihydroxyphenyl)-3-methyl-1-butanone
(L-158,870) [2904]

[67239-25-2] $C_{11}H_{14}O_3$ mol. wt. 194.23

Syntheses
-Obtained by Fries rearrangement of pyrocatechol diisovalerate with aluminium chloride,
*in nitrobenzene for 1 h at 80° (40 %) [2646];
*in the presence of pyrocatechol for 4.5 h at 135–140° (69 %) [2075].

-Also refer to: [885, 899, 2127, 2904].

b.p.$_{.4}$ 200–210° [2075]; m.p. 108° [2646], 106.5–107.5° [2075].

BIOLOGICAL ACTIVITY: Central nervous system depressant [2127]; Agonist specific for the modified β-$_2$AR [2904]; Antimelanoma and skin depigmentation, *in vitro* method for screening [612].

Dimethyl ether [132858-47-0] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Also obtained by reaction of isovaleric acid with veratrole in the presence of polyphosphoric acid for 2.5 h at 60° (91.6 %) [1364].

pale yellow oil [1364]; b.p.$_{0.37}$ 134.5° [1364];
^{1}H NMR [1231], ^{13}C NMR [1231], IR [1231], MS [1231].

Oxime of the dimethyl ether $C_{13}H_{19}NO_3$ mol. wt. 237.30

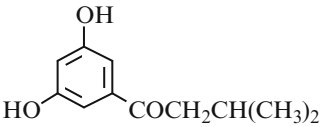
oil [1364].

Semicarbazone of the dimethyl ether [101778-04-5] $C_{14}H_{21}N_3O_3$ mol. wt. 279.34

colourless short thick prisms [1364]; m.p. 183.4–185.7° [1364].

1-(3,5-Dihydroxyphenyl)-3-methyl-1-butanone

[104216-80-0] $C_{11}H_{14}O_3$ mol. wt. 194.23



Synthesis
-Obtained by treatment of its diacetate with 5 % sodium hydroxide at reflux for 4–5 h (45 %) [1406].
m.p. 102° [1406].

Monohydrate $C_{11}H_{14}O_3$, H_2O mol. wt. 212.24

m.p. 44° [1406].

2,4-Dinitrophenylhydrazone [101593-65-1] $C_{17}H_{18}N_4O_6$ mol. wt. 374.35

m.p. 204° (d) [1406].

Diacetate [108715-26-0] $C_{15}H_{18}O_5$ mol. wt. 278.30

-Preparation by reaction of diisobutylcadmium with 3,5-diacetoxybenzoyl chloride in refluxing benzene for 1 h (62 %) [1406].

b.p.$_{0.5}$ 178–182° [1406].

2,4-Dinitrophenylhydrazone of the diacetate

[102661-34-7] $C_{21}H_{22}N_4O_8$ mol. wt. 458.43

m.p. 160° [1406].

Dimethyl ether $C_{13}H_{18}O_3$ mol. wt. 222.28

-Obtained by reaction of isobutylmagnesium bromide with 3,5-dimethoxybenzonitrile (17 %) [1212].

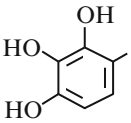
m.p. 143–145° [1212].

Semicarbazone of the dimethyl ether $C_{14}H_{21}N_3O_3$ mol. wt. 279.34

m.p. 195–196° [1212].

3-Methyl-1-[2,3,4-trihydroxyphenyl]-1-butanone

[757408-19-8] $C_{11}H_{14}O_4$ mol. wt. 210.23



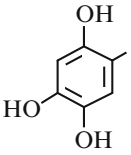
Syntheses
-Obtained by reaction of isovaleric acid with pyrogallol in the presence,
*of boron trifluoride in ethyl ether at 0° for 1 h (72 %) [538, 540];
*of zinc chloride (Nencki reaction) (64 %) [811].

-Also refer to: [1054, 1260, 3349].

$b.p._{0.01}$ 138–140° [811];
m.p. 109° [538, 540], 106–110° [811]; UV [540].

3-Methyl-1-[2,4,5-trihydroxyphenyl]-1-butanone

[79744-63-1] $C_{11}H_{14}O_4$ mol. wt. 210.23



Synthesis
-Refer to: [1508].
^{1}H NMR [1508], ^{13}C NMR [1508].

Trimethyl ether [98230-17-2] $C_{14}H_{20}O_4$ mol. wt. 252.31

m.p. 76.5° [1406]; UV [1406].

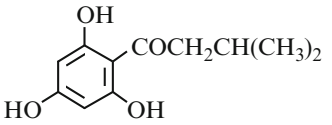
2,4-Dinitrophenylhydrazone of the trimethyl ether

[102458-53-7] $C_{20}H_{24}N_4O_7$ mol. wt. 432.43

m.p. 132° [1406].

3-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone

[26103-97-9] $C_{11}H_{14}O_4$ mol. wt. 210.23



Syntheses

-Preparation by reaction of isovaleryl chloride with phloroglucinol in the presence of aluminium chloride [(88.5 %) 491, (60 %) 621, 2534, 3415],

*in nitrobenzene [334, (60–70 %) 421, (45 %) 898, (30–38 %) 1665, (25 %) 2615, (47 %) 2618, 2646];
*in a methylene chloride/nitromethane mixture [2580];
*in a carbon disulfide/nitrobenzene mixture [(35–38 %) 1066, (46 %) 2113, (47 %) 2620];
*without solvent at 50° (70 %) [335].

-Also obtained by reaction of isovaleronitrile with phloroglucinol (Hoesch reaction) [1608, 1665, (23 %) 2926].
-Also obtained by reaction of isovaleric acid with phloroglucinol in the presence of boron trifluoride etherate [3019, 3020] at 100° for 2 h (27 %) [338].
-Also obtained by acid hydrolysis of its 2-β-D-glucopyranoside in methanol in the presence of 1 N HCl at reflux for 4 h [209].
-Also obtained by acid hydrolysis of its 2,4-di-β-D-glucopyranoside [1089].
-Also obtained by adding phloroglucinol to a solution of phosphorous oxychloride plus aluminium chloride and stirred under nitrogen. 3-Methylbutanoic acid was added and the reaction stirred under nitrogen at 0° for 8 h, then at 6° for 40 h (40–54 %) [3201].
-Also obtained from valerophenone synthase (VPS) which uses isovaleryl-CoA to synthetize phloroisovalerophenone [3482].
-Also refer to: [5, 337, 542, 763, 1254, 1292, 1374, 1983, 2405, 2610, 2614, 2616, 2685, 2686, 2771, 3033, 3120, 3202, 3310, 3481].

Isolation from natural sources

-From hop plant, *Humulos lupulus* (Cannabinaceae) [1066, 2389].
-From hop bittering [2846].

yellow crystals [1066]; b.p.$_{0.01}$ 180–190° [2926];
m.p. 176–178° [1608], 146° [2113],
145° [421, 1374, 1665, 2615, 2618, 2620, 2646, 2771],
144–145° [1066, 2534, 2926],
143–145° [209], 142° [898], 141–143° [541];
^{1}H NMR [209, 421, 541, 898, 1066, 2534, 3019],
^{13}C NMR [3019], IR [421, 898, 3019], UV [898, 1066, 3019],
MS [421, 1066, 2531, 2534, 2846];
GLC [2531]; TLC [1066]; HPLC [1066, 3481].

USE: As bone metabolism improving agent [1042]; Antagonist both thromboxane A_2 and Leukotriene D_4 [3019]; Effects on transpiration and stomatal closure [3408]; In lupulone preparation [3120].

BIOLOGICAL ACTIVITY: Antimicrobial activity against *Bacillus subtilis* [3020]; Antimicrobial activity of, for *Staphylococcus aureus* [3372]; Germination inhibition [421]; Inhibitory effects of treatment with this acylphenol on TPA Induced EBV-EA Activation [3033]; Antifungal [2113]; As bone resorption inhibitor for treatment of bone diseases [2686]; For the prevention and treatment of bone and cartilage diseases [2685].

Monohydrate $C_{11}H_{14}O_4, H_2O$ mol. wt. 228.25

m.p. 95° [1608].

Trimethyl ether [101032-04-6] $C_{14}H_{20}O_4$ mol. wt. 252.31

-Obtained by reaction of isovaleryl chloride with phloroglucinol trimethyl ether in the presence of aluminium chloride [1818] (88 %), in methylene chloride,
*at 0° for 3.5 h (81 %) [3071, 3072];
*at −10 to −5° over 2 h, then at 0° for 30 min (88 %) [1819].

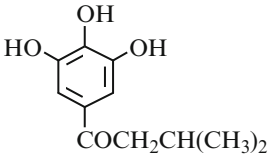
oil [1819]; ^{1}H NMR [1819].

2,4-Dinitrophenylhydrazone $C_{17}H_{18}N_4O_7$ mol. wt. 390.35

m.p. 196° [1665].

3-Methyl-1-(3,4,5-trihydroxyphenyl)-1-butanone

[216300-88-8] $C_{11}H_{14}O_4$ mol. wt. 210.23



Synthesis
-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

Trimethyl ether $C_{14}H_{20}O_4$ mol. wt. 252.31

-Obtained by reaction of 3,4,5-trimethoxybenzonitrile with isobutylmagnesium bromide in toluene at 40° for 5 h (42 %) [1407] or at reflux for 3 h (26 %) [1212].

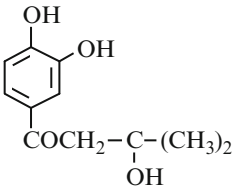
b.p.$_1$ 147–150° [1212], b.p.$_6$ 164–166° [1407];
m.p. 37–39° [1212, 1407].

Semicarbazone of the trimethyl ether $C_{15}H_{23}N_3O_4$ mol. wt. 309.37

m.p. 205° [1212].

1-(3,4-Dihydroxyphenyl)-3-hydroxy-3-methyl-1-butanone

$C_{11}H_{14}O_4$ mol. wt. 210.23



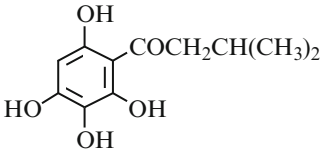
Synthesis

-Obtained by thermal Fries rearrangement of pyrocatechol di-3-methyl-2-butenoate (13 %) [1505].

pale yellow needles [1505];
m.p. 132–133° [1505];
^{1}H NMR [1505], IR [1505], UV [1505].

1-(2,3,4,6-Tetrahydroxyphenyl)-3-methyl-1-butanone

[100059-66-3] $C_{11}H_{14}O_5$ mol. wt. 226.23



Syntheses

-Preparation by total demethylation of 2,4-dihydroxy-3,6-dimethoxyisovalerophenone with aluminium bromide in chlorobenzene at 80–85° for 5 h (83 %) [2610].

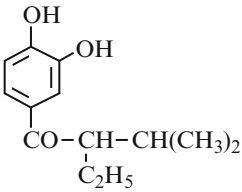
-Also obtained by reaction of isovaleryl chloride with 1,2,3,5-tetrahydroxybenzene in the presence of aluminium chloride in nitrobenzene first at 0°, then at r.t. for 3 days (38 %) [2307].

m.p. 178–179° [2610], 167–168° [2307];
sublimation $_{0.2}$ 130–140° [2610];
^{1}H NMR [2307], UV [2307], MS [2307, 2683].

N.B.: Stability [2610, 2616].

1-(3,4-Dihydroxyphenyl)-2-ethyl-3-methyl-1-butanone

[67114-29-8] $C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis

-Obtained by treatment of its dimethyl ether with pyridinium chloride under nitrogen at 200–220° for 1 h (30 %) [2127].

white crystals [2127]; b.p.$_{0.025}$ 135° [2127];
m.p. 100–101.5° [2127].

BIOLOGICAL ACTIVITY: Central nervous system depressant [2127].

Dimethyl ether [92730-14-8] $C_{15}H_{22}O_3$ mol. wt. 250.34

-Obtained by reaction of 2-ethyl-3-methylbutyryl chloride with veratrole in the presence of aluminium chloride in refluxing benzene for 30 min (39 %) [2127].

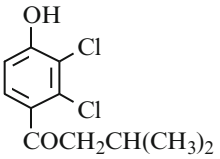
colourless liquid [2127]; b.p.$_{0.025}$ 117° [2127]; $n_D^{25} = 1.5329$ [2127].

BIOLOGICAL ACTIVITY: Central nervous system depressant [2127].

2.3.2 Substituted Hydroxyketones

1-(2,3-Dichloro-4-hydroxyphenyl)-3-methyl-1-butanone

[1506-72-5] $C_{11}H_{12}Cl_2O_2$ mol. wt. 247.12



Syntheses

-Obtained by reaction of isovaleryl chloride with 2,3-dichloroanisole in the presence of aluminium chloride in carbon disulfide (77 %) [2057, 2767].

-Also refer to: [2047, 2048, 2056, 2766].

m.p. 112–114° [2048, 2766], 110–112° [2047, 2056, 2057, 2767].

Methyl ether [53107-50-9] $C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15

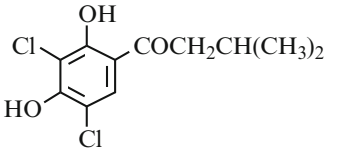
-Preparation by reaction of isovaleryl chloride with 2,3-dichloroanisole in the presence of aluminium chloride (72 %) [3333].

-Also refer to: [732, 734, 736, 737, 2052].

m.p. 54–55° [3333], 49–54° [732, 734, 736, 737, 2052].

1-(3,5-Dichloro-2,4-dihydroxyphenyl)-3-methyl-1-butanone

$C_{11}H_{12}Cl_2O_3$ mol. wt. 263.21



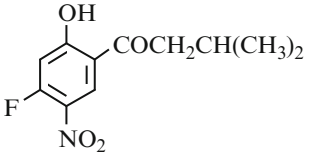
Synthesis

-Refer to: [1052].

BIOLOGICAL ACTIVITY: Bactericide [1052].

1-(4-Fluoro-2-hydroxy-5-nitrophenyl)-3-methyl-1-butanone

[120292-07-1] $C_{11}H_{12}FNO_4$ mol. wt. 241.22

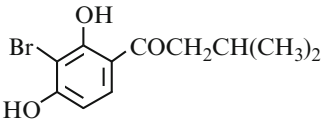


Synthesis

-Refer to: [958].

1-(3-Bromo-2,4-dihydroxyphenyl)-3-methyl-1-butanone

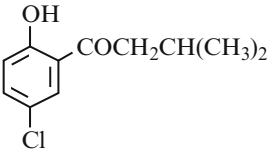
[664376-91-4] $C_{11}H_{13}BrO_3$ mol. wt. 273.13



Syntheses
-Refer to: [2485, 2486].

1-(5-Chloro-2-hydroxyphenyl)-3-methyl-1-butanone

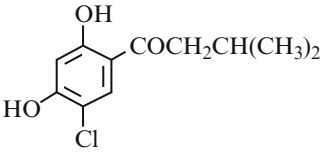
$C_{11}H_{13}ClO_2$ mol. wt. 212.68



Synthesis
-Obtained by Fries rearrangement of 4-chlorophenyl isovalerate with aluminium chloride in tetrachloroethane at 150–160° for 2 h [3170].
b.p.$_{0.20–0.25}$ 98–98.5° [3170]; UV [3170].

1-(5-Chloro-2,4-dihydroxyphenyl)-3-methyl-1-butanone

[216300-97-9] $C_{11}H_{13}ClO_3$ mol. wt. 228.68

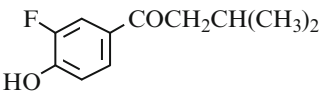


Synthesis
-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

1-(3-Fluoro-4-hydroxyphenyl)-3-methyl-1-butanone

$C_{11}H_{13}FO_2$ mol. wt. 196.22



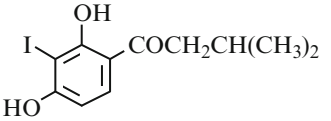
Synthesis
-Obtained by Fries rearrangement with aluminium chloride in carbone disulfide [922].
m.p. 100–101° [922].

Methyl ether [4374-24-7] $C_{12}H_{15}FO_2$ mol. wt. 210.25

b.p.$_{0.09}$ 90° [671].

1-(2,4-Dihydroxy-3-iodophenyl)-3-methyl-1-butanone

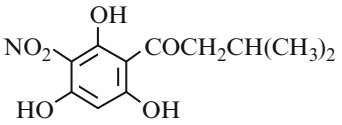
[1204737-61-0] $C_{11}H_{13}IO_3$ mol. wt. 320.13



Synthesis
-Obtained by action of iodine/iodine carbonate in ethanol at 20° (93 %) [1672].
MS [1672].

3-Methyl-1-(2,4,6-trihydroxy-3-nitrophenyl)-1-butanone

[119691-94-0] $C_{11}H_{13}NO_6$ mol. wt. 255.23



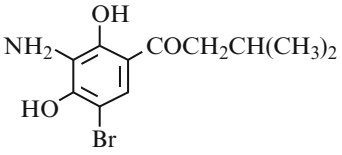
Synthesis
-Obtained by adding hexane, then a mixture of concentrated sulfuric acid and fuming nitric acid at 0° to a solution of 2,4,6-trihydroxyisovalerophenone in concentrated sulfuric acid below 0° (70–80 %) [3414].

bright yellow needles [3414]; m.p. 94–96° [3414];
^{1}H NMR [3414], IR [3414], MS [3414].

BIOLOGICAL ACTIVITY: Germination inhibition [3414];

1-(3-Amino-5-bromo-2,4-dihydroxyphenyl)-3-methyl-1-butanone

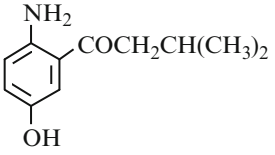
[909255-16-9] $C_{11}H_{14}BrNO_3$ mol. wt. 288.14



Synthesis
-Obtained by reduction of the nitro group of the 3-nitro derivative by zinc and acetic acid in methanol at 20° (73 %) [3350].
m.p. 119–121° [3350]; ^{1}H NMR [3350], ^{13}C NMR [3350].

1-(2-Amino-5-hydroxyphenyl)-3-methyl-1-butanone

[404918-99-6] $C_{11}H_{15}NO_2$ mol. wt. 193.25

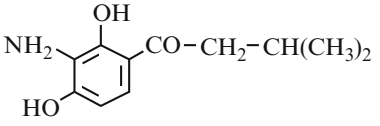


Synthesis
-Refer to: [3331].

USE: Preparation of indazoles having an action similar to that of a thyroid hormone and method for the production thereof, and their use in medicaments [3331].

1-(3-Amino-2,4-dihydroxyphenyl)-3-methyl-1-butanone

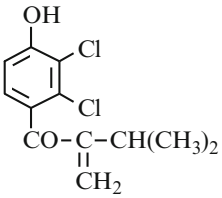
[909255-15-8] $C_{11}H_{15}NO_3$ mol. wt. 209.25



Synthesis
-Obtained by reduction of the nitro group of the 3-nitro derivative by zinc and acetic acid in methanol at 20° (75 %) [3350].
m.p. 117–119° [3350]; ^{1}H NMR [3350], ^{13}C NMR [3350].

1-(2,3-Dichloro-4-hydroxyphenyl)-3-methyl-2-methylene-1-butanone

$C_{12}H_{12}Cl_2O_2$ mol. wt. 259.13



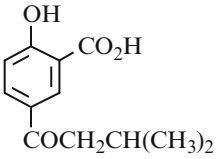
Synthesis
-Refer to: [3333].

Methyl ether [53107-51-0]
$C_{13}H_{14}Cl_2O_2$ mol. wt. 273.16
-Refer to: [732, 734, 736, 737, 2052, 3333 (63 %)].

m.p. 56–58° [3333], 46–51° [732, 734, 736, 737, 2052].

2-Hydroxy-5-(3-methylbutyryl)benzoic acid

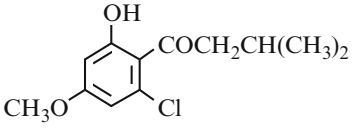
$C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Obtained by alkaline hydrolysis of 5-isovalerylsalicylamide [1158].
m.p. 178° [1158].

1-(2-Chloro-6-hydroxy-4-methoxyphenyl)-3-methyl-1-butanone

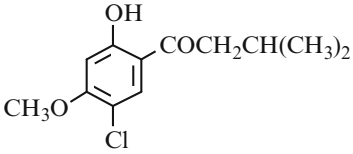
[112954-17-3] $C_{12}H_{15}ClO_3$ mol. wt. 242.70



Syntheses
-Obtained by Friedel-Crafts reaction of isovaleryl chloride with 3-chloro-5-methoxyphenol in the presence of aluminium chloride [1695, 1696].

1-(5-Chloro-2-hydroxy-4-methoxyphenyl)-3-methyl-1-butanone

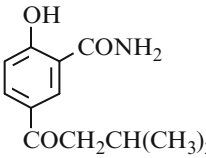
[136741-47-4] $C_{12}H_{15}ClO_3$ mol. wt. 242.70



Synthesis
-Preparation by reaction of isovaleryl chloride with 4-chlororesorcinol dimethyl ether in the presence of aluminium chloride in 1,2-dichloroethane (92 %) [2718].
m.p. 81–82° [2718].

2-Hydroxy-5-(3-methylbutyryl)benzamide

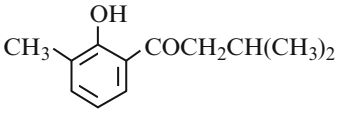
$C_{12}H_{15}NO_3$ mol. wt. 221.26



Synthesis
-Obtained by Fries rearrangement of salicylamide isovalerate in the presence of aluminium chloride in nitrobenzene for 3 h at 20° [1158].
m.p. 182° [1158].

1-(2-Hydroxy-3-methylphenyl)-3-methyl-1-butanone

[105337-84-6] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses
-Obtained by Fries rearrangement of o-cresyl isovalerate with aluminium chloride for 30 min at 160–180° (20 %) [1644].
-Also refer to: [2390].

b.p.$_{.4}$ 127° [2390], b.p.$_{.8}$ 137° [2390], b.p.$_{.11.5}$ 140–146° [1644], b.p.$_{.11}$ 143° [2390].

Phenylhydrazone $C_{18}H_{22}N_2O$ mol. wt. 282.39

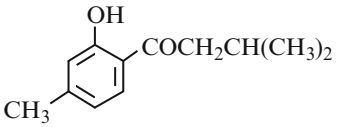
m.p. 114–115° [2390].

2,4-Dinitrophenylhydrazone [109252-17-7] $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 191–192° [2390].

1-(2-Hydroxy-4-methylphenyl)-3-methyl-1-butanone

[105337-38-0] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses
-Obtained by reaction of isovaleric acid with m-cresol in the presence of boron trifluoride for 2 h at 70° (78 %) [1685].

-Also obtained by Fries rearrangement of m-cresyl isovalerate in the presence of aluminium chloride,
*without solvent for 30 min at 120–148° (73 %) [1644] or at 140–150° [906];
*first in refluxing carbon disulfide for 2 h, then at 145–150° for 4 h after solvent elimination, (95 %) [3063].
-Also obtained from 2,2,7-trimethyl-4-chromanone, also named 2,2,7-trimethyl-4-oxo-4*H*-1-benzopyran (4 %) [118, 3063].

b.p.$_{1.5}$ 95–97° [906], b.p.$_{11.5}$ 137–142° [1644], b.p.$_{.21}$ 151–152° [3063], b.p.$_{18}$ 152–156° [1685];
^{1}H NMR [118, 3063], IR [118, 3063]; $n_D^{20} = 1.5295$ [118].

Phenylhydrazone [101784-96-7] $C_{18}H_{22}N_2O$ mol. wt. 282.39

m.p. 107–110° [1644].

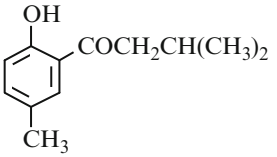
Methyl ether [71898-88-9] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by treatment of 2-hydroxy-4-methylisovalerophenone with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 10 h (96 %) [3063].

$b.p._{10}$ 146° [3063]; ^1H NMR [3063], IR [3063].

1-(2-Hydroxy-5-methylphenyl)-3-methyl-1-butanone

[55813-81-5] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Obtained by Fries rearrangement of p-cresyl isovalerate in the presence of aluminium chloride for 45 min at 130–160° (67 %) [1644].

-Also obtained by treatment of its methyl ether with boiling pyridinium chloride [515, 2089].

-Also obtained by reaction of aluminium chloride with its methyl ether in boiling carbon disulfide [185].

$b.p._{0.1}$ 85° [640], $b.p._{12}$ 138–140° [1644], $b.p._{21}$ 151° [185];
^1H NMR [640], IR [640], UV [640]; $n_D^{18.4} = 1.5685$ [185].

2,4-Dinitrophenylhydrazone $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 174–175.5° [1644].

4-Nitrophenylhydrazone $C_{18}H_{21}N_3O_3$ mol. wt. 327.38

m.p. 136–137° [185].

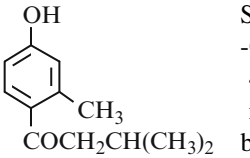
Methyl ether $C_{13}H_{18}O_2$ mol. wt. 206.28

-Preparation by reaction of isovaleryl chloride with 4-methylanisole in the presence of aluminium chloride in carbon disulfide for 24 h at r.t. [515, (50 %) 2089].

pale yellow oil; $b.p._{17}$ 157–158° [515, 2089]; $n_D^{20} = 1.5200$ [515, 2089].

1-(4-Hydroxy-2-methylphenyl)-3-methyl-1-butanone

$C_{12}H_{16}O_2$ mol. wt. 192.26



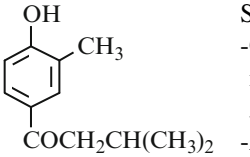
Synthesis

-Obtained by reaction of aluminium chloride with 4-hydroxy-2-methyl-5-isopropylisovalerophenone in chlorobenzene, first 20 h at r.t., then for 4 h at 50° (53 %) [1523].

b.p.$_{0.0008}$ 115–120° [1523]; m.p. 51° [1523].

1-(4-Hydroxy-3-methylphenyl)-3-methyl-1-butanone

[105337-39-1] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Obtained by treatment of p-isovalerocarvacrol with aluminium chloride in chlorobenzene, first at r.t. for 20 h, then at 50° for 4 h (71 %) [1522, 1523].

-Also obtained by Fries rearrangement of o-cresyl isovalerate in the presence of aluminium chloride at 160–180° for 30 min (18 %) [1644].

b.p.$_{10.5}$ 184–188° [1644], b.p.$_{2}$ 188–190° [2390], b.p.$_{18}$ 219–220° [2390]; m.p. 83° [1522, 1523], 76–77° [2390]; IR [2777].

Methyl ether [1096879-14-9] $C_{13}H_{18}O_2$ mol. wt. 206.29

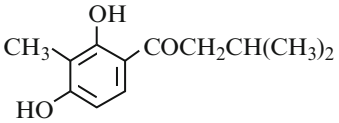
^{1}H NMR [1231], ^{13}C NMR [1231], IR [1231], MS [1231].

2,4-Dinitrophenylhydrazone [109248-77-3] $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 200–201° [2390].

1-(2,4-Dihydroxy-3-methylphenyl)-3-methyl-1-butanone

[664376-65-2] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses

-Obtained (by-product) from methyl 3-(bromomethyl)-benzoate, first with 4-mercaptopyridine in the presence of potassium carbonate in acetone at 45°, then the product obtained by $LiAlH_4$ in tetrahydrofuran at 0° [2485].

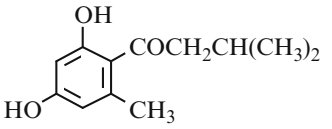
-Also obtained by reaction of isovaleroyl chloride with 2-methylresorcinol in the presence of aluminium chloride in methylene chloride first at 0°, then at r.t. for 16 h (57 %) [2486].

-Also refer to: [773].

white solid [2486].

1-(2,4-Dihydroxy-6-methylphenyl)-3-methyl-1-butanone

[198879-07-1] $C_{12}H_{16}O_3$ mol. wt. 208.26

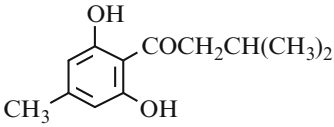


Syntheses
-Refer to: [2684, 2685].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684, 2685].

1-(2,6-Dihydroxy-4-methylphenyl)-3-methyl-1-butanone

[216300-92-4] $C_{12}H_{16}O_3$ mol. wt. 208.26

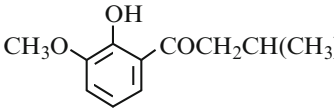


Synthesis
-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

1-(2-Hydroxy-3-methoxyphenyl)-3-methyl-1-butanone

[15116-06-0] $C_{12}H_{16}O_3$ mol. wt. 208.26

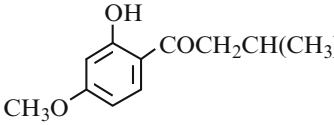


Syntheses
-Obtained by partial demethylation of its methyl ether with aluminium chloride in toluene (50–60 %) [2747].
-Also refer to: [1681].

oil [2747]; b.p.$_{0.2}$ 97–101° [2747].

1-(2-Hydroxy-4-methoxyphenyl)-3-methyl-1-butanone

[193687-88-6] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses
-Obtained by reaction of isovaleryl chloride with resorcinol dimethyl ether in the presence of aluminium chloride in refluxing carbon disulfide (60 %) [1788].

-Preparation by partial methylation of 2,4-dihydroxyisovalerophenone with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 4–6 h (85–90 %) [2501].
-Also obtained from 2,2-dimethyl-7-methoxy-4-chromanone, also named 2,2-dimethyl-7-methoxy-4-oxo-4*H*-1-benzopyran (31 %) [118].

-Also obtained by treatment of 2-(*t*-butyldimethylsilyloxy)-2′-isopropyl-4-methoxyacetophenone (m.p. 110–112°) with $(n\text{-Bu})_4NF$ in THF at 0° for 45 min (82 %) [1467].

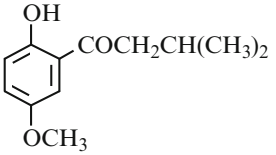
oil [118]; b.p.$_{.4}$ 165° [1788];
m.p. 125–127° [1467];
^{1}H NMR [118, 1467], ^{13}C NMR [1467], IR [118, 1467],
MS [1467]; $n_D^{20} = 1.5475$ [118].

Phenylhydrazone $C_{18}H_{22}N_2O_2$ mol. wt. 298.38

m.p. 85° [1788].

1-(2-Hydroxy-5-methoxyphenyl)-3-methyl-1-butanone

[876511-19-2] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses
-Obtained by reaction of isovaleryl chloride with quinol dimethyl ether in the presence of aluminium chloride [770] in carbon disulfide [161].
-Also obtained by hydrogenation of 1-(2-hydroxy-5-methoxyphenyl)-3-methyl-2-buten-1-one in the presence of 10 % Pd/C in ethanol at r.t. [2540].

-Also refer to: [458]

oil [2540]; b.p.$_{.15}$ 155–163° [161], b.p.$_{.18}$ 177–178° [458].

Na salt $C_{12}H_{15}O_3Na$ mol. wt. 230.24

-Refer to: [770].

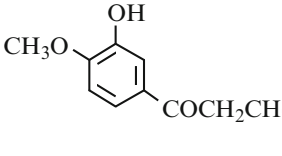
yellow needles [770].

Semicarbazone $C_{13}H_{19}N_3O_3$ mol. wt. 265.31

m.p. 171° [770, 2540].

1-(3-Hydroxy-4-methoxyphenyl)-3-methyl-1-butanone

[99783-85-4] $C_{12}H_{16}O_3$ mol. wt. 208.26

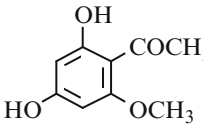


Syntheses
-Obtained from its 3-methylbutanoate by refluxing with 30 % sodium hydroxide for 2 h (92 %) [144].
-Also refer to: [2779].

m.p. 51–53° [2779], 45–48° [144]; ^{1}H NMR [144].

1-(2,4-Dihydroxy-6-methoxyphenyl)-3-methyl-1-butanone

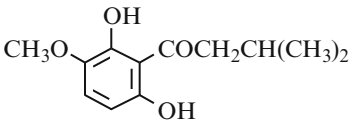
$C_{12}H_{16}O_4$ mol. wt. 224.26



Synthesis
-Refer to: [2356].
m.p. 132° [2356]; UV [2356].

1-(2,6-Dihydroxy-3-methoxyphenyl)-3-methyl-1-butanone

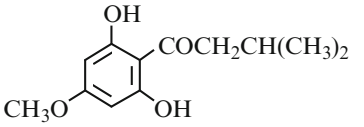
$C_{12}H_{16}O_4$ mol. wt. 224.26



Synthesis
-Refer to: [829].
^{1}H NMR [829].

1-(2,6-Dihydroxy-4-methoxyphenyl)-3-methyl-1-butanone

[91555-33-8] $C_{12}H_{16}O_4$ mol. wt. 224.26



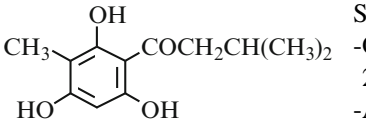
Syntheses
-Refer to: [829, 2356].
Isolation from natural sources
-Refer to: [2707].

-Gradient-enhanced nuclear Overhauser effect spectroscopy (GOESY) in structure elucidation of plant secondary metabolites [2707].

m.p. 96–97° [2356]; ^{1}H NMR [829], UV [2356].

3-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone

[49583-27-9] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Obtained by reaction of isovaleryl chloride with 2,4,6-trihydroxytoluene [3176] according to [641].
-Also obtained by treatment of 1-[2-hydroxy-3-methyl-4,6-bis(1-methylethoxy)phenyl]-3-methyl-1-butanone with titanium tetrachloride in methylene chloride at r.t. for 48 h (83.4 %) [642].

-Also refer to: [361, 769, 1917, 2435, 3405, 3437 (23 %)].

red crystals [642];
m.p. 160–161° [1917], 154–155° [642], 148° [3437];
^{1}H NMR [642, 3437], ^{13}C NMR [642], IR [642, 3437], UV [642], MS [642, 1917, 3437]; GLC [2531].

BIOLOGICAL ACTIVITY: As photosynthetic electron transport (PET) [3405].

Trimethyl ether [149053-77-0] $C_{15}H_{22}O_4$ mol. wt. 266.34

-Refer to: [2435].

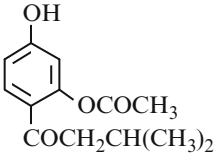
Isolation from natural sources

-From volatile leaf oils of some south-western and southern Australian species of the genus Eucalyptus: Subgenus Symphyomyrtus, section Bisectaria, series Macrocarpae [361].

^{1}H NMR [2435]; GC/MS [361].

1-[2-(Acetyloxy)-4-hydroxyphenyl]-3-methyl-1-butanone

[251463-59-9] $C_{13}H_{16}O_4$ mol. wt. 236.27



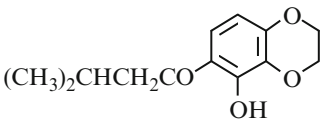
Synthesis

-Obtained by selective deacetylation of 2,4-diacetoxyphenyl isobutyl ketone mediated by porcine pancreatic lipase (PPL) in THF at 42–45° for 48 h in the presence of n-butanol (45 %) [2517].

oil [2517];
^{1}H NMR [2517], ^{13}C NMR [2517], IR [2517], UV [2517], MS [2517].

5-Hydroxy-6-(2-methyl-1-oxobutyl)-1,4-benzodioxane

$C_{13}H_{16}O_4$ mol. wt. 236.27



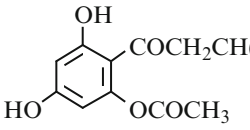
Synthesis

-Obtained by Fries rearrangement of 5-isovaleryloxy-1,4-benzodioxane in the presence of aluminium chloride in nitrobenzene at 20° (62 %) [801].

b.p.$_{0.1}$ 162–164° [801]; m.p. 59–60° [801]; UV [801].

1-[2-(Acetyloxy)-4,6-dihydroxyphenyl]-3-methyl-1-butanone

[62545-33-9] $C_{13}H_{16}O_5$ mol. wt. 252.27

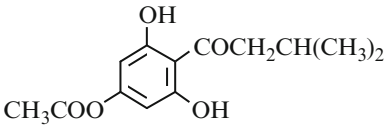


Synthesis

-Obtained by partial acetylation of phloroisobutyrophenone [2580].

1-[4-(Acetyloxy)-2,6-dihydroxyphenyl]-3-methyl-1-butanone

[62545-32-8] $C_{13}H_{16}O_5$ mol. wt. 252.27



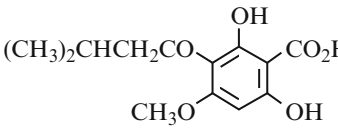
Synthesis

-Obtained by partial acetylation of phloroisobutyrophenone [2580].

m.p. 120° [2580].

2,6-Dihydroxy-3-isovaleryl-4-methoxybenzoic acid

$C_{13}H_{16}O_6$ mol. wt. 268.27



Synthesis

-Refer to: [493].

Methyl ester [162071-05-8]

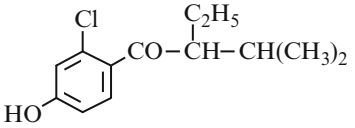
$C_{14}H_{18}O_6$ mol. wt. 282.29

-Obtained by reaction of isovaleryl chloride with methyl 2,6-dihydroxy-4-methoxybenzoate in the presence of aluminium chloride in nitrobenzene at 0°, then 3 days at r.t. (80 %) [493].

m.p. 102–104° [493]; IR [493].

1-(2-Chloro-4-hydroxyphenyl)-2-ethyl-3-methyl-1-butanone

[5590-61-4] $C_{13}H_{17}ClO_2$ mol. wt. 240.73



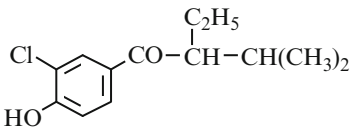
Synthesis

-Obtained by condensation of 2-ethyl-3-methylbutyryl chloride on chloro-3-anisole [2767].

m.p. 75–77° [2047, 2057, 2767].

1-(3-Chloro-4-hydroxyphenyl)-2-ethyl-3-methyl-1-butanone

$C_{13}H_{17}ClO_2$ mol. wt. 240.73



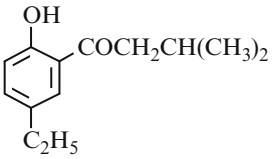
Synthesis

-To 2-isopropylbutyryl chloride, 2-chloroanisole and carbon disulfide was added in small portions at 25°, aluminium chloride; the mixture stirred 1 h at r.t. and 45 min at 55°; pentane and aluminium chloride added, heated 3 h at 80° [2056].

m.p. 75–76° [2056].

1-(5-Ethyl-2-hydroxyphenyl)-3-methyl-1-butanone

[77346-69-1] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses
-Preparation by Fries rearrangement of 4-ethylphenyl 3-methylbutanoate in the presence of aluminium chloride for 2 h at 140° (94 %) [403].
-Also refer to: [2220].

b.p.$_{0.3}$ 96–98° [403]; ^{1}H NMR [403], IR [403].

Isovalerate [77346-70-4] $C_{18}H_{26}O_3$ mol. wt. 290.40

-Obtained by reaction of isovaleryl chloride with 5-ethyl-2-hydroxyisovalerophenone in the presence of pyridine in chloroform at r.t. (96 %) [403].

b.p.$_{.3}$ 180–185° [403]; ^{1}H NMR [403], IR [403].

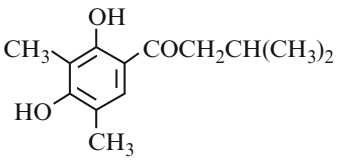
Methyl ether [72247-02-0] $C_{14}H_{20}O_2$ mol. wt. 220.31

-Obtained by reaction of isovaleric acid with p-ethylanisole in the presence of PPA at 80° for 2 h (87 %) [2220, 2701].

b.p.$_4$ 126–127° [2220]; ^{1}H NMR [2220], IR [2220], UV [2220].

1-(2,4-Dihydroxy-3,5-dimethylphenyl)-3-methyl-1-butanone

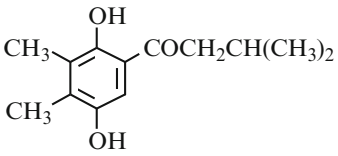
$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Refer to: [829].
^{1}H NMR [829].

1-(2,5-Dihydroxy-3,4-dimethylphenyl)-3-methyl-1-butanone

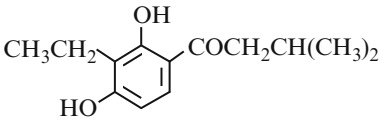
$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Refer to: [2538].
m.p. 138° [2538]; UV [2538].

1-(3-Ethyl-2,4-dihydroxyphenyl)-3-methyl-1-butanone

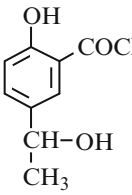
[664376-82-8] $C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Refer to: [773].

1-[5-(1-Hydroxyethyl)-2-hydroxyphenyl]-3-methyl-1-butanone

$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Refer to: [399].
Isolation from natural sources
-From *Brachyclados megalanthus* (Compositae) [3444].

colourless crystals [3444]; m.p. 150° [3444];
$(\alpha)_D^{24} = -4°$ (chloroform) [3444];
^{1}H NMR [3444], IR [3444], MS [3444].

2-Methyl ether [51995-88-1] $C_{14}H_{20}O_3$ mol. wt. 236.31

-Obtained by heating its isovalerianate with methanolic 2 N potassium hydroxide for 1 h at 65° (90 %) [399].

Isolation from natural sources
-From *Verbesina luetzelburgii* (Compositae) [407].

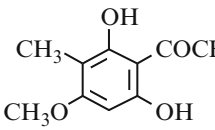
colourless oil [399]; ^{1}H NMR [399], IR [399].

Isovalerianate of the 2-methyl ether $C_{14}H_{20}O_3$ mol. wt. 236.31

-Refer to: [399].

1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-3-methyl-1-butanone
(Aspidinol C)

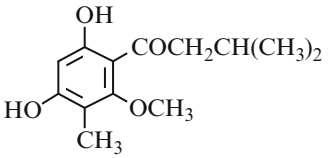
[1257216-80-0] $C_{13}H_{18}O_4$ mol. wt. 238.28



Synthesis
-Refer to: [3268].
m.p. 155–158° [3268]; ^{1}H NMR [3268], ^{13}C NMR [3268], IR [3268], UV [3268], MS [3268].

1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-3-methyl-1-butanone

[55382-31-5] $C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses

-Obtained by reductive alkaline cleavage,

*of kosotoxin (**II**) and protokosin (**III**) from female flowers of *Hagenia abyssinica* (Bruce) Gmelin [1916] (**IVb**);

*of "kosin" (**IV**), from *Flos koso* "Siegfried" by treatment with 15 % potassium hydroxide in the presence of zinc powder on a water bath for 24 h [1915] (**VIIIb**).

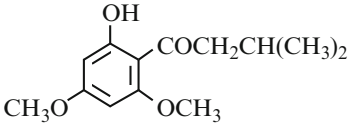
m.p. 59–61° [1915].

N.B.: "Kosin" (**IV**), others names: Methylene-bis-pseudo-aspidinol; pseudo-aspidin. [1911].

m.p. 148–150° [1915];
^{1}H NMR [1915], IR [1915], UV [1915], MS [1915].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-methyl-1-butanone

[68754-16-5] $C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses

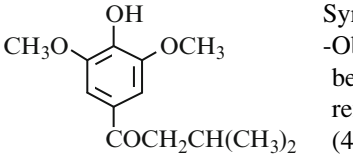
-Preparation by reaction of 3-isovaleric acid with 3,5-dimethoxyphenol in the presence of boron trifluoride etherate at 80° for 2 h (98 %) [643].

-Also refer to: [176, 177, 3085, 3086].

m.p. 50–50.5° [1005], 48° [2356], 32° [643];
^{1}H NMR [643], ^{13}C NMR [643], IR [643, 1005], UV [643, 1005, 2356], MS [643].

1-(4-Hydroxy-3,5-dimethoxyphenyl)-3-methyl-1-butanone

[873380-96-2] $C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses

-Obtained by reaction of 3,4,5-trimethoxy-benzonitrile with isobutylmagnesium bromide in refluxing toluene for 3 h (25 %) [1212] or for 5 h (40 %) [1407].

-Also obtained by treatment of its methyl ether with concentrated sulfuric acid at 35–40° for 20 h (85 %) [1407].

m.p. 94° [1212], 93–93.5° [1407].

Oxime $C_{13}H_{19}NO_4$ mol. wt. 253.30

m.p. 110° [1212].

Semicarbazone $C_{14}H_{21}N_3O_4$ mol. wt. 295.34

m.p. 162.5° [1212].

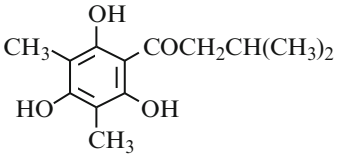
Benzoate $C_{20}H_{22}O_5$ mol. wt. 342.39

-Obtained by reaction of benzoyl chloride with the title ketone in the presence of pyridine in boiling benzene for 1 h (70 %) [1212].

m.p. 111° [1212].

3-Methyl-1-(2,4,6-trihydroxy-3,5-dimethylphenyl)-1-butanone
(Kunzeaphlogin D aglycone)

$C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses
-Obtained by reductive alkaline cleavage of kosotoxin (**II**) and protokosin (**III**) from female flowers of *Hagenia abyssinica* (Bruce) Gmelin [1916] (**XIXb**).

-Also obtained by reaction of isovaleric acid with 2,4-dimethylphloroglucinol in the presence of boron trifluoride in carbon tetrachloride during 3 h on the steam bath (51 %) [440].
-Also obtained from *Kunzeaphlogin* D, isolated from the leaves of *Kunzea ambigua* (SM) Bruce (Myrtaceae) [1612].
-Also refer to: [1838].

brown oil [1612]; ^{1}H NMR [1612, 1838].

BIOLOGICAL ACTIVITY: Refer to: [1838].

Trimethyl ether [3567-96-2] $C_{16}H_{24}O_4$ mol. wt. 280.36
(Torquatone)

Synthesis
-Obtained by treatment of triphenol above with excess dimethyl sulfate in the presence of potassium carbonate in acetone solution [440].

Isolation from natural sources

-From volatile leaf oils of,
**Eucalyptus incrassata* Labill. [367] (1.56 %), [1106];
**Eucalyptus angulosa* Schau [367] (1.37 %), [1106];
**Eucalyptus ceratocorys* (Blakely) L. A. S. Johnson & K. D. Hill [367, 1106];
**Eucalyptus erythrandra* Blakely & Steedm. [367, 1106];

**Eucalyptus flocktoniae* Maiden [440, 1106];
**Eucalyptus tetraptera* Turcz. [367, 1106];
**Eucalyptus stoatei* Gardner [367, 1106];
**Eucalyptus brachycalyx* Blakely [360]; Maiden [1106];
**Eucalyptus rugosa* R.Br. ex Blakely [360, 1106];
**Eucalyptus griffithsii* Maiden [360, 1106];
**Eucalyptus concinna* Maiden & Blakely [360, 1106];
**Eucalyptus corrugata* Luehm. [360, 1106];
**Eucalyptus torquata* Luehm. [360 (40.91 %), 439, 1106, 2037];
**Eucalyptus pimpiniana* Maiden [360, 1106];
**Eucalyptus caesia* Benth. [439, 1106];
**Eucalyptus calygona* Turcz. [461 (3.6 %), 1106];
**Eucalyptus celastroides* Turcz. ssp. *celastroides* [461 (4.2 %), 1106];
**Eucalyptus clelandii* (Maiden) Maiden [461 (7.2 %), 1106];
**Eucalyptus salubris* var. *glauca* Maiden [461 (10.2 %), 1106];
**Eucalyptus stricklandii* Maiden [461 (32.9 %), 1106];
**Eucalyptus woodwardii* Maiden [461 (6.2 %), 1106];
**Eucalyptus macrocarpa* subsp. *macrocarpa* Hopper [361 (6.68 %)];
**Eucalyptus carnabyi* Blakely & Steedm. ex. Blakely [361 (1.96 %)];
**Eucalyptus rhodantha* Blakely & Steedm. [361 (0.84 %)];
**Eucalyptus pachyphylla* F. Muell. [361 (0.98 %)];
**Eucalyptus oxymitra* Blakely [361 (0.75 %)];
**Eucalyptus spathulata* Hook ssp. *grandiflora* Benth [440, 1106];
**Eucalyptus chartaboma* (chemotype II) (3 %) and *Eucalyptus miniata* (1.6 %) (Myrtaceae) [1453];
**Eucalyptus torquata folage* [439, 1838];
**Eucalyptus* leaf essential oils in relation to taxonomy [924].
-From essential oil of *Eucalyptus apodophylla* (Myrtaceae) [2046].
-From genus *Angophora taxa* (Myrtaceae) [923],
*on volatile leaf oils of 8 south-western and southern Australian species of the genus *Eucalyptus* [357, 358, 365, 925].
-Also refer to: [362–364, 1107].

colourless crystalline solid [439]; cubes [1107];
m.p. 40–41° [439], 38–39° [440];
^{1}H NMR [1107, 1453, 2046], ^{13}C NMR [1107, 1453, 2046],
IR [439, 440, 461, 2046], UV [439], MS [361, 461, 1453, 2046];
X-ray crystal data [1107];
GC [357, 358, 361, 461, 925]; GC-MS [357, 358].

N.B.: The formula mentioned in the paper [439] (page 444), 3-methyl-1-(2,4,6-trimethoxy-3,5-dimethylphenyl)-**2**-butanone was erroneous.

BIOLOGICAL ACTIVITY: Antiherbivore Chemistry of Eucalyptus-Cues and Deterrents for Marsupial Folivores [2138]; Inhibition of drug metabolism enzymes [1154].

-Also refer to: [1838].

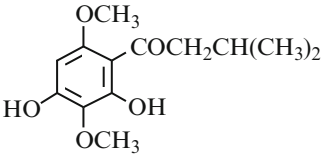
2,4-Dinitrophenylhydrazone of the trimethyl ether

[111979-31-8] $C_{22}H_{28}N_4O_7$ mol. wt. 460.49

m.p. 204–205° [440], 202° [439].

1-(2,4-Dihydroxy-3,6-dimethoxyphenyl)-3-methyl-1-butanone
(3,6-Dimethoxy-resisovalerophenone)

[106276-13-5] $C_{13}H_{18}O_5$ mol. wt. 254.28

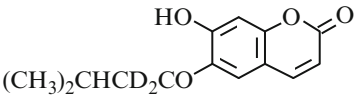


Synthesis
-Obtained by reaction of isovaleryl chloride with 2,5-dimethoxyresorcinol (**XI**) (88 %, m.p. 86–88°) in the presence of aluminium chloride in a carbon disulfide/nitrobenzene mixture [2610].

m.p. 93.5° [2610]; sublimation $_{0.1}$ 85° [2610].

7-Hydroxy-6-(2,2-dideuterio-3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one
(Dideuterogeijerin)

$C_{14}H_{12}D_2O_4$ mol. wt. 248.26



Synthesis
-Refer to: [1944].

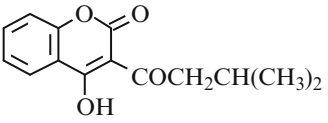
Methyl ether [38409-24-4] $C_{15}H_{14}D_2O_4$ mol. wt. 262.27

-Refer to: [1944].

MS [1944].

4-Hydroxy-3-(3-methyl 1-oxobutyl)-2*H*-1-benzopyran-2-one

[4139-75-7] $C_{14}H_{14}O_4$ mol. wt. 246.26



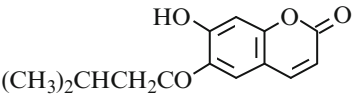
Syntheses
-Obtained by reaction of isovaleryl chloride with 4-hydroxycoumarin in pyridine containing one drop of piperidine for 3 h on a water bath (33 %) [3174].

-Also refer to: [525, 3144].

m.p. 75–76° [3174].

7-Hydroxy-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

[109966-52-1] $C_{14}H_{14}O_4$ mol. wt. 246.26



Syntheses

-Obtained by Fries rearrangement of 7-iso-valeroxycoumarin with aluminium chloride in nitrobenzene first at 120–130° overnight. The next day, the mixture was heated at 160–170° for 1 h [2823].

-Also refer to: [886].

m.p. 168–170° and 146–148° (dimorphic forms) [2823].

Methyl ether [450-16-8] $C_{15}H_{16}O_4$ mol. wt. 260.29
(Geijerin)

-Obtained by dehydrogenation of 3,4-dihydro-7-methoxy-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one in the presence of Pd/C in refluxing a diphenyl oxide/1-dodecene (5 equiv.) mixture (66 %) [529].
-Also obtained by cyclization of methyl 3-[2-hydroxy-4-methoxy-5-(3-methyl-1-oxobutyl)-phenyl]propanoate in the presence of Pd/C in refluxing diphenyl oxide (66 %) [529].
-Also obtained by treatment of 6-isovaleryl-7-hydroxycoumarin with methyl iodide in the presence of potassium carbonate in refluxing acetone for 6 h (89.9 %) [2823].
-Also refer to: [530, 886, 1814, 1944].

Isolation from natural sources

-From the bark of *Geijera salicifolia* Schott (Rutaceae) [529, (0.6 %) 1814].

flat colourless prisms [1814]; colourless needles [2823];
m.p. 121–123° [2823], 121° [1814];
^{1}H NMR [529, 530], IR [530], UV [530], MS [530, 1944].

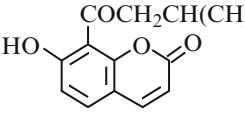
2,4-Dinitrophenylhydrazone of the methyl ether

[16850-97-8] $C_{21}H_{20}N_4O_7$ mol. wt. 440.41

m.p. 187° [2823], 181° [1814].

7-Hydroxy-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

[109966-03-2] $C_{14}H_{14}O_4$ mol. wt. 246.26



Synthesis

-Obtained by Fries rearrangement of 7-isovaleroxycoumarin with aluminium chloride in nitrobenzene for 1 h at 150° (18 %) [2823].

m.p. 103–105° [2823].

Methyl ether [109068-12-4] $C_{15}H_{16}O_4$ mol. wt. 260.29
(Isogeijerin)

-Obtained by treatment of 8-isovaleryl-7-hydroxycoumarin with methyl iodide in the presence of potassium carbonate in refluxing acetone for 6 h [2823].

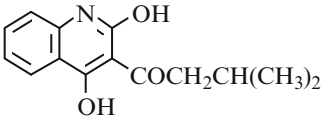
m.p. 94–96° [2823].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{21}H_{20}N_4O_7$ mol. wt. 440.41

m.p. 194–195° [2823].

1-(2,4-Dihydroxy-3-quinolinyl)-3-methyl-1-butanone

$C_{14}H_{15}NO_3$ mol. wt. 245.28



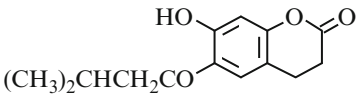
Synthesis
-Obtained by reaction of isovaleryl chloride with 2,4-dihydroxyquinoline in the presence of aluminium chloride in nitrobenzene on the steam bath for 3 h (26 %) [3123].

m.p. 195–198° [3123]; UV [3123].

BIOLOGICAL ACTIVITY: Antibacterial properties (Staphylococcus aureus and Escherichia coli) [3123].

3,4-Dihydro-7-hydroxy-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

$C_{14}H_{16}O_4$ mol. wt. 248.28



Synthesis
-Refer to: [529].

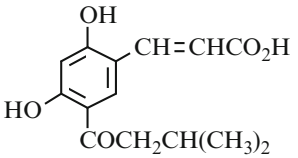
Methyl ether [117285-87-7] $C_{15}H_{18}O_4$ mol. wt. 262.31

-Obtained by cyclization of methyl 3-[2-hydroxy-4-methoxy-5-(3-methyl-1-oxobutyl)phenyl]-propanoate in refluxing diphenyl oxide (90 %) [529].
-Also refer to: [530, 1814].

m.p. 86.5–87.5° [530], 84° [1814];
^{1}H NMR [530], IR [530], UV [530], MS [530].

2,4-Dihydroxy-5-isovalerylcinnamic acid

$C_{14}H_{16}O_5$ mol. wt. 264.28



Synthesis
-Refer to: [2823].

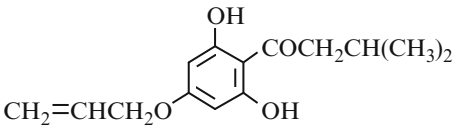
Dimethyl ether [101430-14-2]
$C_{16}H_{20}O_5$ mol. wt. 292.33
Methylgeijerinic acid

-Obtained by heating 6-isovaleryl-7-methoxycoumarin with dimethyl sulfate in aqueous alkali (20 per cent) on a steam bath for 4 h [2823].
-Also refer to: [1814].

colourless needles [2823]; m.p. 158° [1814], 157–158° [2823].

1-[2,6-Dihydroxy-4-(2-propen-1-yloxy)phenyl]-3-methyl-1-butanone

[918814-68-3] $C_{14}H_{18}O_4$ mol. wt. 250.29



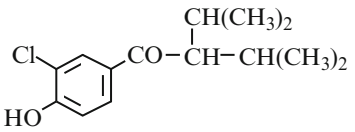
Synthesis
-Obtained by Friedel-Crafts acylation of phloroglucinol monoallyl ether with isopentanoyl chloride in the presence of titanium tetrachloride (20 %) [337].

light brown viscous oil [337];
^{1}H NMR [337], IR [337], MS [337].

BIOLOGICAL ACTIVITY: Antiprotozoal and antimicrobial [337].

1-(3-Chloro-4-hydroxyphenyl)-3-methyl-2-(1-methylethyl)-1-butanone

$C_{14}H_{19}ClO_2$ mol. wt. 254.76

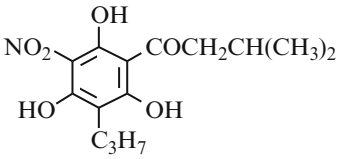


Synthesis
-To diisopropylacetyl chloride, 2-chloroanisole and carbon disulfide was added in small portions at 25°, aluminium chloride; the mixture stirred 1 h at r.t. and 45 min at 55°; pentane and aluminium chloride added, heated 3 h at 80° [2056].

m.p. 123–124.5° [2056].

3-Methyl-1-(2,4,6-trihydroxy-3-nitro-5-propylphenyl)-1-butanone

[119692-00-1] $C_{14}H_{19}NO_6$ mol. wt. 297.31



Synthesis

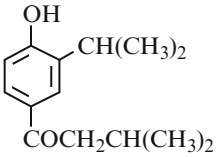
-Obtained by adding a mixture of fuming nitric acid and acetic acid to the solution of 3-methyl-1-(2,4,6-tri-hydroxy-3-propylphenyl)-1-butanone in acetic acid at 60° for 30 min (30–40 %) [3414].

m.p. 53–55° [3414]; ^{1}H NMR [3414], IR [3414], MS [3414].

BIOLOGICAL ACTIVITY: Germination inhibition [3414]; PET inhibition [3414].

1-[4-Hydroxy-3-(1-methylethyl)phenyl]-3-methyl-1-butanone

[95185-73-2] $C_{14}H_{20}O_2$ mol. wt. 220.31

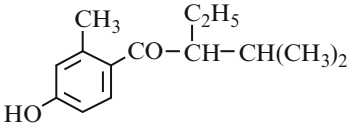


Synthesis

-Obtained by Fries rearrangement of 2-isopropylphenyl isovalerate with aluminium chloride in nitrobenzene, first 2 h at 30°, then at r.t. for 24 h [2704].

1-(4-Hydroxy-2-methylphenyl)-2-ethyl-3-methyl-1-butanone

$C_{14}H_{20}O_2$ mol. wt. 220.31



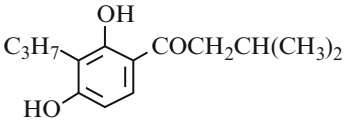
Synthesis

-Refer to: [2057].

m.p. 123–124.5° [2057].

1-(2,4-Dihydroxy-3-propylphenyl)-3-methyl-1-butanone

[664376-79-8] $C_{14}H_{20}O_3$ mol. wt. 236.31



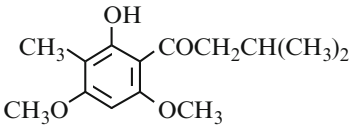
Syntheses

-Obtained by reaction of isovaleroyl chloride with 2-propylresorcinol in the presence of aluminium chloride in methylene chloride first at 0°, then at r.t. for 16 h [2486].

-Also refer to: [773].

1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-3-methyl-1-butanone
(Homobaeckeol, Pallidusol)

[60831-55-2] $C_{14}H_{20}O_4$ mol. wt. 252.31



Synthesis
-Obtained by treatment of 2,4,6-trimethoxytoluene with isovaleric acid and boron trifluoride, after hydrolysis of 1-oxa-3-oxonia-2-boratanaphthalene, which on hydrolysis gave homobaeckeol (61 %) [2743].

Isolation from natural sources
-From the leaves of *Mallotus palliduss* (Euphorbiaceae) [2988].

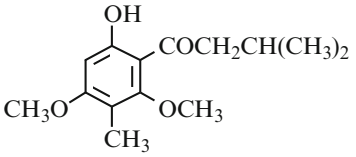
pale yellow [2743]; m.p. 109° [2743], 101–102° [2988];
^{1}H NMR [2743, 2988], ^{13}C NMR [2988], IR [2988],
UV [2743, 2988], MS [2988].

Na salt $C_{14}H_{19}O_4Na$ mol. wt. 274.29

-Refer to: [2988].

1-(6-Hydroxy-2,4-dimethoxy-3-methylphenyl)-3-methyl-1-butanone
(Homoisobaeckeol)

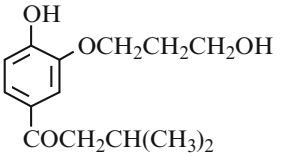
[126211-12-9] $C_{14}H_{20}O_4$ mol. wt. 252.31



Isolation from natural sources
-From the essential oil of *Thryptomene saxicola* (Myrtaceae) [803].
-From *Eucalyptus* species (Myrtaceae) [1106].

1-[3-(3-Hydroxypropoxy)-4-hydroxyphenyl]-3-methyl-1-butanone

$C_{14}H_{20}O_4$ mol. wt. 252.31



Synthesis
-Refer to: [2779].

4-methyl ether [919995-26-9]
$C_{15}H_{22}O_4$ mol. wt. 266.34
-Refer to: [2779].

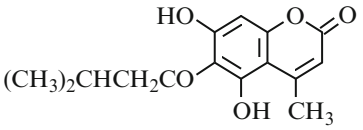
Dimethyl ether [919995-27-0] $C_{16}H_{24}O_4$ mol. wt. 280.36

-Refer to: [1085, 2206, 2779].

^{1}H NMR [1231, 2206], ^{13}C NMR [1231], IR [1231], MS [1085, 1231].

5,7-Dihydroxy-6-(3-methyl-1-oxobutyl)-4-methyl-2*H*-1-benzopyran-2-one

$C_{15}H_{16}O_5$ mol. wt. 276.29



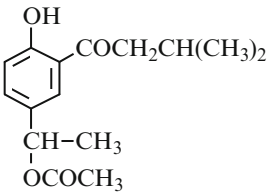
Syntheses
-Preparation from 2,4,6-trihydroxy isovalerophenone (54 %) [1884].
-Preparation [650] according to the method [1884].

canary-yellow solid [1884]; m.p. 272–274° [1884];
^{1}H NMR [1884], ^{13}C NMR [1884], IR [1884], MS [1884]; TLC [1884].

BIOLOGICAL ACTIVITY: Inhibition of growth (Escherichia coli, Staphylococcus aureus, Klebsiella pneumoniae, Pseudomonas aeruginosa, Salmonella typhimurium) [650].

1-[5-(Acetoxyethyl)-2-hydroxyphenyl]-3-methyl-1-butanone

$C_{15}H_{20}O_4$ mol. wt. 264.32



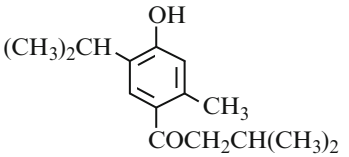
Synthesis
-Refer to: [2701].

Methyl ether [77311-66-1]
$C_{16}H_{22}O_4$ mol. wt. 278.35
-Obtained by treatment of 5-ethyl-2-methoxy-isovalerophenone with BTAP (benzyltriethyl-ammonium permanganate) in acetic acid at 30° for 2 days (8.6 %) [2701].

b.p.$_1$ 153–155° [2701]; ^{1}H NMR [2701], IR [2701].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-3-methyl-1-butanone

[80356-12-3] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Obtained by treatment of its methyl ether with boiling pyridinium chloride (205–215°) for 2 h (20 %) [2660].
-Also obtained by photo-Fries rearrangement of thymyl isovalerate in methanol for 6 h at 25° under nitrogen (28 %) (**2b**) [2421].

-Also obtained by Fries rearrangement of thymyl isovalerate with aluminium chloride in nitrobenzene for 12 h at 30° (92 %) [2647].
-Also refer to: [2648].

b.p.$_{13}$ 198° [2660], b.p.$_{13}$ 202° [2647];
m.p. 119° [2421], 108° [2647, 2648], 106° [2660];
^{1}H NMR [2421], IR [2421].

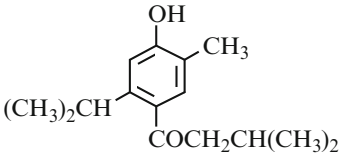
Methyl ether (VI) $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by reaction of isovaleryl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (71 %) [2660].

b.p.$_{16}$ 179–180° [2660]; $n_D^{20.5} = 1.523$ [2660].

1-[4-Hydroxy-5-methyl-2-(1-methylethyl)phenyl]-3-methyl-1-butanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses

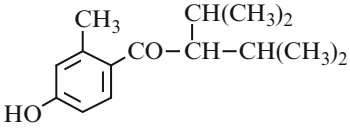
-Obtained by reaction of isovaleryl chloride with carvacrol in the presence of aluminium chloride in nitrobenzene at r.t. for 48 h (5 %) [1522].

-Also obtained by Fries rearrangement of carvacryl isovalerate with aluminium chloride in nitrobenzene for 12 h at 30° (88 %) [2647].

b.p.$_{13}$ 201° [2647]; m.p. 108° [2647], 86° [1522].

1-(4-Hydroxy-2-methylphenyl)-3-methyl-2-(1-methylethyl)-1-butanone

[5310-91-8] $C_{15}H_{22}O_2$ mol. wt. 234.34



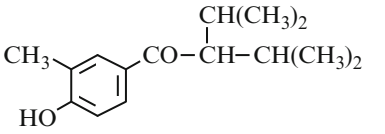
Synthesis

-Refer to: [2047].

m.p. 123–124.5° [2047].

1-(4-Hydroxy-3-methylphenyl)-3-methyl-2-(1-methylethyl)-1-butanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



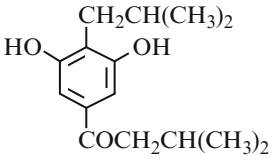
Synthesis

-Refer to: [2767].

m.p. 123–124.5° [2767].

1-[3,5-Dihydroxy-4-(2-methylpropyl)phenyl]-3-methyl-1-butanone

$C_{15}H_{22}O_3$ mol. wt. 250.34



Synthesis

-Refer to: [1407].

Dimethyl ether

$C_{17}H_{26}O_3$ mol. wt. 278.39

-Obtained by reaction of 3,4,5-trimethoxybenzonitrile with a greater excess of isobutylmagnesium bromide in refluxing toluene for 5 h (28 %) [1407].

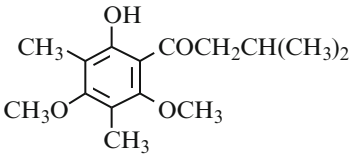
b.p.$_5$ 163–167° [1407].

Semicarbazone of the dimethyl ether $C_{18}H_{29}N_3O_3$ mol. wt. 335.45

m.p. 183–184° [1407].

1-(2-Hydroxy-4,6-dimethoxy-3,5-dimethylphenyl)-3-methyl-1-butanone
(Miniatone)

[808751-12-4] $C_{15}H_{22}O_4$ mol. wt. 266.34

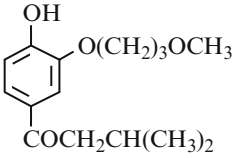


Isolation from natural sources
-Compound of leaf essential oils of *Eucalyptus chartaboma* (chemotype II) (4.6 %) and *Eucalyptus miniata* (3.2 %) (Myrtaceae) [1453].

^{1}H NMR [1453], ^{13}C NMR [1453], MS [1453].

1-[4-Hydroxy-3-(3-methoxypropoxy)phenyl]-3-methyl-1-butanone

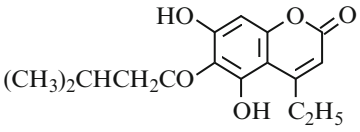
$C_{15}H_{22}O_4$ mol. wt. 266.34



Synthesis
-Refer to: [2206].

5,7-Dihydroxy-4-ethyl-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

$C_{16}H_{18}O_5$ mol. wt. 290.32



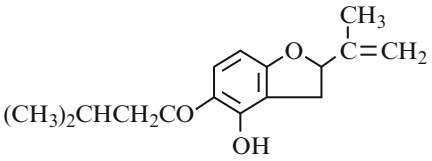
Syntheses
-Preparation from 2,4,6-trihydroxy-isovalerophenone (36 %) [1884].
-Preparation [650] according to the method [1884].

canary-yellow solid [1884]; m.p. 229–232° [1884];
^{1}H NMR [1884], ^{13}C NMR [1884], IR [1884], MS [1884]; TLC [1884].

BIOLOGICAL ACTIVITY: Inhibition of growth (Escherichia coli, Staphylococcus aureus, Klebsiella pneumoniae, Pseudomonas aeruginosa, Salmonella typhimurium) [650].

1-[2,3-Dihydro-4-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-3-methyl-1-butanone (−)

[596805-44-6] $C_{16}H_{20}O_3$ mol. wt. 260.33

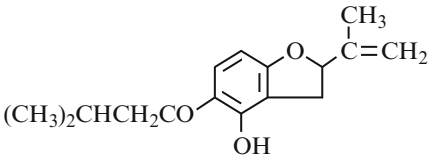


Synthesis
-Refer to: [1300].

BIOLOGICAL ACTIVITY: Antitumor [1300].

1-[2,3-Dihydro-4-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-3-methyl-1-butanone (+)

[596805-43-5] $C_{16}H_{20}O_3$ mol. wt. 260.33

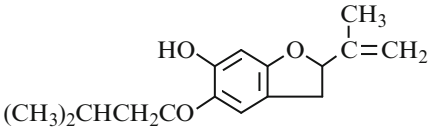


Synthesis
-Refer to: [1300].

BIOLOGICAL ACTIVITY: Antitumor [1300].

1-[(2*R*)-2,3-Dihydro-6-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-3-methyl-1-butanone

[596805-35-5] $C_{16}H_{20}O_3$ mol. wt. 260.33

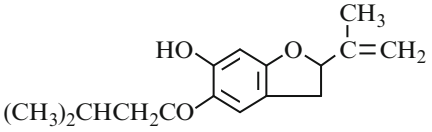


Synthesis
-Refer to: [1300].

BIOLOGICAL ACTIVITY: Antitumor [1300].

1-[(2*S*)-2,3-Dihydro-6-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-3-methyl-1-butanone

[596805-36-6] $C_{16}H_{20}O_3$ mol. wt. 260.33

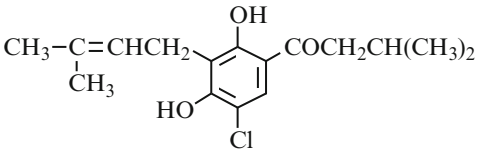


Synthesis
-Refer to: [1300].

BIOLOGICAL ACTIVITY: Antitumor [1300].

1-[5-Chloro-2,4-dihydroxy-3-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone

[216301-00-7] $C_{16}H_{21}ClO_3$ mol. wt. 296.79

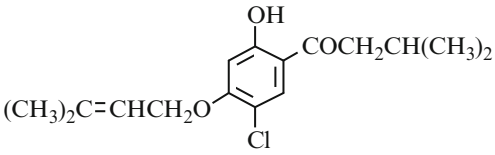


Synthesis
-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

1-[5-Chloro-2-hydroxy-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone

[216300-99-1] $C_{16}H_{21}ClO_3$ mol. wt. 296.79

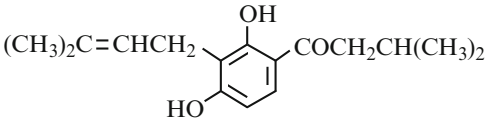


Synthesis
-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

1-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone

[198879-03-7] $C_{16}H_{22}O_3$ mol. wt. 262.35

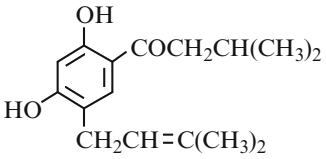


Syntheses
-Refer to: [1300, 2685].

BIOLOGICAL ACTIVITY: Antitumor [1300]; For the prevention and treatment of bone and cartilage diseases [2685].

1-[2,4-Dihydroxy-5-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone

[198879-04-8] $C_{16}H_{22}O_3$ mol. wt. 262.35



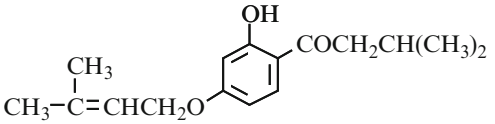
Syntheses
-Refer to: [1300, 2685].

BIOLOGICAL ACTIVITY: Antitumor [1300].

-For the prevention and treatment of bone and cartilage diseases [2685].

1-[2-Hydroxy-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone

[198879-02-6] $C_{16}H_{22}O_3$ mol. wt. 262.35

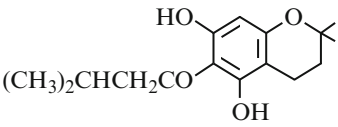


Synthesis
-Refer to: [2685].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2685].

1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-3-methyl-1-butanone

[20870-01-3] $C_{16}H_{22}O_4$ mol. wt. 278.35



Syntheses

-Obtained by treatment of 3-methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl) phenyl]-1-butanone with p-toluenesulfonic acid in refluxing benzene [2042].

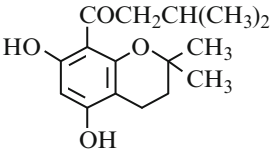
-Also obtained by reaction of isovaleronitrile with 5,7-dihydroxy-2,2-dimethylchroman (Hoesch reaction) [2481].

-Also refer to: [702, 1611].

Pale yellow needles [2042]; Almost colourless needles [2481];
m.p. 144–145° [2481], 142° [702, 2614], 141–142° [2042];
^{1}H NMR [2042], IR [2042], UV [702].

1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-3-methyl-1-butanone

[20869-99-2] $C_{16}H_{22}O_4$ mol. wt. 278.35



Syntheses

-Obtained by treatment of 3-methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone with p-toluenesulfonic acid in refluxing benzene (40 %) [2042].

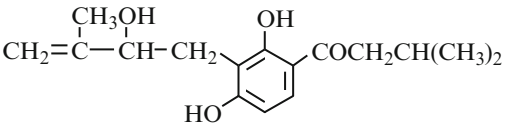
-Also obtained by reaction of isovaleronitrile with 5,7-dihydroxy-2,2-dimethylchroman (Hoesch reaction) (70 %) [2481].

-Also refer to: [702, 708, 1611].

pale yellow prisms [2042]; pale greenish-yellow plates [2481];
m.p. 138° [2481], 136° [702], 135–136° [2042],
^{1}H NMR [2042], IR [2042], UV [702].

1-[2,4-Dihydroxy-3-(2-hydroxy-3-methyl-3-butenyl)phenyl]-3-methyl-1-butanone

[596805-37-7] $C_{16}H_{22}O_4$ mol. wt. 278.35



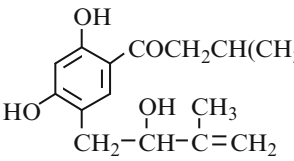
Synthesis

-Refer to: [1300].

BIOLOGICAL ACTIVITY: Antitumor [1300].

1-[2,4-Dihydroxy-5-(2-hydroxy-3-methyl-3-butenyl)phenyl]-3-methyl-1-butanone

[596805-39-9] $C_{16}H_{22}O_4$ mol. wt. 278.35

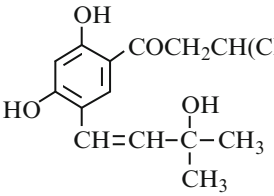


Synthesis
-Refer to: [1300].

BIOLOGICAL ACTIVITY: Antitumor [1300].

1-[2,4-Dihydroxy-5-(3-hydroxy-3-methyl-1-butenyl)phenyl]-3-methyl-1-butanone

[596805-40-2] $C_{16}H_{22}O_4$ mol. wt. 278.35

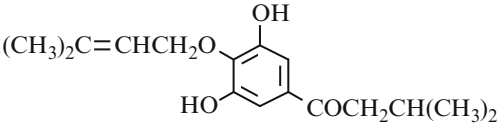


Synthesis
-Refer to: [1300].

BIOLOGICAL ACTIVITY: Antitumor [1300].

1-[3,5-Dihydroxy-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone

[216300-90-2] $C_{16}H_{22}O_4$ mol. wt. 278.35

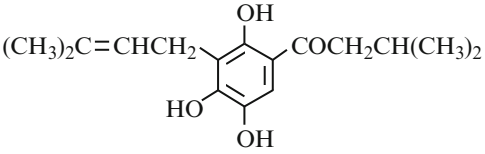


Synthesis
-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

3-Methyl-1-[2,4,5-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone

[198878-84-1] $C_{16}H_{22}O_4$ mol. wt. 278.35

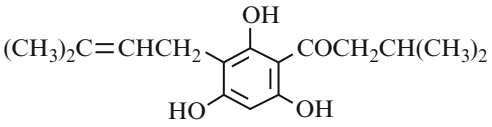


Syntheses
-Refer to: [2685, 2686].

BIOLOGICAL ACTIVITY: As bone resorption inhibitor for treatment of bone diseases [2686]; For the prevention and treatment of bone and cartilage diseases [2685].

3-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone

[54614-64-1] $C_{16}H_{22}O_4$ mol. wt. 278.35



Syntheses

-Obtained by reaction of prenyl bromide with phloroisovalerophenone,

*in the presence of sodium methoxide in an ethyl ether/methanol solution [1254], (9 %) [2616];

*in the presence of potassium hydroxide in water at 0° for 22 h under argon (13 %) [1066];

*in the presence of 10 % aqueous potassium hydroxide containing crushed ice (21 %) [2042].

-Also prepared by adding at 5° a solution of sodium methoxide in methanol, followed by isopentenyl bromide in ethyl ether to a solution of 3-methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone in benzene and ethyl ether; then the mixture was stirred at r.t. for 6 h (17 %) [2113].

-Also obtained from isoprenyl pyrophosphate and 6-isovaleryl-3,5-diketocapronyl-CoA [909].

-Also refer to: [542, 2609, 2614, 2685, 2686, 3481].

Isolation from natural sources

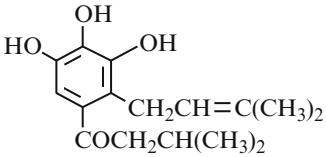
-From hop plant, *Humulos lupulus* (Cannabinaceae) [1066].

yellow crystals [1066]; pale yellow prisms [2042];
m.p. 140° [2113], 139–140° [2609], 138.5–140° [2616], 138.5–139.5° [1066], 138–139° [2042], 134–141° [541];
^{1}H NMR [541, 1066, 2042], IR [2042], UV [1066],
MS [1066]; TLC [1066]; HPLC [1066, 3481].

BIOLOGICAL ACTIVITY: Antifungal [2113]; As bone resorption inhibitor for treatment of bone diseases [2686]; For the prevention and treatment of bone and cartilage diseases [2685].

3-Methyl-1-[3,4,5-trihydroxy-2-(3-methyl-2-butenyl)phenyl]-1-butanone

[216300-91-3] $C_{16}H_{22}O_4$ mol. wt. 278.35



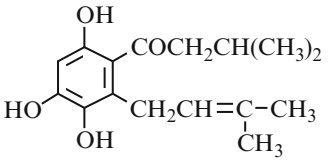
Synthesis

-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

3-Methyl-1-[3,4,6-trihydroxy-2-(3-methyl-2-butenyl)phenyl]-1-butanone

$C_{16}H_{22}O_4$ mol. wt. 278.35



Synthesis
-Refer to: [2685].

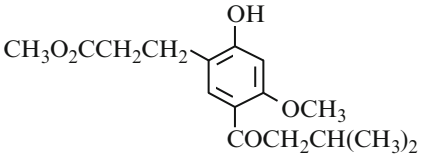
3-Mono(3-methyl-2-butenyl) ether
[198965-98-9]
$C_{21}H_{30}O_4$ mol. wt. 346.47

^{1}H NMR [2683].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2685].

Methyl 3-(2-hydroxy-5-isovaleroyl-4-methoxyphenyl)propanoate

[117285-75-3] $C_{16}H_{22}O_5$ mol. wt. 294.35



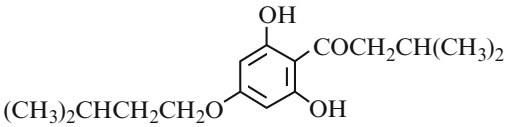
Syntheses
-Preparation by Fries rearrangement of methyl 3-(2-isovaleroyloxy-4-methoxyphenyl)-propanoate with aluminium chloride (5 equiv.) in nitromethane at r.t. (65 %) [529].

-Also refer to: [530].

m.p. 117–119° [530];
^{1}H NMR [530], IR [530], UV [530], MS [530].

1-[2,6-Dihydroxy-4-[(3-methylbutoxyl)]phenyl]-3-methyl-1-butanone

[918814-70-7] $C_{16}H_{24}O_4$ mol. wt. 280.36



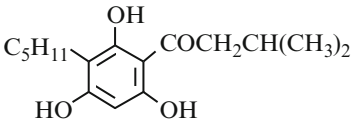
Synthesis
-Obtained by Friedel-Crafts acylation of phloroglucinol monoisopentyl ether with isopentanoyl chloride in the presence of titanium tetrachloride (35 %) [337].

off white solid [337]; m.p. 168–172° [337];
^{1}H NMR [337], IR [337], MS [337].

BIOLOGICAL ACTIVITY: Antiprotozoal and antimicrobial [337].

3-Methyl-1-(2,4,6-trihydroxy-3-pentylphenyl)-1-butanone

[74478-03-8] $C_{16}H_{24}O_4$ mol. wt. 280.36



Synthesis

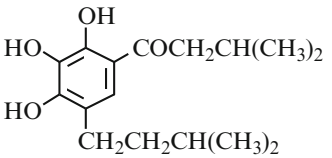
-Obtained by adding a solution of isopentanoyl chloride in nitrobenzene to a suspension, of 2,4,6-trihydroxy-pentylbenzene and aluminium chloride in carbon disulfide at r.t., then stirring the mixture for 6 h at 30–35° (54 %) [2113].

m.p. 155° [2113].

BIOLOGICAL ACTIVITY: Antifungal [2113].

1-[2,3,4-Trihydroxy-5-(3-methylbutyl)phenyl]-3-methyl-1-butanone

$C_{16}H_{24}O_4$ mol. wt. 280.36



Syntheses

-Obtained by reaction of isovaleric acid with 4-iso-amylpyrogallol in the presence of zinc chloride for 3 h at 130–140° [811].

-Also refer to: [1054].

$b.p._{.0.01}$ 148–160° [811]; m.p. 94° [811].

Tribenzoate $C_{37}H_{36}O_7$ mol. wt. 592.69

-Obtained treatment of the title ketone with benzoyl chloride in the presence of pyridine [811].

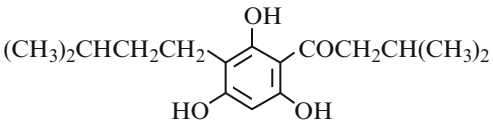
-Also refer to: [1054].

m.p. 170° [811].

3-Methyl-1-[2,4,6-trihydroxy-3-(3-methylbutyl)phenyl]-1-butanone

2′,4′,6′-Trihydroxy-3′-isopentylisovalerophenone (**XIII**)

[26104-01-8] $C_{16}H_{24}O_4$ mol. wt. 280.36



Syntheses

-Obtained by reaction of isovaleryl chloride with 2-isopentylphloroglucinol in the presence of aluminium chloride in nitrobenzene (52 %) (**II**) [2610], at 0° for 3 days (41 %) (**XIII**) [898].

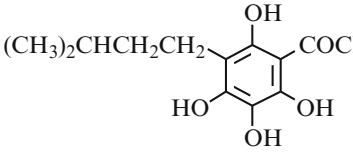
-Preparation by hydrogenation of 3-prenylphloroisovalerophenone (**XV**) with hydrogen in acetic acid in the presence of Pd (**XVI**) (81 %) [2616].
-Preparation by hydrogenation of 2,4,6-trihydroxy-3-(3-methyl-2-butenyl) isovalerophenone,
*in methanol over 5 % Pd/C (91 %) [542];
*in the presence of PtO_2 in methanol under a hydrogen atmosphere at r.t. for 1 h (86 %) [2113].
-Also obtained by hydrogenation of 3,5-dihydroxy-2-isovaleryl-6,6-bis(3-methyl-2-butenyl)-cyclohexa-2,4-dien-1-ol in methanol over 5 % Pd/C (42 %) [542].
-Also obtained by condensation of isobutyl cyanide with isoamylphloroglucinol (Hoesch reaction) (5 %) [811].

m.p. 173–175° [898], 172–174° [542], 171° [2113], 169–170° [2616], 167–169° [2610], 163–165° [541], 103° [811];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [541, 898], IR [898], UV [898].

BIOLOGICAL ACTIVITY: Antifungal [2113].

3-Methyl-1-[2,3,4,6-tetrahydroxy-5-(3-methylbutyl)phenyl]-1-butanone
*(Humulo-hydrochinon) (**IV**), (Humuloquinol)*

[107152-23-8] $C_{16}H_{24}O_5$ mol. wt. 296.36



Syntheses
-Obtained (**II**) by treatment of humuloquinone (**III**) with sulfur dioxide in 80 % ethanol for 90 min (92 %) [2610].

-Also obtained by hydrogenation of Humulon (II) in the presence of palladium chloride in methanol [1255, 2613, 3329].
-Also refer to: [3304–3306].

Isolation from natural sources

-Refer to: [1254, 2613, 3330].

b.p.$_{0.2}$ 135–140° [2610];
m.p. 128–130° [2610], 126–128° [1254, 1255],
123–125° [3329, 3330], 118° [2613, 3304, 3305]; UV [1255].

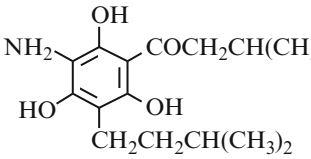
Tetrabenzoate [103567-06-2] $C_{44}H_{40}O_9$ mol. wt. 712.80

-Obtained by reaction of benzoyl chloride with humuloquinol in the presence of pyridine [1255].
-Also refer to: [2610, 3329, 3330].

m.p. 172–172.5° [2610], 168° [3329, 3330], 167° [1255]; UV [1255].

1-[3-Amino-2,4,6-trihydroxy-5-(3-methylbutyl)phenyl]-3-methyl-1-butanone
5-Amino-3-isoamyl-phlorisovalerophenone

$C_{16}H_{25}NO_4$ mol. wt. 295.38



Synthesis
-Refer to: [2610].

Hydrochloride
$C_{16}H_{25}NO_4$, HCl mol. wt. 331.84

-Obtained by treatment of 5-phenylazo-3-isoamylphloroisovalerophenone with stannous chloride dihydrate in the presence of concentrated hydrochloric acid in boiling acetic acid for 10 min (77 %) [2610].

m.p. 125–130° [2610].

Tetrabenzoate $C_{44}H_{41}NO_8$ mol. wt. 711.80

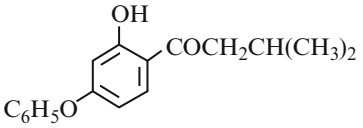
-Refer to: [2610].

Pentabenzoate $C_{51}H_{45}NO_9$ mol. wt. 815.90

-Refer to: [2610].

1-(2-Hydroxy-4-phenoxyphenyl)-3-methyl-1-butanone

[307000-33-5] $C_{17}H_{18}O_3$ mol. wt. 270.32



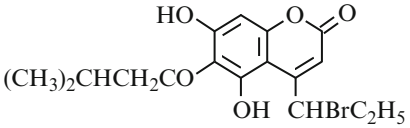
Syntheses
-Refer to: [1018–1022, 1345].

USE: Cosmetic compounds containing derivs of hydroxydiphenyl ether for inhibiting body odours [1018–1022].

BIOLOGICAL ACTIVITY: Antimicrobial [1345].

4-(1-Bromopropyl)-5,7-dihydroxy-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

[98498-59-0] **racemic** $C_{17}H_{19}BrO_5$ mol. wt. 383.24
[111249-67-3]



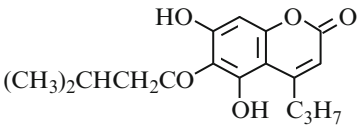
Syntheses
-Obtained by condensation of 2-(3-methylbutyryl)phloroglucinol with ethyl 4-bromo-3-oxohexanoate (small amount) [347].

-Obtained from a Pechmann reaction (low yield) [766].

yellow-brown solid [347]; m.p. 205–206° (d) [347];
^{1}H NMR [763], IR [763], UV [763], MS [763].

5,7-Dihydroxy-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

[98192-61-1] $C_{17}H_{20}O_5$ mol. wt. 304.34



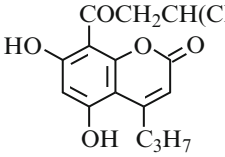
Syntheses
-Obtained by reaction of ethyl 3-oxohexanoate with 1-(2,4,6-trihydroxyphenyl)-3-methyl-1-butanone in the presence of concentrated sulfuric acid in acetic acid at r.t. for 2 days (35 %) [753].

-Also refer to: [762].

m.p. 228–229° [1005], 223–224° [753];
^{1}H NMR [753], IR [753], UV [753], MS [753].

5,7-Dihydroxy-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

[98192-67-7] $C_{17}H_{20}O_5$ mol. wt. 304.34

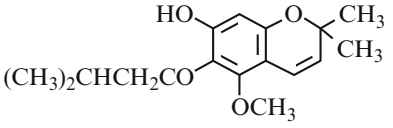


Syntheses
-Obtained by reaction of ethyl 3-oxohexanoate with 1-(2,4,6-trihydroxyphenyl)-3-methyl-1-butanone in the presence of concentrated sulfuric acid in acetic acid at r.t. for 2 days (4 %) [753].
-Also refer to: [553, 762].

m.p. 219° [753];
^{1}H NMR [753], IR [753], UV [553, 753], MS [753].

1-(7-Hydroxy-5-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-3-methyl-1-butanone
(Rhynchonin A)

[163734-37-0] $C_{17}H_{22}O_4$ mol. wt. 290.36

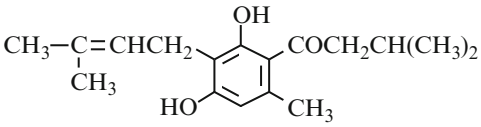


Synthesis
-Refer to: [493].
m.p. 34.5–36° [493];
^{1}H NMR [493], ^{13}C NMR [493], IR [493], UV [493].

BIOLOGIC ACTIVITY: Bioactive chromenes from *Rhyncholacis penicillata* [493].

1-[2,4-Dihydroxy-6-methyl-3-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone

[198878-99-8] $C_{17}H_{24}O_3$ mol. wt. 276.38

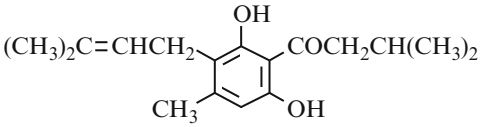


Synthesis
-Refer to: [2685].

BIOLOGICAL ACTIVITY: As preventive and therapeutic agent for bone and cartilage diseases [2685].

1-[2,6-Dihydroxy-4-methyl-3-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone

[216300-95-7] $C_{17}H_{24}O_3$ mol. wt. 276.38

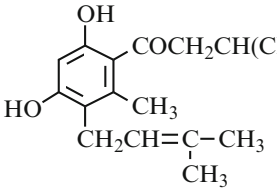


Synthesis
-Refer to: [2684].

BIOLOGICAL ACTIVITY: Prevention and treatment of bone and cartilage diseases [2684].

1-[4,6-Dihydroxy-2-methyl-3-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone

[198879-00-4] $C_{17}H_{24}O_3$ mol. wt. 276.38

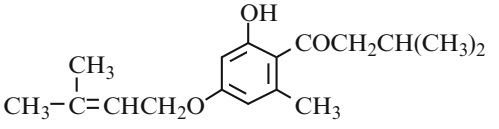


Synthesis
-Refer to: [2685].

BIOLOGICAL ACTIVITY: As preventive and therapeutic agent for bone and cartilage diseases [2685].

1-[2-Hydroxy-6-methyl-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone

[198878-98-7] $C_{17}H_{24}O_3$ mol. wt. 276.38

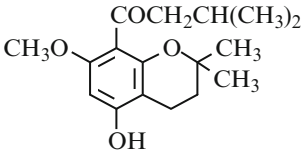


Synthesis
-Refer to: [2685].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2685].

1-(3,4-Dihydro-5-hydroxy-7-methoxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-3-methyl-1-butanone

$C_{17}H_{24}O_4$ mol. wt. 292.37



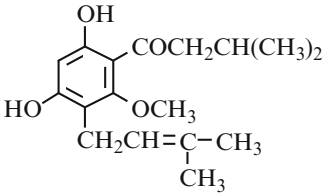
Synthesis

-Obtained by hydrogenation of 5-benzyloxy-7-methoxy-2,2-dimethyl-8-isovaleroylchroman in the presence of palladium chloride in acetic acid for 20 min at r.t. (81 %) [2481].

small needles [2481]; m.p. 142–143° [2481].

1-[4,6-Dihydroxy-2-methoxy-3-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone

[162071-07-0] $C_{17}H_{24}O_4$ mol. wt. 292.37



Synthesis

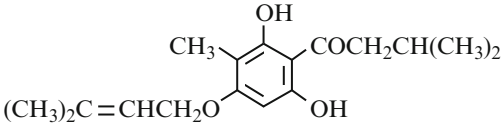
-Obtained by refluxing methyl 2,6-dihydroxy-3-isovaleryl-4-methoxy-5-(3-methyl-2-butenyl) benzoate with 5 % aqueous KOH for 4 h under nitrogen (75 %) [493].

m.p. 80–82° [493]; IR [493].

BIOLOGICAL ACTIVITY: Bioactive chromenes from *Rhyncholacis penicillata* [493].

1-[2,6-Dihydroxy-3-methyl-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone

[140400-68-6] $C_{17}H_{24}O_4$ mol. wt. 292.37



Isolation from natural sources

-From the aerial parts of *Hypericum calycinum* (Clusiacees, Guttuferes) [337, 836].

pale yellow needles [836]; m.p. 118–121° [836];
^{1}H NMR [836], ^{13}C NMR [836], IR [836], UV [836], MS [836]; TLC [836].

BIOLOGICAL ACTIVITY: Antiprotozoal and antimicrobial activities [337]; *In vitro* malarial activity [334, 337, 836]; Fungicide [337, 836].

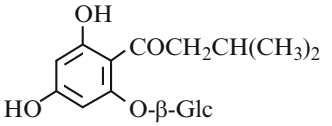
Diacetate [140400-69-7] $C_{21}H_{28}O_6$ mol. wt. 376.45

-Obtained by reaction of acetic anhydride with the title ketone in the presence of pyridine at r.t. for 25 h [836].

colourless oil [836];
^{1}H NMR [836], ^{13}C NMR [836], MS [836]; TLC [836].

1-[2-(β-D-Glucopyranosyloxy)-4,6-dihydroxyphenyl]-3-methyl-1-butanone
(Lysidiciside A, Lysidiside A)

[718608-83-4] $C_{17}H_{24}O_9$ mol. wt. 372.37



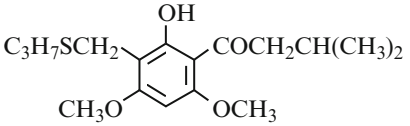
Isolation from natural sources
-From strawberry Fruit, *Fragaria ananassa* Duch. cv. Tochiotome [3154].
-From the whole plant of *Indigofera heterantha* (Leguminosae) [209].
-From the roots of *Lysidice rhodostega* Hance (Fabaceae) [1089, 1091].
-In hop extracts [3396].
-From *Lysidice brevicalyx* [2536].

colourless gummy solid [209]; light yellow amorphous powder [1089];
m.p. 112–115° [1089];
^{1}H NMR [209, 1089, 2536, 3154], ^{13}C NMR [209, 1089, 3154],
IR [209, 1089, 3154], UV [209, 1089, 2536, 3154],
MS [209, 1089, 2536, 3154]; HPLC [2536];
$(\alpha)_D^{26} = -55°$ (methanol) [3154]; $(\alpha)_D^{25} = -63.4°$ (acetone) [1089].

BIOLOGICAL ACTIVITY: Lipoxygenase enzyme inhibitor [209]; Cytochrome P 450 inhibitor [3154]; Vasodilator [1089].

1-[2-Hydroxy-4,6-dimethoxy-3-[(propylthio)methyl]phenyl]-3-methyl-1-butanone

[179630-66-1] $C_{17}H_{26}O_4S$ mol. wt. 326.46

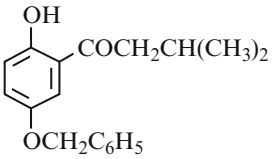


Synthesis
-Obtained in two steps: First, treatment of 2-hydroxy-4,6-dimethoxy-3-(1-oxo-3-methyl-butyl)benzaldehyde with $NaBH_3CN$ in methanol at r.t. for 3 h. Then, after evaporation, the residue was treated with propane-1-thiol in methylene chloride in the presence of zinc iodide for 16 h at r.t. (88 %) [643].

oil [643];
^{1}H NMR [643], ^{13}C NMR [643], IR [643], UV [643], MS [643].

1-[2-Hydroxy-5-(phenylmethoxy)phenyl]-3-methyl-1-butanone

$C_{18}H_{20}O_3$ mol. wt. 284.36

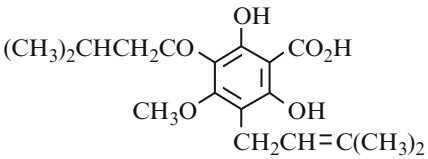


Synthesis
-Obtained from a mixture of 2,5-dihydroxyisovalerophenone, benzyl chloride and sodium ethoxide in refluxing ethanol for 8 h (58 %) [770].

yellow rhombs. [770]; b.p.$_2$ 160–170° [770]; m.p. 60° [770].

2,6-Dihydroxy-3-isovaleryl-4-methoxy-5-(3-methyl-2-butenyl)benzoic acid

$C_{18}H_{24}O_6$ mol. wt. 336.38



Synthesis
-Refer to: [493].

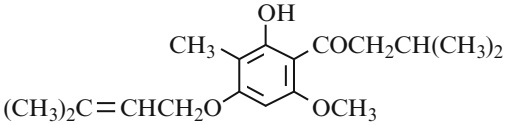
Methyl ester [162071-06-9]
$C_{19}H_{26}O_6$ mol. wt. 350.41

-Obtained by treatment of methyl 2,6-dihydroxy-3-isovaleryl-4-methoxybenzoate with 2-methyl-3-buten-2-ol in the presence of boron trifluoride etherate in dioxane at r.t. for 48 h (50 %) [493].

oil [493]; IR [493].

1-[2-Hydroxy-6-methoxy-3-methyl-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone

[140400-70-0] $C_{18}H_{26}O_4$ mol. wt. 306.40

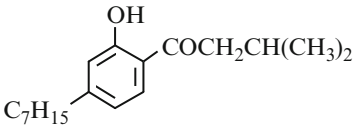


Synthesis
-Obtained by treatment of 1-[2,6-dihydroxy-3-methyl-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone with diazomethane in ethyl ether at r.t. for 30 h [836].

colourless crystals [836]; m.p. 63–67° [836];
^{1}H NMR [836], ^{13}C NMR [836], MS [836]; TLC [836].

1-(4-Heptyl-2-hydroxyphenyl)-3-methyl-1-butanone

[101873-66-9] $C_{18}H_{28}O_2$ mol. wt. 276.42



Syntheses

-Obtained by Fries rearrangement of 3-heptylphenyl isovalerate with aluminium chloride at 140° for 15 min (66 %) [855].

-Also obtained by Friedel-Crafts acylation of 3-heptylanisole with isovaleryl chloride in the presence of aluminium chloride in carbon disulfide between −5 and −10°, then boiling for 5 h after solvent elimination (76 %) [551].

b.p.$_{1.7}$ 173–174° [551], b.p.$_{0.8–0.9}$ 177° [551], b.p.$_{1.5}$ 183° [551];
$n_D^{20} = 1.5148$ [551].

p-Nitrophenylhydrazone [102812-21-5] $C_{24}H_{33}N_3O_3$ mol. wt. 411.54

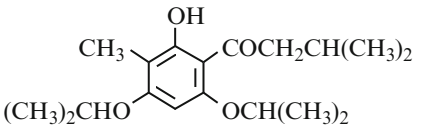
m.p. 130–131° [551].

2,4-Dinitrophenylhydrazone [102897-71-2] $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 112–113° [551].

1-[2-Hydroxy-3-methyl-4,6-bis(1-methylethoxy)phenyl]-3-methyl-1-butanone

[181227-34-9] $C_{18}H_{28}O_4$ mol. wt. 308.42



Syntheses

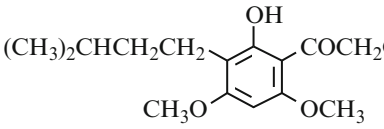
-Obtained by reaction of isovaleryl chloride with 2-methyl-3,5-diisopropoxyphenol in the presence of titanium tetrachloride [641] in methylene chloride at 0° C under argon.

The mixture was allowed to stand at r.t. for 30 min (84.6 %) [642].

yellow oil [642];
^{1}H NMR [642], ^{13}C NMR [642], IR [642], UV [642],
MS [642].

1-[2-Hydroxy-4,6-dimethoxy-3-(3-methylbutyl)phenyl]-3-methyl-1-butanone
3-Isoamyl-phlorisovalerophenon-4,6-dimethylether

[101874-06-0] $C_{18}H_{28}O_4$ mol. wt. 308.42



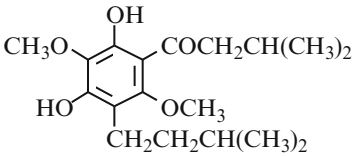
Syntheses
-Obtained by reaction of methyl iodide with 3-isoamylphloro-isovalerophenone in the presence of potassium carbonate in refluxing acetone for 6 h (27 %) [2610].

-Also refer to: [778].

yellow prisms [2610]; b.p.$_{0.2}$ 100° [2610]; m.p. 86° [2610].

1-[2,4-Dihydroxy-3,6-dimethoxy-5-(3-methylbutyl)phenyl]-3-methyl-1-butanone
(Humulo-hydrochinon-dimethyläther) (**XII**)

[101874-19-5] $C_{18}H_{28}O_5$ mol. wt. 324.42

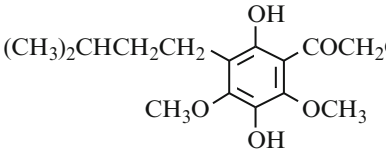


Synthesis
-Obtained by reaction of isovaleryl chloride with 2,5-dimethoxy-4-isoamylresorcinol in the presence of aluminium chloride in a carbon disulfide/nitrobenzene mixture (55 %) (**XII**) [2610].

yellow oil [2610]; b.p.$_{0.2}$ 120–140° [2610]; UV [2610].

1-[2,5-Dihydroxy-4,6-dimethoxy-3-(3-methylbutyl)phenyl]-3-methyl-1-butanone

$C_{18}H_{28}O_5$ mol. wt. 324.42

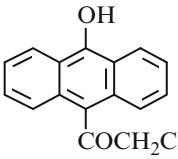


Syntheses
-Obtained (**XIII**) by reaction of diazomethane with natural humulo-hydroquinone (2,4,5,6-tetrahydr-oxy-3-isopentylisovalerophenone) in ethyl ether [1255, 2610].

b.p.$_{0.01}$ 100–115° [1255, 2610].

9-Hydroxy-10-isovalerylanthracene

$C_{19}H_{18}O_2$ mol. wt. 278.35

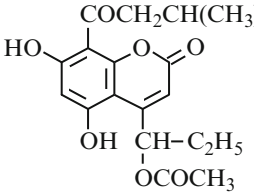


Synthesis

-Obtained by Fries rearrangement of 9-isovaleryloxyanthracene with various metal halides in benzene under reflux, but it is rapidly transformed into 10-isovalerylanthrone [3052].

4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

[98498-78-3] racemic $C_{19}H_{22}O_7$ mol. wt. 362.38



Syntheses

-Obtained by reaction of isovaleroyl chloride with 4-[1-(acetyloxy)propyl]-5,7-dihydroxy-2*H*-1-benzopyran-2-one in the presence of aluminium chloride in carbon disulfide/nitrobenzene for 4 days at 20° (33 %) [766].

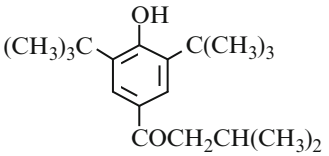
-Also refer to: [764].

m.p. 210–212° [764];

^{1}H NMR [764], IR [764], UV [764], MS [764].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-methyl-1-butanone

[14102-16-0] $C_{19}H_{30}O_2$ mol. wt. 290.45



Syntheses

-Preparation by reaction of isovaleryl chloride with 2,6-di-tert-butylphenol in the presence of,

*aluminium chloride at −10° for 1–13 min (88 %) [2506];

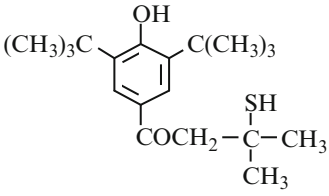
*titanium tetrachloride [1468].

-Also refer to: [951].

m.p. 110–113° [2506], 110–111° [951].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-mercapto-3-methyl-1-butanone

[174635-35-9] $C_{19}H_{30}O_2S$ mol. wt. 322.51



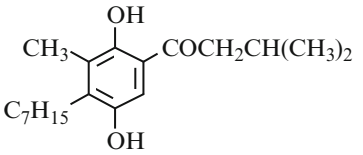
Synthesis

-Refer to: [2482].

BIOLOGICAL ACTIVITY: As antiinflammatory and analgesic agent [2482].

1-(2,5-Dihydroxy-4-heptyl-3-methylphenyl)-3-methyl-1-butanone
(Dihydroflavoglaucine)

$C_{19}H_{30}O_3$ mol. wt. 306.45



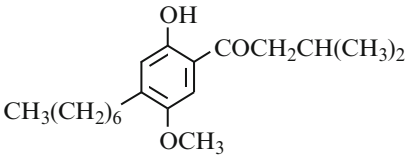
Syntheses
-Obtained by hydrogenation of flavoglaucine* [2882] in the presence of 10 % Pd/C in ethanol at r.t. [2540].
-Also obtained by hydrogenation of Auroglaucine* [2882].

***Flavoglaucine**: 1-(2,5-dihydroxy-4-heptyl-3-methylphenyl)-3-methyl-2-buten-1-one
***Auroglaucine**: 1-[2,5-dihydroxy-3-methyl-4-(1,3,5-heptanetriene)phenyl]-3-methyl-2-buten-1-one
-Also refer to: [2541].

UV [2882].

1-(4-Heptyl-2-hydroxy-5-methoxyphenyl)-3-methyl-1-butanone

[102020-42-8] $C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Obtained by reaction of isovaleryl chloride with heptylhydroquinone dimethyl ether in the presence of aluminium chloride in carbon disulfide for 2 h (39 %) [2391].

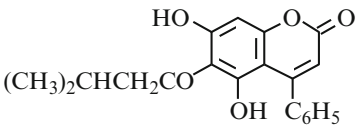
b.p.$_{0.5}$ 191–192° [2391], b.p.$_{3-4}$ 199–204° [2391].

2,4-Dinitrophenylhydrazone $C_{25}H_{34}N_4O_6$ mol. wt. 486.57

m.p. 134° [2391].

5,7-Dihydroxy-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one

[98192-57-5] $C_{20}H_{18}O_5$ mol. wt. 338.36



Syntheses
-Preparation as a mixture (36 %) from (3-methyl-butyryl)phloroglucinol and ethyl benzoylacetate [762] in acetic acid/concentrated sulfuric acid set aside or 5 days [754].
-Also obtained by reaction of benzoyl acetic ester with phloroisovalerophenone in acetic acid in the presence of concentrated sulfuric acid at r.t. for 3 days (31 %) [236].

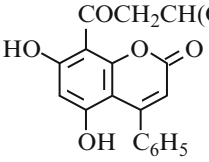
-Also obtained from *Ochrocarpin* B [1884].
-Also refer to: [650, 765, 1884 (12 %)].

yellow needles [762]; canary-yellow solid [1884];
long colourless needles [236];
m.p. 257–258° [762], 253–255° [1884], 244–245° [754], 242–244° [236];
^{1}H NMR [754, 762, 1884], ^{13}C NMR [1884],
IR [754, 762, 1884], UV [754, 762],
MS [754, 762, 1884]; TLC [236, 1884].

BIOLOGICAL ACTIVITY: Inhibition of growth (Escherichia coli, Staphylococcus aureus, Klebsiella pneumoniae, Pseudomonas aeruginosa, Salmonella typhimurium) [650]; Antioxidant [1884]; Cytotoxicity [1884].

5,7-Dihydroxy-8-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
(Isodispar B)

[98192-64-4] $C_{20}H_{18}O_5$ mol. wt. 338.36



Syntheses
-Preparation as a mixture (36 %) from (3-methylbutyryl)-phloroglucinol and ethyl benzoylacetate [762] in acetic acid/concentrated. sulfuric acid set aside for 5 days [754].
-Also refer to: [236, 278, 650, 765, 1178, 1906].

white crystals [762];
m.p. 200–202° [762], 196–197° [754];
^{1}H NMR [754, 762, 1178], ^{13}C NMR [1178], IR [754, 762, 1178],
UV [754, 762, 1178], MS [754, 762, 1178].

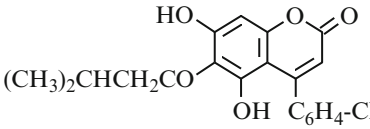
Isolation from natural sources

-From the leaves of *Marila pluricostata* [1906].
-From the fruits and the stem bark of *Calophyllum dispar* (Clusiaceae) [1178].

BIOLOGICAL ACTIVITY: Inhibition of growth (Escherichia coli, Staphylococcus aureus, Klebsiella pneumoniae, Pseudomonas aeruginosa, Salmonella typhimurium) [650]; Antiviral, anti HIV [278]; Antioxidant [1884]; Cytotoxicity [278, 1178, 1906].

5,7-Dihydroxy-6-(3-methyl-1-oxobutyl)-4-(4-methylphenyl)-2*H*-1-benzopyran-2-one

$C_{21}H_{20}O_5$ mol. wt. 352.39



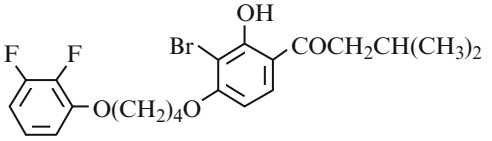
Syntheses
-Preparation from 2,4,6-trihydroxy-isovalerophenone (24 %) [1884].
-Preparation [650] according to the method [1884].

canary-yellow solid [1884]; m.p. 253–255° [1884];
^{1}H NMR [1884], ^{13}C NMR [1884], IR [1884], MS [1884]; TLC [1884].

BIOLOGICAL ACTIVITY: Inhibition of growth (Escherichia coli, Staphylococcus aureus, Klebsiella pneumoniae, Pseudomonas aeruginosa, Salmonella typhimurium) [650].

1-[3-Bromo-4-[4-(2,3-difluorophenoxy)butoxy]-2-hydroxyphenyl]-3-methyl-1-butanone

[811801-19-1] $C_{21}H_{23}BrF_2O_4$ mol. wt. 457.31

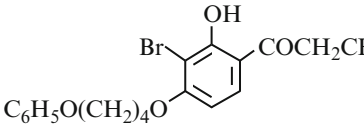


Synthesis
-Refer to: [2485].
^{1}H NMR [2485], MS [2485].

BIOLOGICAL ACTIVITY: Study of its activity as allosteric potentiator of metabotropic glutamate receptor 2 (mGlu2) [2485].

1-[3-Bromo-2-hydroxy-4-(4-phenoxybutoxy)phenyl]-3-methyl-1-butanone

[811801-17-9] $C_{21}H_{25}BrO_4$ mol. wt. 421.33

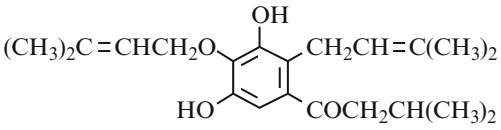


Synthesis
-Refer to: [2485].
^{1}H NMR [2485], MS [2485].

BIOLOGICAL ACTIVITY: Study of its activity as allosteric potentiator of metabotropic glutamate receptor 2 (mGlu2) [2485].

1-[3,5-Dihydroxy-2-(3-methyl-2-butenyl)-4-[(3-methyl-2-butenyl)oxy]phenyl]-3 methyl-1-butanone

[216300-89-9] $C_{21}H_{30}O_4$ mol. wt. 346.47

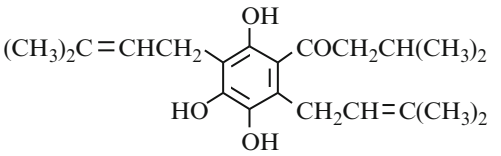


Synthesis
-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

3-Methyl-1-[2,4,5-trihydroxy-3,6-bis(3-methyl-2-butenyl)phenyl]-1-butanone

[198878-83-0] $C_{21}H_{30}O_4$ mol. wt. 346.47

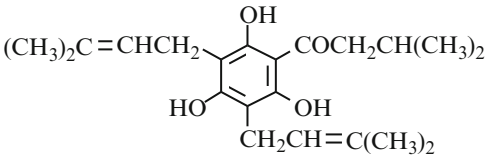


Synthesis
-Refer to: [2686].

BIOLOGICAL ACTIVITY: As bone resorption inhibitor for treatment of bone diseases [2686].

3-Methyl-1-[2,4,6-trihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-1-butanone
(3,5-Bis(Ÿ,Ÿ-dimethylallyl)phloroisovalerophenone)
(4-Desoxyhumulone) (Deoxycohumulone)

[4374-93-0] $C_{21}H_{30}O_4$ mol. wt. 346.47



Syntheses
-Obtained by reaction of prenyl bromide with phloroisovalerophenone in aqueous potassium hydroxide (13 %) [2609].

-Also obtained from phloroisovalerophenone which, in 2 N KOH and chlorobenzene containing Aliquat 336 as phase-transfer catalyst and the mixture adjusted to pH 12 with 2 N HCl, was prenylated with prenyl bromide at 0° for 4 h (54.8 %) [491].
-Also obtained by reaction of prenyl bromide with 2,6-disodium salt of phloroisovalerophenone in benzene suspension at 0° under nitrogen [2615].
-Also obtained by thermal rearrangement of 2-isovaleryl-4,4-bis(3-methylbut-2-enyl)-cyclohexane-1,3,5-trione in a sealed vial at 170° for 4 h (10 %) [703].
-Also obtained by treatment of phloroisovalerophenone in dioxan with 3-hydroxy-3-methylbutene and boron trifluoride etherate [705] at 20° for 8 h (24 %) [704].
-Also obtained by reaction of phloroisovalerophenone with 1-bromo-3-methyl-2-buten (3 mol) in the presence of the weakly basic resin DeAcidite H-IP (OH^- form) in boiling benzene (12.1 %) [708]. **N.B.**: The yield was similar at this obtained by using 2-methyl-3-buten-2-ol but the isolation was simpler [708].

-Also obtained by reaction of phloroisovalerophenone with 1-chloro-3-methyl-2-butene (2 molar parts), magnesium oxide (0.5 equiv.) and potassium iodide (1 %) [3309, 3310].
-Also refer to: [542, 907, 908, 1254, 1292, 2532, 2580, 2685, 2686, 3481].

Isolation from natural source

-From the hop (0.2–0.5 %) [2608] and the hop resins [164].

oil [703];
m.p. 86° [708], 82–84° [541, 704], 81–83° [2609], 81–82° [2608];
^{1}H NMR [541, 703], UV [703], MS [703];
HPLC [3481]; TLC [703].

BIOLOGICAL ACTIVITY: As bone resorption inhibitor for treatment of bone diseases [2686]; for the prevention and treatment of bone and cartilage diseases [2685].

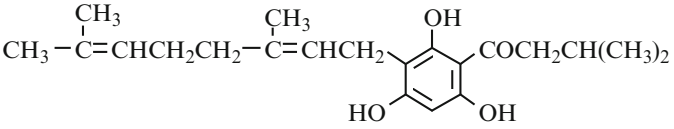
Tribenzoate [121426-03-7] $C_{42}H_{42}O_7$ mol. wt. 658.79

m.p. 138–139° [1401, 2609], 127° [702].

3-Methyl-1-[2,4,6-trihydroxy-3-(3,7-dimethyl-2,6-octanediene)phenyl]-1-butanone

3-Geranyl-1-(3-methylbutanoyl)phloroglucinol

[144785-80-8] $C_{21}H_{30}O_4$ mol. wt. 346.47



Isolation from natural sources

-From the aerial parts of *Hypericum jovis* [169].
-From the leaves of *Hypericum styphelloides* (Clusiaceae) [1083].
-From the leaves of *Esenbeckia nesiotica* Stand. (Rutaceae) [2625].
-From *Helichrysum species* (monticola and anomalym) [1488].
-From the aerial parts of *Helichrysum stenopterum* [1487].
-From the aerial parts of *Helichrysum platypterum* [1487].
-From the aerial parts of *Achyrocline alata* [406].
-From *Helichrysum infaustum* [401].
-Also refer to: [1782, 3269].

^{1}H NMR [2625, 3269], ^{13}C NMR [169, 2625, 3269],
IR [3269], MS [2625, 3269].

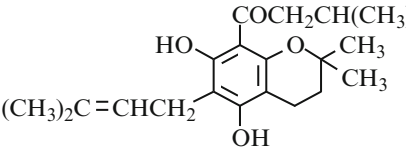
BIOLOGICAL ACTIVITY: Antioxidant (human skin fibroblasts) [169].

Triacetate [144785-84-2] $C_{27}H_{36}O_7$ mol. wt. 472.58

-Refer to: [2625]; ^{1}H NMR [2625].

3-Methyl-1-(3,4-dihydro-5,7-dihydroxy-2,2-dimethyl-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-8-yl)-1-butanone

[53771-36-1] $C_{21}H_{30}O_4$ mol. wt. 346.47



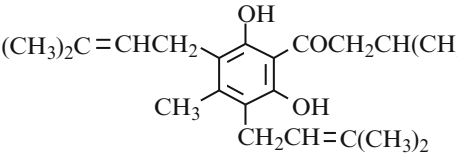
Synthesis

-Obtained by thermal rearrangement of 2-isovaleryl-4,4-bis(3-methylbut-2-enyl) cyclohexane-1,3,5-trione in a sealed vial at 170° for 4 h (16 %) [703].

oil [703]; ^{1}H NMR [703], UV [703], MS [703];
TLC [703]; GLC [703].

1-[2,6-Dihydroxy-4-methyl-3,5-bis(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone

[216300-96-8] $C_{21}H_{32}O_3$ mol. wt. 332.48



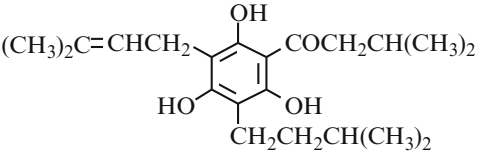
Synthesis

-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

3-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)-5-(3-methylbutyl)-phenyl]-1-butanone
(Prehumulone)

[93796-34-0] $C_{21}H_{32}O_4$ mol. wt. 348.48



Syntheses

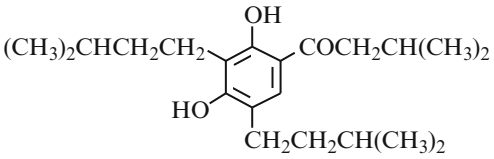
-Obtained by adding boron trifluoride etherate to a solution of 2,4,6-trihydroxy-3-isopentyl-isovalerophenone and 2-methyl-3-buten-2-ol in dioxane and stirring the mixture at 20° for 7 h (22 %) [542].

-Also obtained by reaction of 4-bromo-2-methyl-2-butene with phlor-4-methyl-pentanophenone in the presence of potassium hydroxide in dilute methanol first at 0°, then at r.t. for 25 h (4 %) [2624].

oil [542]; yellow oil [2624];
^{1}H NMR [542], UV [542], MS [542].

1-[2,4-Dihydroxy-3,5-bis(3-methylbutyl)phenyl]-3-methyl-1-butanone

[25915-31-5] $C_{21}H_{34}O_3$ mol. wt. 334.50



Syntheses

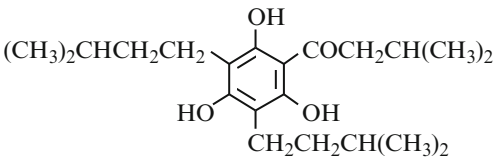
-Obtained by perhydrogenation of (−) tetrahydrohumulone in methanol in the presence of 5 % PtO2 (Adam's catalyst) and 2 % Pt as chloroplatinic acid (35–40 %) [828].

-Also refer to: [829].

white crystals [828]; m.p. 70–70.5° [828];
^{1}H NMR [828, 829], IR [828], UV [828].

3-Methyl-1-[2,4,6-trihydroxy-3,5-bis(3-methylbutyl)phenyl]-1-butanone
(4-Deoxytetrahydrohumulone), (3,5-diisoamyl-phloroisovalerophenone) (**III**)

[22748-59-0] $C_{21}H_{34}O_4$ mol. wt. 350.50



Syntheses

-Obtained by hydrogenation of Lupulon (m.p. 93–94°) [557],
*in the presence of palladium [811, 2615];

*in the presence of palladium chloride in methanol [557, 1254, 1255, 2613, 3330].
-Also refer to: [898, 1181, 2685, 2686, 3304, 3306, 3330, 3339].

^{1}H NMR [898], UV [557, 898, 3330].

BIOLOGICAL ACTIVITY: As bone resorption inhibitor for treatment of bone diseases [2686]; For the prevention and treatment of bone and cartilage diseases [2685].

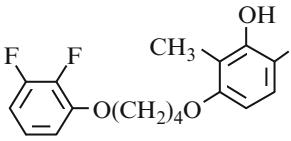
Tribenzoate [26104-08-5] $C_{42}H_{46}O_7$ mol. wt. 662.83

-Obtained by reaction of benzoyl chloride with the title ketone in the presence of pyridine for 3 days at r.t. under CO_2 atmosphere [813].
-Also refer to: [811, 898, 2609, 3330].

m.p. 167–168° [898], 165–166° [2609], 164–165° [3330], 164° [813], 163–164° [811]; UV [898].

1-[4-[4-(2,3-Difluorophenoxy)butoxy]-2-hydroxy-3-methylphenyl]-3-methyl-1-butanone

[811801-08-8] $C_{22}H_{26}F_2O_4$ mol. wt. 392.44

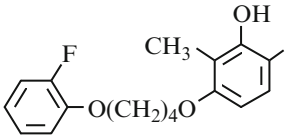


Synthesis
-Refer to: [2485].
^{1}H NMR [2485], MS [2485].

BIOLOGICAL ACTIVITY: Study of its activity as allosteric potentiator of metabotropic glutamate receptor 2 (mGlu2) [2485].

1-[4-[4-(2-Fluorophenoxy)butoxy]-2-hydroxy-3-methylphenyl]-3-methyl-1-butanone

[811801-06-6] $C_{22}H_{27}FO_4$ mol. wt. 374.45

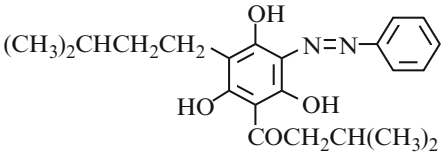


Synthesis
-Refer to: [2485].
^{1}H NMR [2485], MS [2485].

BIOLOGICAL ACTIVITY: Study of its activity as allosteric potentiator of metabotropic glutamate receptor 2 (mGlu2) [2485].

3-Methyl-1-(2,4,6-trihydroxy-3-isopentyl-5-phenylazophenyl)-1-butanone

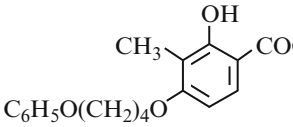
[115120-54-2] $C_{22}H_{28}N_2O_4$ mol. wt. 384.48



Synthesis
-Refer to: [2610].
m.p. 143° [2610].

1-[2-Hydroxy-3-methyl-4-(4-phenoxybutoxy)phenyl]-3-methyl-1-butanone

[811801-04-4] $C_{22}H_{28}O_4$ mol. wt. 356.46

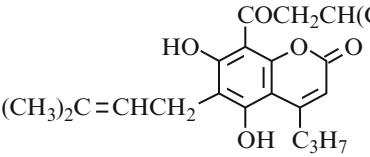


Synthesis
-Refer to: [2485].
^{1}H NMR [2485], MS [2485].

BIOLOGICAL ACTIVITY: Study of its activity as allosteric potentiator of metabotropic glutamate receptor 2 (mGlu2) [2485].

5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one
(Mammein) (Mammea B/BA)

[521-38-0] $C_{22}H_{28}O_5$ mol. wt. 372.46



Syntheses

-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of 10 % aqueous potassium hydroxide at 0° (30–45 %) [765], (23 %) [762].

Isolation from natural sources

-From kernels of the fruit of *Mammea americana* L. and *Mammea africana* (Guttiferae) [765, 1006].
-From only seed of *Mammea africana* (Guttiferae) [751].
-From the seed of *Mammea americana* L. (Guttiferae) [753, 758, 759, 886, 887, 1001, 1003, 1004, 1007].
-From the bark of *Mammea africana* G. Don (Guttiferae) [553, 1082].

needles [751, 753]; white needles [762]; transparent prisms [887];
m.p. 128.5–129.5° [887], 128–129° [762], 128° [751], 127° [753, 754, 1006];
^{1}H NMR [751, 753, 762], ^{13}C NMR [751], IR [751, 753, 762],
UV [751, 753, 762, 886, 887], MS [751, 753, 762]; GC-MS [1082].

USE: Insecticide [753, 758, 759, 765, 1001, 1003, 1004].

BIOLOGICAL ACTIVITY: Antitumor [1006].

Hydrochloride $C_{22}H_{28}O_5$, HCl mol. wt. 408.96

-Obtained by treatment of mammein in ethyl ether with hydrogen chloride for 1.5 h (70 %) [887].

m.p. 142–144° [887]; UV [887].

Diacetate [38789-16-1] $C_{26}H_{32}O_7$ mol. wt. 456.54

-Preparation by reaction of acetic anhydride with mammein in the presence of pyridine at r.t. overnight [887].
-Also refer to: [753, 756].

m.p. 118–120° [753, 756], 105–107.5° [887];
IR [753, 756, 887], UV [887].

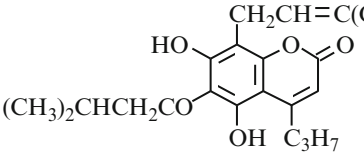
Dimethyl ether [119042-58-9] $C_{24}H_{32}O_5$ mol. wt. 400.52

-Preparation by treatment of mammein with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 1.5 h (74 %) [887].
-Also obtained by reaction of diazomethane in ethyl ether with mammein in acetone at 0°, then at r.t. for 24 h [887].

m.p. 103–103.5° [887]; UV [887].

5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one
(Isomammein, Mammea B/AA)

[478-67-1] $C_{22}H_{28}O_5$ mol. wt. 372.46



Syntheses
-Obtained by reaction of prenyl bromide with 5,7-dihydroxy-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one in the presence of 10 % aqueous potassium hydroxide at 0° (30–45 %) [765], (22 %) [762].
-Also obtained by treatment of 5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one (*mammein*) with methanolic potassium hydroxide at r.t. overnight, followed by acidification [886], (61 %) [887].
-Also obtained by saponification of mammein diacetate with 1 N methanolic potassium hydroxide overnight at r.t. [887].
-Also obtained by isomerization of 5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one (mammea B/BA) by treatment with methanolic 5 % potassium hydroxide at 20° overnight (80 %) [757].
-Also obtained by treatment of 5,7-dihydroxy-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one with 2-methyl-3-buten-2-ol in the presence of boron trifluoride-ether complex [757] in dioxane solution at r.t. for 24 h (2 %) [1081].

Isolation from natural sources

-From kernels of the fruit of *Mammea americana* L. [757, 1007] and *Mammea africana* (Guttiferae) [765].
-From only seed of *Mammea africana* (Guttiferae) (small amount) [751].
-From *Mammea africana* G. Don (Guttiferae) [1082].

yellow compound [886]; yellow needles [762];
m.p. 122.5–123° [1081], 119–121° [757], 119–120° [762, 887];
^{1}H NMR [751, 757, 762], IR [757, 762, 887],
UV [757, 762, 887], MS [751, 757, 762];
GC-MS [1082]; TLC [757].

USE: Insecticide [757, 765].

Diacetate $C_{26}H_{32}O_7$ mol. wt. 456.54

-Obtained by treatment of isomammein with acetic anhydride in the presence of pyridine at r.t. overnight [887].

colourless crystals [887]; m.p. 98–99° [887]; UV [887].

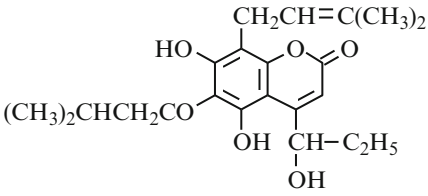
Dimethyl ether [114002-07-2] $C_{24}H_{32}O_5$ mol. wt. 400.52

-Preparation by reaction of dimethyl sulfate with isomammein in the presence of potassium hydroxide in refluxing acetone for 25.5 h (57 %) [887].

colourless oil [887]; IR [887], UV [887].

5,7-Dihydroxy-4-(1-hydroxypropyl)-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

[38534-76-8] $C_{22}H_{28}O_6$ mol. wt. 388.46



Syntheses

-The 4-[1-(acetyloxy)propyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one was isomerised and deacylated when treated with methanolic 5 % potassium hydroxide at 20° overnight [758].

-Also refer to: [756].

IR [756, 758], UV [756, 758], MS [756, 758].

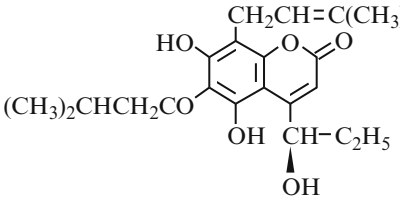
Triacetate [38534-63-3] $C_{28}H_{34}O_9$ mol. wt. 514.57

-Obtained by treatment of the titled compound with pyridine-acetic anhydride mixture [758].
-Also refer to: [756].

IR [756, 758], UV [756, 758], MS [758].

5,7-Dihydroxy-4-(1-hydroxypropyl)-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (1S)
(Kayeassamin G)

[1080509-35-8] $C_{22}H_{28}O_6$ mol. wt. 388.46



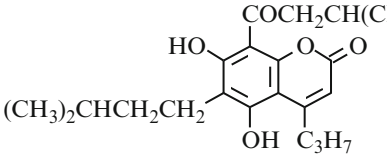
Isolation from natural sources
-From flowers of Kayea assamica [3315].
yellow [3315];
$(\alpha)_D^{23} = -33.23°$ (chloroform) [3315].

^{1}H NMR [3315], ^{13}C NMR [3315], IR [3315], UV [3315], MS [3315].

BIOLOGICAL ACTIVITY: Cytotoxicity [3315].

5,7-Dihydroxy-6-(3-methylbutyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one
(Dihydromammein)

[37975-69-2] $C_{22}H_{30}O_5$ mol. wt. 374.48



Syntheses
-Obtained by hydrogenation of 5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one (*mammein*) [886], (75 %) [887].

-Also refer to: [1005].

m.p. 133–134.5° [1005], 132–133° [887]; UV [886, 887].

Diacetate [120363-74-8] $C_{26}H_{34}O_7$ mol. wt. 458.55

-Obtained by hydrogenation of mammein diacetate in the presence of PtO_2 in methanol (90 %) [3014].
-Also obtained by acetylation of dihydromammein with acetic anhydride at r.t. (45 %) [1005].

m.p. 86–87° [887]; IR [887], UV [887].

Dimethyl ether [120363-73-7] $C_{24}H_{34}O_5$ mol. wt. 402.53

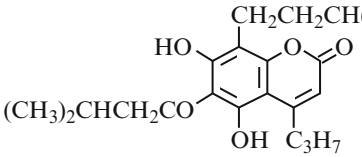
-Obtained by hydrogenation of mammein dimethyl ether in the presence of PtO_2 in methanol (76 %) [3014].
-Also obtained by methylation of dihydromammein with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 4 h (86 %) [887].

m.p. 89–90° [887]; UV [887].

5,7-Dihydroxy-8-(3-methylbutyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one

(Isodihydromammein) (Dihydroisomammein)

[123127-70-8] $C_{22}H_{30}O_5$ mol. wt. 374.48



Syntheses

-Obtained by hydrogenation of 5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one (*isomammein*) [886], (89 %) [887].

-Could also be obtained by isomerization of 5,7-dihydroxy-6-(3-methylbutyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one (dihydromammein) with potassium hydroxide in methanol at r.t. overnight [886], (81 %) [887].

m.p. 122–124° [887]; IR [887], UV [887].

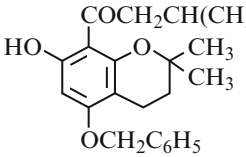
Dimethyl ether [120363-75-9] $C_{24}H_{34}O_5$ mol. wt. 402.53

-Preparation by reaction of dimethyl sulfate with dihydroisomammein in the presence of potassium carbonate in refluxing acetone [887].

m.p. 82–84° [887]; IR [887], UV [886, 887].

1-[3,4-Dihydro-7-hydroxy-5-(phenylmethoxy)-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-3-methyl-1-butanone

[854465-73-9] $C_{23}H_{28}O_4$ mol. wt. 368.47



Synthesis

-Obtained by reaction of benzyl bromide with 5,7-dihydroxy-2,2-dimethyl-8-isovaleroylchroman in the presence of potassium carbonate in boiling acetone for 2 h (53 %) [2481].

prisms or plates [2481]; m.p. 92–93° [2481].

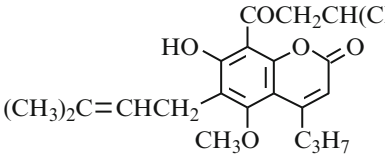
Methyl ether [854465-70-6] $C_{24}H_{30}O_4$ mol. wt. 382.50

-Preparation by reaction of 5-benzyloxy-7-hydroxy-2,2-dimethyl-8-isovaleroylchroman with methyl iodide in the presence of potassium carbonate in boiling acetone during 60 h (92 %) [2481].

rectangular prisms [2481]; m.p. 90–91° [2481].

7-Hydroxy-6-(3-methyl-2-butenyl)-5-methoxy-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one
(Mammein monomethyl ether)

$C_{23}H_{30}O_5$ mol. wt. 386.49

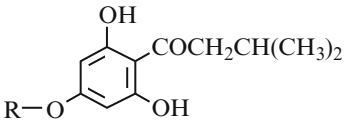


Synthesis
-Obtained by reaction of diazomethane in ethyl ether with mammein in acetone at 0°, then at r.t. for 24 h (37 %) [887].

pale yellow needles [887];
m.p. 80–82° [887]; IR [887], UV [887].

1-[4-[[6-O-(6-Deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-2,6-dihydroxy-phenyl]-3-methyl-1-butanone
(Lysidiside D)

[1000210-35-4] $C_{23}H_{34}O_{13}$ mol. wt. 518.52



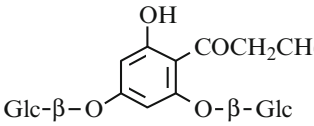
R = [6-O-(6-Deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]

Isolation from natural sources
-From the roots of *Lysidice rhodostegia* Hance (family Fabaceae).

yellow powder [1090];
m.p. 201–203° [1090]; ^{1}H NMR [1090], ^{13}C NMR [1090], IR [1090], UV [1090], MS [1090]; TLC [1090]; HPLC [1090];
$(\alpha)_D^{25} = -8.5°$ (acetone) [1090].

1-[2,4-Bis(β-D-glucopyranosyloxy)-6-hydroxyphenyl]-3-methyl-1-butanone
(Lysidiciside B) (Lysidiside B)

[718608-84-5] $C_{23}H_{34}O_{14}$ mol. wt. 534.51



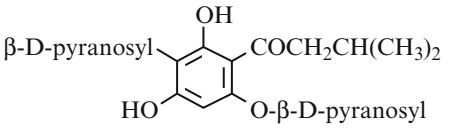
Isolation from natural sources
-From the roots of *Lysidice rhodostega* (Fabaceae) [1089, 1091].

Yellow amorphous powder [1089];
m.p. 142–144° [1089];
^{1}H NMR [1089], ^{13}C NMR [1089], IR [1089], UV [1089], MS [1089];
$(\alpha)_D^{25} = -86°$ (acetone) [1089].

BIOLOGICAL ACTIVITY: Vasodilator [1089].

1-[3-β-D-Glucopyranosyl-6-(β-D-glucopyranosyloxy)-2,4-dihydroxyphenyl]-3-methyl-1-butanone

[1000210-34-3] $C_{23}H_{34}O_{14}$ mol. wt. 534.51



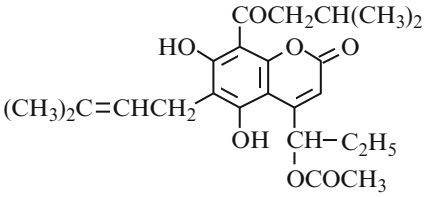
Isolation from natural sources
-From the roots of *Lysidice rhodostegia* Hance (family Fabaceae).
yellow powder [1090];

m.p. 157–150° [1090];
^{1}H NMR [1090], ^{13}C NMR [1090], IR [1090], UV [1090], MS [1090]; TLC [1090]; HPLC [1090];
$(\alpha)_D^{25} = -25.2°$ (acetone) [1090].

USE: Antioxidant [1090].

4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one
(Mammea E/BA)

[98498-81-8] racemic $C_{24}H_{30}O_7$ mol. wt. 430.50
[26477-64-5]
[111321-13-2]



Syntheses
-Obtained by reaction of prenyl bromide with 4-[1-(acetyloxy)propyl]-5,7-dihydroxy-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one in the presence of aqueous potassium hydroxide at 0° (40 %) [766].
-Also refer to: [373, 762].

Isolation from natural sources

-From *Mammea americana* [758, 766].
-From *Mammea africana* seeds [759].

m.p. 50–51° [758];
^{1}H NMR [758, 759], IR [758, 759], UV [758, 759], MS [758, 759].

BIOLOGICAL ACTIVITY: Insecticidal [758, 759, 766]; Toxicity [759].

Diacetate [38534-84-8] $C_{28}H_{34}O_9$ mol. wt. 514.57

-Obtained by treatment of the titled ketone with pyridine-acetic anhydride at 100° temperature overnight [758].

m.p. 20–22° [756, 758];
IR [756, 758], UV [758], MS [756, 758].

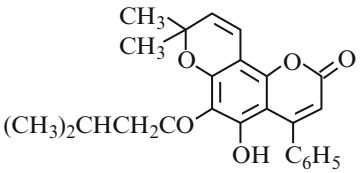
Dimethyl ether [26481-09-4] $C_{26}H_{34}O_7$ mol. wt. 458.55

-Refer to: [756, 758, 759].

m.p. 88–90° [756, 758, 759];
IR [756, 758], UV [756, 758], MS [756, 758].

5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*;8*H*-pyrano [2,3-f]chromen-2-one
(Mammea A/AA cyclo D) (Mammeigin)

[2289-11-4] $C_{25}H_{24}O_5$ mol. wt. 404.46

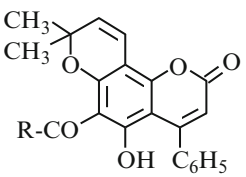


Isolation from natural sources
-From mamey seed oil of *Mammea americana* L (Guttiferae) [1003].
-From *flowers of Kayea assamica* [3315].
-From the fruit of *Kilmeyera pumila* Pohl [901].
-From Mammea americana L (Clusiaceae) [1004], seeds (Fruit and Spice Park) [3381].
-From the leaves of *Marila pluricostata* [1906].
-CO_2 extract of *Mesua ferrea* L. (Guttiferae) [236, 582, 3219].
-From Mammea harmandi (Pierre) Kosterm (Guttiferae), leaves and twigs [2589].
-From *Kielmeyera elata* [1156].
-From *Kielmeyera pumila* [2218].
-Also refer to: [553, 1006, 1081].

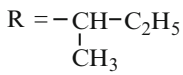
yellow crystalline substance [1003];
m.p. 150–151° [1081], 149–150° [582], 148–150° [2218], 146–147° [1006], 145–146° [553], 144–146° [236, 1003, 1004], 140–142° [2589];
^{1}H NMR [553, 1003, 1004, 2218, 3219],
^{13}C NMR [3219], IR [553, 1003, 1004, 2218],
UV [236, 553, 1003, 1004, 2218], MS [553, 2218].

BIOLOGICAL ACTIVITY: Antiviral [278]; Cytotoxicity [278, 1906, 2589, 3315, 3381].

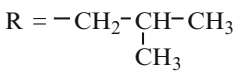
mixture (composition completely given)	Chemical Name	p. cent	
-mammea A/AB cyclo D	mammeigin	67 %	[3219]
-mammea A/AA cyclo D	mammea A/AA cyclo D	20 %	[3219]
-mammea A/AD cyclo D	mesuagin	13 %	[3219]



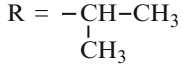
mammea A/AB cyclo D



mammea A/AA cyclo D



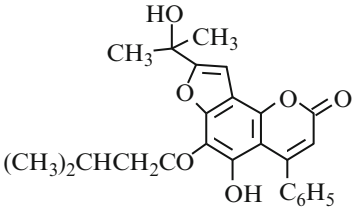
mammea A/AD cyclo D



BIOLOGICAL ACTIVITY: Antibacterial [3219]; Antiprotozoal [3219].

5-Hydroxy-8-(1-hydroxy-1-methylethyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2′,3′:5,6]benzo[1,2-b]pyran-2-one
(Ochrocarpin B)

$C_{25}H_{24}O_6$ mol. wt. 420.46

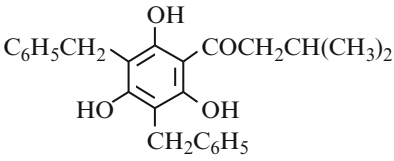


Isolation from natural sources
-From the bark of *Ochrocarpos punctatus* H. Perrier (Clusiaceae = Guttiferae) [616, 1884].
viscous liquid [616];
^{1}H NMR [616], ^{13}C NMR [616],
IR [616], UV [616];
$(\alpha)_D^{20} = 0.12°$ (chloroform) [616].

BIOLOGICAL ACTIVITY: Anticancer [1884]; Against ovarian cancer cells [616, 1884]; Cytotoxicity [616].

3-Methyl-1-[2,4,6-trihydroxy-3,5-bis(phenylmethyl)phenyl]-1-butanone

[198878-91-0] $C_{25}H_{26}O_4$ mol. wt. 390.48



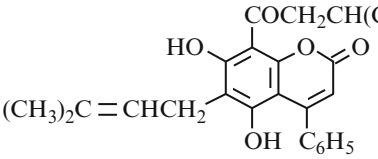
Syntheses
-Refer to: [2685, 2686].

BIOLOGICAL ACTIVITY: As bone resorption inhibitor for treatment of bone diseases [2686]; For the prevention and treatment of bone and cartilage diseases [2685].

^{1}H NMR [2683].

5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
(Mammea A/BA)

[5224-54-4] $C_{25}H_{26}O_5$ mol. wt. 406.48



Synthesis
-Obtained by reaction of 3-methyl-2-butenyl bromide with 5,7-dihydroxy-8-(3-methyl-butyryl)-4-phenylcoumarin in the presence of 10 % potassium hydroxide at 0° under nitrogen over 1.5 h (22 %) [762].

Isolation from natural sources

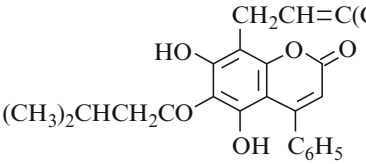
-From kernels of the fruit of *Mammea americana* L. [754, 758, 759, 1007] and *Mammea africana* (Guttiferae) [765].
-From the Bark of *Mammea africana* G. Don (Guttiferae) [553].

white needles [762]; colourless needles [754];
m.p. 125–126° [754], 123–125° [762], 122–124° [2591];
^{1}H NMR [754, 762, 2591, 3219], ^{13}C NMR [3219], IR [754, 762, 2591], UV [754, 762], MS [754, 762, 2591, 3219].

USE: Insecticide [758, 759, 765].

5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one
(Mammeisin) (Mammea A/AA)

[18483-64-2] $C_{25}H_{26}O_5$ mol. wt. 406.48



Syntheses
-Obtained by reaction of 3-methyl-2-butenyl bromide with 5,7-dihydroxy-6-(3-methyl-butyryl)-4-phenylcoumarin in the presence of 10 % potassium hydroxide at 0° under nitrogen over 1.5 h (20 %) [762].

-Also obtained by adding 2-methyl-3-buten-2-ol to a solution of 4-phenyl-5,7-dihydroxy-6-isovalerylcoumarin in dioxane and boron trifluoride etherate for 90 min at 50° [236].

Isolation from natural sources

-From kernels of the fruit of *Mammea americana* L. [754, 758, 759, 1004, 1007] and *Mammea africana* (Guttiferae) [765, 1006].
-From the peelings of the fruit of *Mammea americana* L. (Guttiferae) [1003].

-From both bark and seed of *Mammea africana* (Guttiferae) [751].
-From the Bark of *Mammea africana* G. Don (Guttiferae) [553].
-From *Mesua ferrea* (Guttiferae) [236].
-From the fruit peels (pericarpa of *Kayea assamica*) (Guttiferae) [428].

yellow needles [751, 754, 762]; yellow powdery solid [1007];
yellow substance [1001]; yellow crystalline solid [428];
m.p. 98–109° [1001, 1007], 98–102° [762], 98–100° [2547], 97° [428], 92–112° [236],
89–100° [751], 83–84° [754, 1007], 83° [553];
^{1}H NMR [428, 553, 751, 754, 762, 1004, 3219], ^{13}C NMR [751, 3219],
IR [236, 428, 553, 751, 754, 762, 1007],
UV [428, 553, 751, 754, 762, 1001, 1007, 2547], MS [428, 553, 751, 754, 762];
$(\alpha)_D^{31} = +22°$ (ethanol) [428].

USE: Insecticide [758, 759, 765, 1003, 1004].

BIOLOGICAL ACTIVITY: Antitumor [1006]; Toxicity [1007].

Diacetate [27127-44-2] $C_{29}H_{30}O_7$ mol. wt. 490.55

-Obtained by reaction of acetic anhydride with 5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one in the presence of pyridine (80 %) [1007].
-Also refer to: [278, 1028, 1906, 2547].

m.p. 122–124° [1001, 1007], 118–120° [2547], 86° [754];
^{1}H NMR [754, 1906], ^{13}C NMR [1906],
IR [754, 1007, 1906], UV [1007], MS [754].

BIOLOGICAL ACTIVITY: Antiviral, anti HIV [278]; Cytotoxicity [278, 1906].

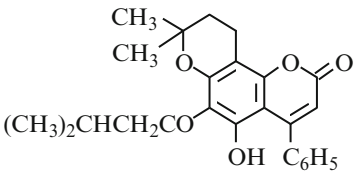
Dimethyl ether [103033-88-1] $C_{27}H_{30}O_5$ mol. wt. 434.53

-Obtained by reaction of dimethyl sulfate with 5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one in the presence of potassium carbonate in acetone (25 %) [1007].
-Also obtained by treatment of 5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one in ethyl ether with diazomethane [1007].
-Also refer to: [1001, 1177].

m.p. 87° [754], 86–89° [1001, 1007];
^{1}H NMR [754], IR [754, 1007], UV [754, 1007],
MS [754].

9,10-Dihydro-8,8-dimethyl-5-hydroxy-6-(3-methyl-1-oxobutyl)-4-phenyl-8*H*-pyrano-[2,3-*f*]chromen-2-one
(Dihydromammeigin)

[2289-30-7] $C_{25}H_{26}O_5$ mol. wt. 406.48



Syntheses
-Obtained by hydrogenation of mammeigin in the presence of Pd-C in ethanol-THF at r.t. and atmosphere pressure [1003].
-Also obtained by treatment of mammeisin in acetic acid containing a trace of H_2SO_4 [1003].

-Also refer to: [760, 1004, 2547].

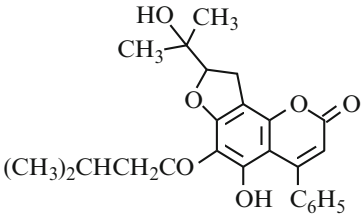
m.p. 164–165° [1003], 158–159° [2547];
IR [1004, 2547], UV [760, 1004, 2547].

Methyl ether $C_{26}H_{28}O_5$ mol. wt. 420.50

-Refer to: [2547]; m.p. 132° [2547].

8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2′,3′:5,6]benzo[1,2-b]pyran-2-one
(Mammea A/AA cyclo F) (Cyclomammeisin)

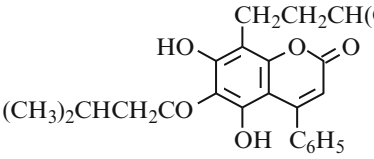
[30563-62-3] $C_{25}H_{26}O_6$ mol. wt. 422.48
[188817-92-7]
[111821-09-1] (racemic)



Isolation from natural sources
-From the fruit peels (pericarpa of *Kayea assamica*) (Guttiferae), compound **3** [428].
m.p. 131–132° [762], 115–117° [756], 105° [428];
^{1}H NMR [428, 756, 762],
IR [428, 756, 762], UV [428, 756], MS [428, 756, 762].

5,7-Dihydroxy-8-(3-methylbutyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one

[37972-55-7] $C_{25}H_{28}O_5$ mol. wt. 408.49



Syntheses

-Obtained by hydrogenation of 5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one in ethanol in the presence of 10 % Pd/C for 3 h at 28° [1001], (47 %) [1007].

yellow derivative [1001];
m.p. 99–103° [1001, 1007];
IR [1001, 1007], UV [1001, 1007].

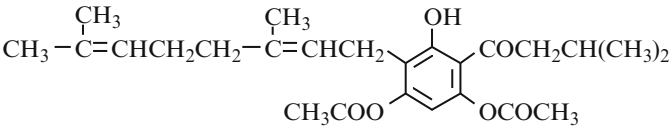
Diacetate [103209-93-4] $C_{29}H_{32}O_7$ mol. wt. 492.57

-Obtained by reaction of acetic anhydride with 5,7-dihydroxy-8-(3-methylbutyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one in the presence of pyridine (28 %) [1007].

m.p. 98–102° [1007]; IR [1007], UV [1007].

1-[4,6-(Diacetyloxy)-2-hydroxy-3-(3,7-dimethyl-2,6-octanediene)phenyl]-3-methyl-1-butanone

[144785-82-0] $C_{25}H_{34}O_6$ mol. wt. 430.54



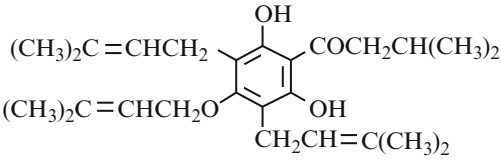
Isolation from natural sources

-Refer to: [2625].

^{1}H NMR [2625].

1-[2,6-Dihydroxy-3,5-bis(3-methyl-2-butenyl)-4-(3-methyl-2-butenyloxy) phenyl]-3-methyl-1-butanone
(Lupulone)

$C_{26}H_{38}O_4$ mol. wt. 414.58



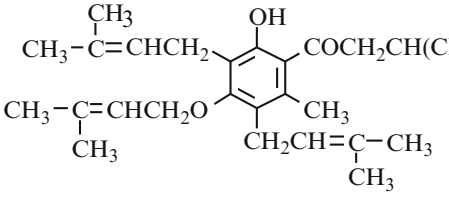
Syntheses

-Obtained by reaction of prenyl bromide with 2,6-dihydroxy 3-prenyl-4-prenyloxyisovalerophenone in the presence of sodium ethoxide [1254].

-Also obtained by treatment of isovalerylphloroglucinol with 3-methyl-1-chloro-2-butene in sodium methoxide-methanol (24.5 %) [3120].

1-[2-Hydroxy-6-methyl-3,5-bis(3-methyl-2-butenyl)]-4-[(3-methyl-2-butenyloxy)phenyl]-3-methyl-1-butanone

[198879-01-5] $C_{27}H_{40}O_3$ mol. wt. 412.61

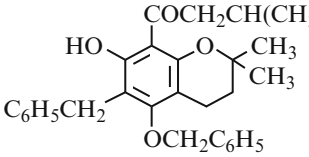


Synthesis
-Refer to: [2685].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2685].

1-[3,4-Dihydro-7-hydroxy-5-(phenylmethoxy)-6-(phenylmethyl)-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-3-methyl-1-butanone

$C_{30}H_{34}O_4$ mol. wt. 458.60

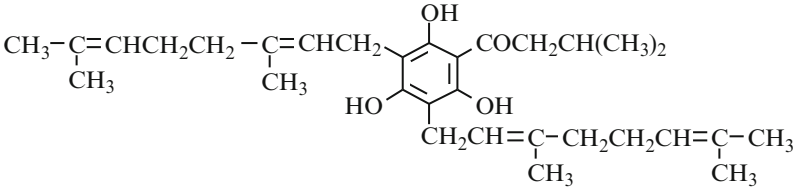


Synthesis
-Obtained by reaction of benzyl bromide with 5,7-dihydroxy-2,2-dimethyl-8-isovaleroylchroman in the presence of potassium carbonate in boiling acetone for 2 h [2481].

long, thin, pale greenish prisms [2481]; m.p. 117° [2481].

1-[3,5-Bis(3,7-dimethyl-2,6-octadienyl)-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

[198878-75-0] $C_{31}H_{46}O_4$ mol. wt. 482.70

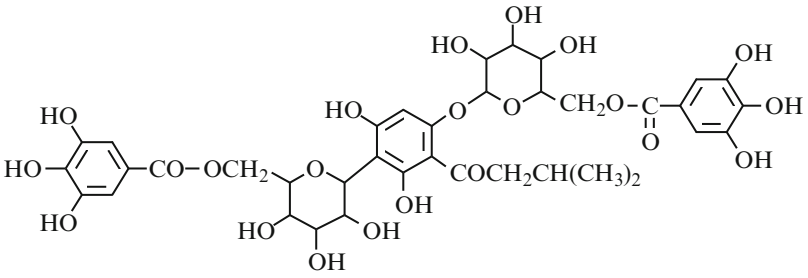


Syntheses
-Refer to: [2685, 2686].

BIOLOGICAL ACTIVITY: As bone resorption inhibitor for treatment of bone diseases [2686]; As preventive and therapeutic agent for bone and cartilage diseases [2685].

1-[2,4-Dihydroxy-3-[6-O-(3,4,5-trihydroxybenzoyl)-β-D-glucopyranosyl]-6-[[6-O-(3,4,5-trihydroxybenzoyl)-β-D-glucopyranosyl]oxy]phenyl]-3-methyl-1-butanone
(Kunzeaphlogin B)

[1109229-46-0] $C_{37}H_{42}O_{22}$ mol. wt. 838.73



Isolation from natural sources

-From the leaves of Kunzen ambigua (Myrtaceae) [1612].

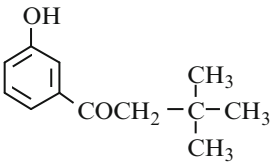
pale yellow amorphous powder [1612];
^{1}H NMR [1612], ^{13}C NMR [1612], UV [1612], MS [1612];
$(\alpha)_D^{23} = -45°$ (methanol) [1612].

2.4 From 3,3-Dimethyl-1-Butanoic Acid

2.4.1 Unsubstituted Hydroxyketones

1-(3-Hydroxyphenyl)-3,3-dimethyl-1-butanone

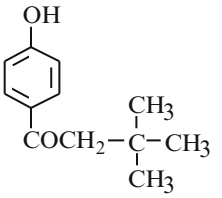
[940307-82-4] $C_{12}H_{16}O_2$ mol. wt. 192.26



Synthesis
-Refer to: [1465].

1-(4-Hydroxyphenyl)-3,3-dimethyl-1-butanone

[14392-74-6] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses
-Obtained by Fries rearrangement of phenyl 3,3-dimethylbutyrate in the presence of BF_3-H_2O in a closed pressure tube at 80° for 1 h (88 %) [2514].
-Also obtained by treatment of its methyl ether with pyridinium chloride at 190° [627].
-Also refer to: [414, 415].

m.p. 102–105° [414], 105° [415];
^{1}H NMR [2514], ^{13}C NMR [2514], MS [2514].

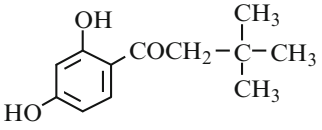
Methyl ether [85157-92-2] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of 3,3-dimethylbutanoic acid with anisole in the presence of PPA at 80° (76–100 %) [627].
-Also obtained by reaction of 3,3-dimethylbutanoyl chloride with anisole [549] in the presence of aluminium chloride in methylene chloride at 0° (76–100 %) [627].
-Also obtained from a mixture of palladium(II) chloride and 4-methoxy-β-tert-butylstyrene in aqueous N,N-dimethylformamide at 100° until completion shown by TLC [1096].
-Also refer to: [963, 1227, 1680].

b.p.$_1$ 130–132° [549];
^{1}H NMR [549, 1096, 1680], ^{13}C NMR [1680], MS [1227].

1-(2,4-Dihydroxyphenyl)-3,3-dimethyl-1-butanone

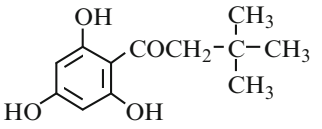
[1204737-56-3] $C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis
-Refer to: [1672].
^{1}H NMR [1672].

1-(2,4,6-Trihydroxyphenyl)-3,3-dimethyl-1-butanone

$C_{12}H_{16}O_4$ mol. wt. 224.26



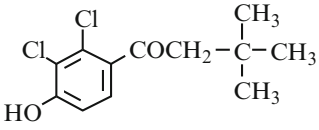
Synthesis
-Obtained by reaction of tert-butylacetyl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene at 60° (70 %) [1884].

yellow solid [1884];
^{1}H NMR [1884], ^{13}C NMR [1884], MS [1884].

2.4.2 Substituted Hydroxyketones

1-(2,3-Dichloro-4-hydroxyphenyl)-3,3-dimethyl-1-butanone

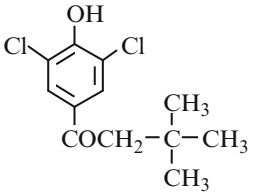
[55507-71-6] $C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15



Synthesis
-Refer to: [739].
m.p. 156.5–157.5° [739].

1-(3,5-Dichloro-4-hydroxyphenyl)-3,3-dimethyl-1-butanone

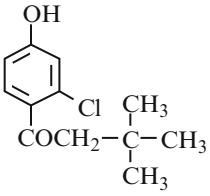
$C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15



Synthesis
-Obtained by treatment of 2,6-dichlorophenyl trimethylacetate, first in carbon disulfide, then at 135–145° for 2 h after carbon disulfide elimination (28 %) [3078].
m.p. 94–95.5° [3078].

1-(2-Chloro-4-hydroxyphenyl)-3,3-dimethyl-1-butanone

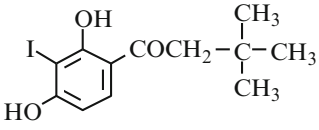
[1506-73-6] $C_{12}H_{15}ClO_2$ mol. wt. 226.70



Syntheses
-Refer to: [2047, 2048, 2057, 2766, 2767].
$b.p._{0.8}$ 128–165° [2767];
m.p. 97–98° [2047, 2048, 2057, 2766, 2767].

1-(2,4-Dihydroxy-3-iodophenyl)-3,3-dimethyl-1-butanone

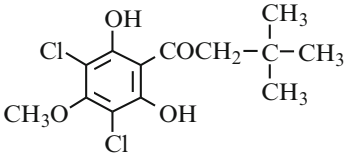
[1204737-68-7] $C_{12}H_{15}IO_3$ mol. wt. 334.15



Syntheses
-Refer to: [1672].
^{1}H NMR [1672].

1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-3,3-dimethyl-1-butanone
(DIF-1) (3M)

[861889-83-0] $C_{13}H_{16}Cl_2O_4$ mol. wt. 307.17



Syntheses

-Preparation by adding a solution of sulfuryl chloride (1.5 equiv.) in ethanol to a solution of 1-(2,6-dihydroxy-4-methoxyphenyl)-3,3-dimethyl-1-butanone in chloroform at r.t.; then, the solution was stirred for 1 h at r.t. [1129].

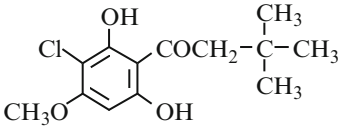
-Also refer to: [1772, 1773, 1777].

Yellow amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-3,3-dimethyl-1-butanone
(DIF-3) (3M)

[861889-91-0] $C_{13}H_{17}ClO_4$ mol. wt. 272.73



Syntheses

-Preparation by adding a solution of sulfuryl chloride (1.5 equiv.) in ethanol to a solution of 1-(2,6-dihydroxy-4-methoxyphenyl)-3,3-dimethyl-1-butanone in chloroform at r.t., then, the solution was stirred for 1 h at r.t. [1129].

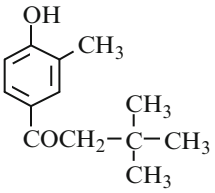
-Also refer to: [1772, 1777].

Yellow amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(4-Hydroxy-3-methylphenyl)-3,3-dimethyl-1-butanone

$C_{13}H_{18}O_2$ mol. wt. 206.28

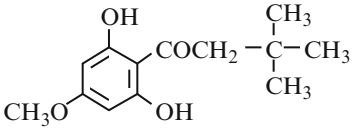


Synthesis
-Refer to: [218].
Methyl ether [927911-90-8]
$C_{14}H_{20}O_2$ mol. wt. 220.31
-Obtained by reaction of 3,3-dimethylbutanoic acid with 2-methylanisole in the presence of $HSiMe_2Cl$ and $InCl_3$ in 1,2-dichloroethane, first 1 h at r.t., then heated at 80° for 4 h (81 %) [218].

^{1}H NMR [218], ^{13}C NMR [218], IR [218], MS [218].

1-(2,6-Dihydroxy-4-methoxyphenyl)-3,3-dimethyl-1-butanone

[861889-78-3] $C_{13}H_{18}O_4$ mol. wt. 238.28

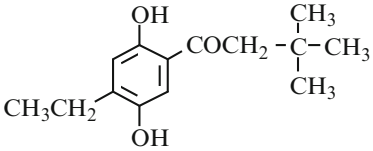


Synthesis
-Preparation by reaction of 3,3-dimethylbutyryl chloride with phloroglucinol monomethyl ether in the presence of aluminium chloride in methylene chloride at r.t. [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(4-Ethyl-2,5-dihydroxyphenyl)-3,3-dimethyl-1-butanone

$C_{14}H_{20}O_3$ mol. wt. 236.31

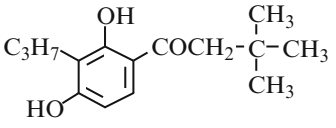


Synthesis
-Refer to: [2441].
Dimethyl ether [153756-53-7]
$C_{16}H_{24}O_3$ mol. wt. 264.37

Obtained by acylation of 2-ethyl-1,4-dimethoxybenzene with 3,3-dimethylbutanoic acid in the presence of trifluoroacetic anhydride [2441].

1-(2,4-Dihydroxy-3-propylphenyl)-3,3-dimethyl-1-butanone

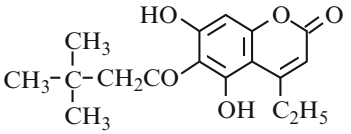
[194855-72-6] $C_{15}H_{22}O_3$ mol. wt. 250.34



Syntheses
-Refer to: [18, 20, 21, 23, 307, 1534].
^{1}H NMR [21].

5,7-Dihydroxy-4-ethyl-6-(3,3-dimethyl-1-oxobutyl)-2*H*-1-benzopyran-2-one

$C_{17}H_{20}O_5$ mol. wt. 304.34



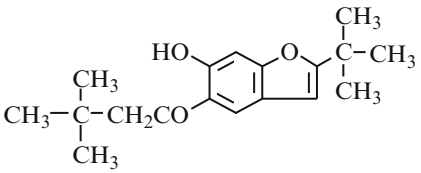
Syntheses
-Preparation from (3,3-dimethylbutyryl) phloroglucinol (39 %) [1884].
-Preparation [650] according to the method [1884].

canary-yellow solid [1884]; m.p. 231–234° [1884];
^{1}H NMR [1884], ^{13}C NMR [1884], IR [1884], MS [1884]; TLC [1884].

BIOLOGICAL ACTIVITY: Inhibition of growth (Escherichia coli, Staphylococcus aureus, Klebsiella pneumoniae, Pseudomonas aeruginosa, Salmonella typhimurium) [650].

1-[2-(1,1-Dimethylethyl)-6-hydroxy-5-benzofuranyl]-3,3-dimethyl-1-butanone

$C_{18}H_{24}O_3$ mol. wt. 288.39

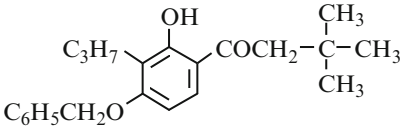


Synthesis
-Obtained by treatment of 2,4-bis(tert-butylethynyl)-1,5-diacetoxybenzene with NaOH (6 equiv.) in THF/MeOH/H_2O at 80° (31 %) [1875].

^{1}H NMR [1875], ^{13}C NMR [1875], IR [1875].

1-[2-Hydroxy-4-(phenylmethoxy)-3-propylphenyl]-3,3-dimethyl-1-butanone

[194855-33-9] $C_{22}H_{28}O_3$ mol. wt. 340.46



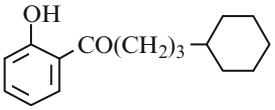
Syntheses
-Refer to: [18, 19].

2.5 *From 4-Cyclohexyl-1-Butanoic Acid*

2.5.1 Unsubstituted Hydroxyketones

4-Cyclohexyl-1-(2-hydroxyphenyl)-1-butanone

[25804-66-4] $C_{16}H_{22}O_2$ mol. wt. 246.35



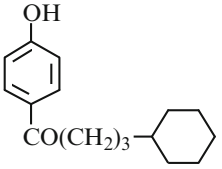
Synthesis
-Obtained by Fries rearrangement of phenyl cyclohexylbutyrate with aluminium chloride at 140° [3116].
b.p.$_{1.5}$ 158° [2513]. b.p.$_{.5}$ 220° [3116].

2,4-Dinitrophenylhydrazone [25804-67-5] $C_{22}H_{26}N_4O_5$ mol. wt. 426.47

m.p. 237° [2513], 125° [3116].

4-Cyclohexyl-1-(4-hydroxyphenyl)-1-butanone

[1760-65-2] $C_{16}H_{22}O_2$ mol. wt. 246.35



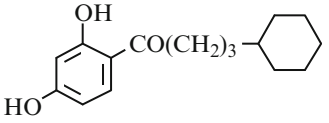
Synthesis
-Obtained by Fries rearrangement of phenyl cyclohexylbutyrate with aluminium chloride at 110° (60 %) [3115].
m.p. 136–137° [2513], 137° [3115], 153–154° [2927]; IR [2927].

2,4-Dinitrophenylhydrazone [25804-69-7] $C_{22}H_{26}N_4O_5$ mol. wt. 426.47

m.p. 110° [3115], 127° [2513].

4-Cyclohexyl-1-(2,4-dihydroxyphenyl)-1-butanone

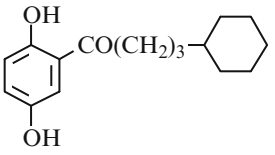
[709032-85-9] $C_{16}H_{22}O_3$ mol. wt. 262.35



Synthesis
-Obtained by reaction of 4-cyclohexylbutyric acid on resorcine in the presence of boron trifluoride [2036].
m.p. 98–107° [2036]

4-Cyclohexyl-1-(2,5-dihydroxyphenyl)-1-butanone

[408310-63-4] $C_{16}H_{22}O_3$ mol. wt. 262.35

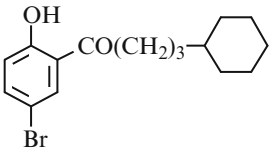


Synthesis
-Obtained by reaction of 4-cyclohexylbutyric acid on hydroquinone in the presence of boron trifluoride [2036].
m.p. 109–110° [2036]

2.5.2 Substituted Hydroxyketones

4-Cyclohexyl-1-(5-bromo-2-hydroxyphenyl)-1-butanone

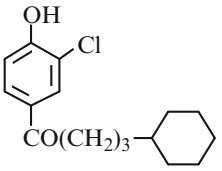
$C_{16}H_{21}BrO_2$ mol. wt. 325.25



Synthesis
-Obtained by Fries rearrangement of 4-bromophenylcyclo-hexylbutyrate with aluminium chloride at 110° (59 %) [3115].
b.p.$_1$ 160° [3115].

4-Cyclohexyl-1-(3-chloro-4-hydroxyphenyl)-1-butanone

$C_{16}H_{21}ClO_2$ mol. wt. 280.79



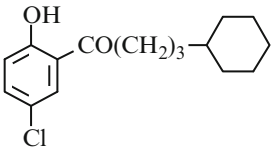
Synthesis
-Obtained by Fries rearrangement of 2-chlorophenyl cyclohexylbutyrate with aluminium chloride at 110° (50 %) [3115].
b.p.$_5$ 230° [3115].

2,4-Dinitrophenylhydrazone $C_{22}H_{25}ClN_4O_5$ mol. wt. 460.92

m.p. 135° [3115].

4-Cyclohexyl-1-(5-chloro-2-hydroxyphenyl)-1-butanone

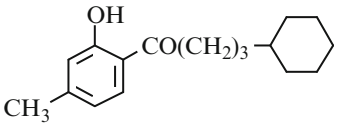
$C_{16}H_{21}ClO_2$ mol. wt. 280.79



Synthesis
-Obtained by Fries rearrangement of 4-chlorophenyl cyclohexylbutyrate with aluminium chloride at 110° (52 %) [3115].
b.p.$_1$ 195° [3115].

4-Cyclohexyl-1-(2-hydroxy-4-methylphenyl)-1-butanone

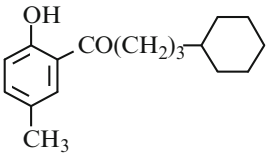
[132180-62-2] $C_{17}H_{24}O_2$ mol. wt. 260.38



Synthesis
-Refer to: [2036].
b.p.$_{0.2}$ 160° [2036]; m.p. 29.5–30° [2036].

4-Cyclohexyl-1-(2-hydroxy-5-methylphenyl)-1-butanone

[25804-40-4] $C_{17}H_{24}O_2$ mol. wt. 260.38



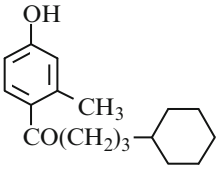
Synthesis
-Obtained by Fries rearrangement of 4-methylphenyl cyclohexylbutyrate with aluminium chloride at 110° (64 %) [3115].
b.p.$_3$ 185° [2513], b.p.$_3$ 193° [3115].

2,4-Dinitrophenylhydrazone [25804-41-5] $C_{23}H_{28}N_4O_5$ mol. wt. 440.50

m.p. 180° [3115], 174–175° [2513].

4-Cyclohexyl-1-(4-hydroxy-2-methylphenyl)-1-butanone

[132180-63-3] $C_{17}H_{24}O_2$ mol. wt. 260.38



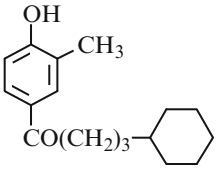
Synthesis
-Obtained by Fries rearrangement of 3-methylphenyl cyclohexylbutyrate with aluminium chloride at 110° (55 %) [3115].
b.p.$_2$ 196–197° [3115].

2,4-Dinitrophenylhydrazone $C_{23}H_{28}N_4O_5$ mol. wt. 440.50

m.p. 160° [3115].

4-Cyclohexyl-1-(4-hydroxy-3-methylphenyl)-1-butanone

[25804-38-0] $C_{17}H_{24}O_2$ mol. wt. 260.38



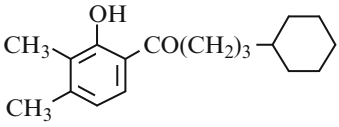
Synthesis
-Obtained by Fries rearrangement of 2-methylphenyl cyclohexylbutyrate with aluminium chloride at 110° (45 %) [3115].
b.p.$_1$ 146° [2513]; m.p. 145° [3115].

2,4-Dinitrophenylhydrazone [25804-39-1] $C_{23}H_{28}N_4O_5$ mol. wt. 440.50

m.p. 241° [2513], 201° [3115].

4-Cyclohexyl-1-(2-hydroxy-3,4-dimethylphenyl)-1-butanone

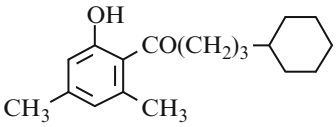
[855620-89-2] $C_{18}H_{26}O_2$ mol. wt. 274.40



Synthesis
-Refer to: [2036].
m.p. 38–40° [2036].

4-Cyclohexyl-1-(2-hydroxy-4,6-dimethylphenyl)-1-butanone

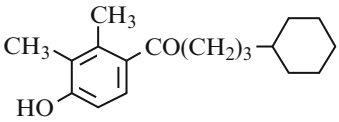
[854866-87-8] $C_{18}H_{26}O_2$ mol. wt. 274.40



Synthesis
-Refer to: [2036].
m.p. 45;2–46° [2036].

4-Cyclohexyl-1-(4-hydroxy-2,3-dimethylphenyl)-1-butanone

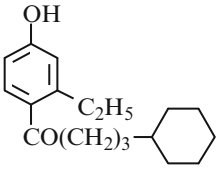
$C_{18}H_{26}O_2$ mol. wt. 274.40



Synthesis
-Refer to: [2036].
m.p. 77.7–78.4° [2036].

4-Cyclohexyl-1-(2-ethyl-4-hydroxyphenyl)-1-butanone

$C_{18}H_{26}O_2$ mol. wt. 274.40



Synthesis
-Obtained by Fries rearrangement of 3-ethylphenyl cyclohexylbutyrate with aluminium chloride at 110° (50 %) [3115].
$b.p._{.7}$ 220° [3115].

2,4-Dinitrophenylhydrazone $C_{24}H_{30}N_4O_5$ mol. wt. 454.53

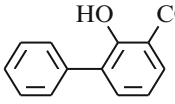
m.p. 155° [3115].

3 Aromatic Hydroxyketones Derived from Diphenyle

3.1 Unsubstituted Hydroxyketones

1,1′-(2-Hydroxy[1,1′-biphenyl]-3-yl)-1-butanone

$C_{16}H_{16}O_2$ mol. wt. 240.30



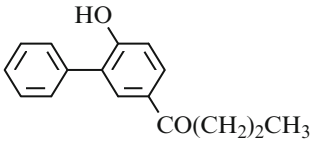
Syntheses
-Obtained by Fries rearrangement of 2-(butyryloxy)-biphenyl with aluminium chloride at 160° for 30–45 min (15 %) [1257].

-Also refer to: [661].

$b.p._{.3.5}$ 185–190° [1257].

1,1′-(2-Hydroxy[1,1′-biphenyl]-5-yl)-1-butanone

[95185-62-9] $C_{16}H_{16}O_2$ mol. wt. 240.30



Syntheses
-Obtained by Fries rearrangement of 2-(butyryloxy)-biphenyl with aluminium chloride at 160° for 30–45 min (40 %) [1257].
-Also obtained by treatment of its methyl ether with pyridinium chloride for 1 h at reflux [504].

-Also refer to: [661, 2704].

shiny colourless leaflets [504];
m.p. 123° [504], 122° [2704], 116–117° [1257].

USE: As colour developer [2704].

Methyl ether [854870-93-2] $C_{17}H_{18}O_2$ mol. wt. 254.33

-Preparation by reaction of butyryl chloride with 2-methoxydiphenyl in the presence of aluminium chloride in carbon disulfide for 4 h at r.t. (90 %) [504].

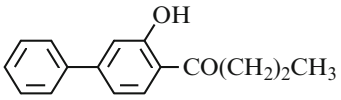
colourless leaflets [504]; b.p.$_{18}$ 243–245° [504]; m.p. 64° [504].

Semicarbazone of the methyl ether $C_{18}H_{21}N_3O_2$ mol. wt. 311.38

m.p. 186° [504].

1,1′-(3-Hydroxy[1,1′-biphenyl]-4-yl)-1-butanone

[131252-71-6] $C_{16}H_{16}O_2$ mol. wt. 240.30

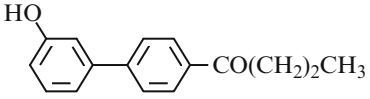


Synthesis
-Preparation by reaction of butyryl chloride with 3-methoxybiphenyl in the presence of aluminium chloride in refluxing methylene chloride (59 %) [443].

m.p. 80.5–81° [443].

1,1′-(3′-Hydroxy[1,1′-biphenyl]-4-yl)-1-butanone

$C_{16}H_{16}O_2$ mol. wt. 240.30



Synthesis
-Refer to: [443].

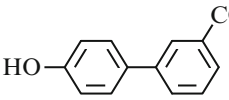
Methyl ether $C_{17}H_{18}O_2$ mol. wt. 254.33

-Obtained by reaction of butyryl chloride with 3-methoxybiphenyl in the presence of aluminium chloride in ethylene chloride at 35° for 45 min (64 %) [443].

irregular white plates [443]; m.p. 62–63° [443].

1,1′-(4′-Hydroxy[1,1′-biphenyl]-3-yl)-1-butanone

$C_{16}H_{16}O_2$ mol. wt. 240.30



Synthesis
-Obtained by diazotization of 4′-amino-3-butyryl-diphenyl [1879].

^{1}H NMR [1879], IR [1879], MS [1879].

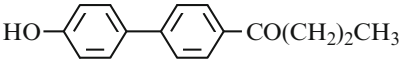
Methyl ether $C_{17}H_{18}O_2$ mol. wt. 254.33

-Refer to: [1879].

^{1}H NMR [1879], IR [1879], MS [1879].

1,1′-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-butanone

[32339-35-8] $C_{16}H_{16}O_2$ mol. wt. 240.30



Syntheses
-Obtained by Fries rearrangement of 4-butyryl-oxybiphenyl with aluminium chloride in nitrobenzene, first at 20° for 12 h, then at 60° for 1 h [522].

-Also obtained by diazotization of 4′-amino-3-butyryldiphenyl [1879].
-Also refer to: [514].

prisms colourless [522];
m.p. 165° [514, 522];
^{1}H NMR [1879], IR [1879], MS [1879].

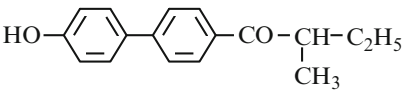
Methyl ether [32339-34-7] $C_{17}H_{18}O_2$ mol. wt. 254.33

-Refer to: [847, 1879].

^{1}H NMR [1879], IR [1879], MS [1879].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-2-methyl-1-butanone (S)

[120837-08-3] $C_{17}H_{18}O_2$ mol. wt. 254.33



Synthesis
-Refer to: [1752].
m.p. 95.5–98.5° [1457].

Methyl ether (S) [112231-64-8] $C_{18}H_{20}O_2$ mol. wt. 268.36

Methyl ether [132041-56-6] $C_{18}H_{20}O_2$ mol. wt. 268.36

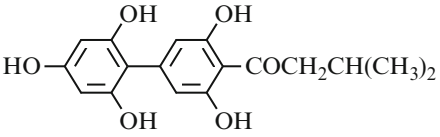
-Refer to: [1752].

10-Undecenyl ether (S) [175797-78-1] $C_{28}H_{38}O_2$ mol. wt. 406.61

-Refer to: [1752].

1,1′-(3,5,2′,4′,6′-Pentahydroxy[1,1′-biphenyl]-4-yl)-3-methyl-1-butanone

[26103-99-1] $C_{17}H_{18}O_6$ mol. wt. 318.33



Synthesis
-Obtained by reaction of isovaleryl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene at 0° for 3 days [898].

Monohydrate $C_{17}H_{18}O_6$, H_2O mol. wt. 336.34

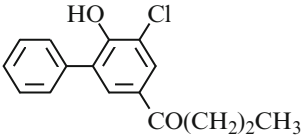
-Refer to: [898] (**X**) (smaller amounts).

m.p. 256° (d) [898]; ^{1}H NMR [898], UV [898].

3.2 Substituted Hydroxyketones

1,1′-(3-Chloro-2-hydroxy[1,1′-biphenyl]-5-yl)-1-butanone

$C_{16}H_{15}ClO_2$ mol. wt. 274.75



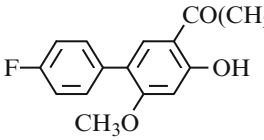
Synthesis
-Refer to: [502].
Methyl ether $C_{17}H_{17}ClO_2$ mol. wt. 288.77

-Obtained by reaction of butyryl chloride with 3-chloro-2-methoxybiphenyl in the presence of aluminium chloride in carbon disulfide. After 12 h standing at r.t., the mixture was heated on a water bath (69 %) [502].

oil [502]; b.p.$_{15}$ 230° [502].

1-[4′-Fluoro-4-hydroxy-6-methoxy[1,1′-biphenyl]-3-yl]-1-butanone

[152609-12-6] $C_{17}H_{17}FO_3$ mol. wt. 288.32

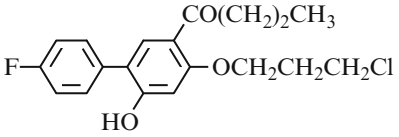


Syntheses
-Refer to: [94, 233].

BIOLOGICAL ACTIVITY: As leukotriene antagonist for the treatment or prevention of Alzheimer' disease [94].

1-[4-(3-Chloropropoxy)-4′-fluoro-6-hydroxy[1,1′-biphenyl]-3-yl]-1-butanone

$C_{19}H_{20}ClFO_3$ mol. wt. 350.82



Synthesis
-Refer to: [94].

Methyl ether [152609-14-8]
$C_{20}H_{22}ClFO_3$ mol. wt. 364.84

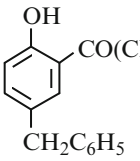
BIOLOGICAL ACTIVITY: As leukotriene antagonist for the treatment or prevention of Alzheimer' disease [94].

4 Aromatic Hydroxyketones Derived from Diphenylmethane

4.1 Unsubstituted Hydroxyketones

1-[2-Hydroxy-5-(phenylmethyl)phenyl]-1-butanone

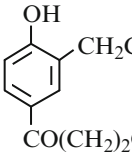
$C_{17}H_{18}O_2$ mol. wt. 254.33



Synthesis
-Obtained by Fries rearrangement of 4-hydroxydiphenylmethane butyrate in the presence of aluminium chloride [3326].
m.p. 52° [3326].

1-[4-Hydroxy-3-(phenylmethyl)phenyl]-1-butanone

$C_{17}H_{18}O_2$ mol. wt. 254.33



Synthesis
-Obtained by Fries rearrangement of 2-hydroxydiphenylmethane butyrate with aluminium chloride in nitrobenzene, first at r.t. overnight, then between 50 and 60° for 4 h [3326].
m.p. 142° [3326].

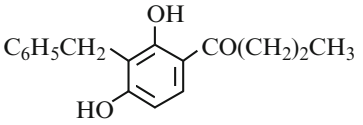
Methyl ether $C_{18}H_{20}O_2$ mol. wt. 268.36

-Obtained by reaction of dimethyl sulfate with 5-butyryl-2-hydroxydiphenylmethane in the presence of sodium hydroxide in dilute ethanol [3326].

m.p. 106° [3326].

1-[2,4-Dihydroxy-3-(phenylmethyl)phenyl]-1-butanone

$C_{17}H_{18}O_3$ mol. wt. 270.33



Syntheses

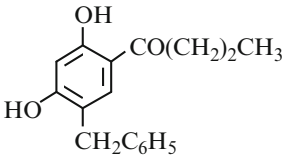
-Obtained treatment of 2-hydroxy-3-benzyl-4-benzyloxybutyrophenone with concentrated hydrochloric acid in boiling acetic acid [2181].

-Also obtained by reaction of 2-benzylresorcinol with butyronitrile (Hoesch reaction) (11 %) [2181].

m.p. 140–142° [2181].

1-[2,4-Dihydroxy-5-(phenylmethyl)phenyl]-1-butanone

$C_{17}H_{18}O_3$ mol. wt. 270.33



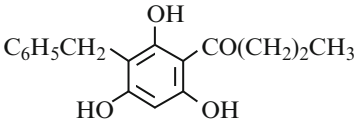
Synthesis

-Preparation by Fries rearrangement of 2,4-dihydroxydiphenylmethane dibutyrate with aluminium chloride in nitrobenzene (85 %) [3326].

m.p. 72° [3326].

1-[2,4,6-Trihydroxy-3-(phenylmethyl)phenyl]-1-butanone

$C_{17}H_{18}O_4$ mol. wt. 286.33



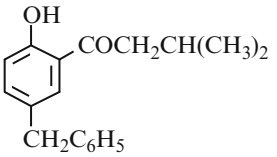
Synthesis

-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and benzyl chloride to a solution of phlorobutyrophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

^{1}H NMR [1026], ^{13}C NMR [1026], IR [1026].

1-[2-Hydroxy-5-(phenylmethyl)phenyl]-3-methyl-1-butanone

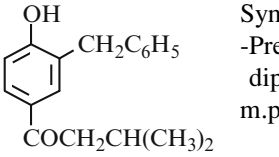
$C_{18}H_{20}O_2$ mol. wt. 268.36



Synthesis
-Preparation by Fries rearrangement of 4-hydroxydiphenylmethane isovalerate [3326].
b.p.$_{22}$ 223° [3326].

1-[4-Hydroxy-3-(phenylmethyl)phenyl]-3-methyl-1-butanone

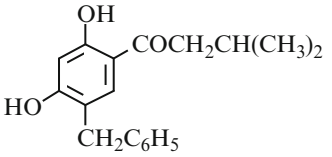
$C_{18}H_{20}O_2$ mol. wt. 268.36



Synthesis
-Preparation by Fries rearrangement of 2-hydroxydiphenylmethane isovalerate [3326].
m.p. 121° [3326].

1-[2,4-Dihydroxy-5-(phenylmethyl)phenyl]-3-methyl-1-butanone

$C_{18}H_{20}O_3$ mol. wt. 284.36



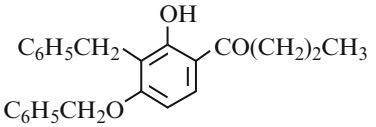
Synthesis
-Preparation by Fries rearrangement of 2,4-dihydroxy-diphenylmethane diisovalerate in the presence of 2,4-dihydroxydiphenylmethane and aluminium chloride in nitrobenzene (78 %) [3326].

m.p. 115° [3326].

4.2 Substituted Hydroxyketones

1-[2-Hydroxy-4-(phenylmethoxy)-3-(phenylmethyl)phenyl]-1-butanone

$C_{24}H_{24}O_3$ mol. wt. 360.45



Synthesis
-Obtained by reaction of benzyl chloride with resbutyrophenone in the presence of potassium hydroxide in methanol, first at r.t. overnight, then at reflux for 5 h (7 %) [2181].

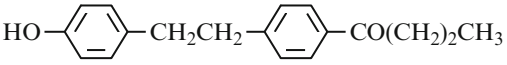
m.p. 108–109° [2181].

5 Aromatic Hydroxyketones Derived from 1,2-Diphenylethane

5.1 Unsubstituted Hydroxyketones

1-(4′-Hydroxy)-4-(1-oxobutyl)-1,2-diphenylethane

$C_{18}H_{20}O_2$ mol. wt. 268.36



Synthesis
-Obtained by diazotization of 4′-amino-4-butyryl-1,2-diphenylethane [1879].

^{1}H NMR [1879], IR [1879], MS [1879].

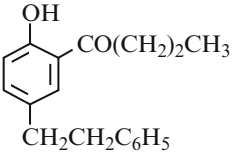
Methyl ether $C_{19}H_{22}O_2$ mol. wt. 282.38

-Refer to: [1879];

^{1}H NMR [1879], IR [1879], MS [1879].

1-[2-Hydroxy-5-(2-phenylethyl)phenyl]-1-butanone

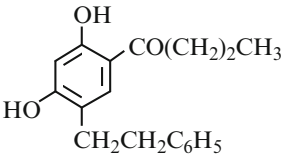
$C_{18}H_{20}O_2$ mol. wt. 268.36



Synthesis
-Obtained by Fries rearrangement of 4-hydroxydiphenylethane butyrate with aluminium chloride in chlorobenzene [3326].
b.p.$_{18}$ 240–242° [3326].

1-[2,4-Dihydroxy-5-(2-phenylethyl)phenyl]-1-butanone

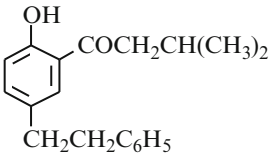
$C_{18}H_{20}O_3$ mol. wt. 284.36



Synthesis
-Obtained by action of aluminium chloride with a 2,4-dihydroxydiphenylethane dibutyrate and 2,4-dihydroxydiphenyethane mixture in nitrobenzene [3326].
m.p. 85–86° [3326].

1-[2-Hydroxy-5-(2-phenylethyl)phenyl]-3-methyl-1-butanone

$C_{19}H_{22}O_2$ mol. wt. 282.38



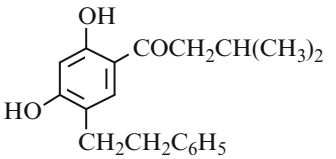
Synthesis

-Preparation by Fries rearrangement of 4-hydroxy-diphenylethane isovalerate in the presence of aluminium chloride in boiling chlorobenzene for 30 min [3326].

b.p.$_{19}$ 247° [3326].

1-[2,4-Dihydroxy-5-(2-phenylethyl)phenyl]-3-methyl-1-butanone

$C_{19}H_{22}O_3$ mol. wt. 298.38



Synthesis

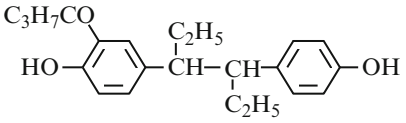
-Preparation by Fries rearrangement of 2,4-dihydroxy-diphenylethane diisovalerate in the presence of 2,4-dihydroxydiphenylethane and aluminium chloride in nitrobenzene at 50° for 3–4 h [3326].

m.p. 102° [3326].

5.2 Substituted Hydroxyketones

3-(4-Hydroxyphenyl)-4-[4-hydroxy-3-(1-oxobutyl)phenyl]hexane
(3-n-Butyrylhexestrol)

$C_{22}H_{28}O_3$ mol. wt. 340.46



Synthesis

-Obtained by treatment of its dimethyl ether by means of pyridinium chloride [510].

colourless needles; m.p. 134° [510].

Dimethyl ether $C_{24}H_{32}O_3$ mol. wt. 368.52

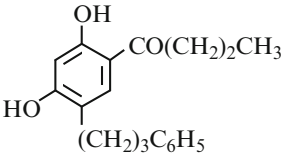
-Obtained by reaction of butyryl chloride with hexestrol dimethyl ether in the presence of aluminium chloride in nitrobenzene for 3 h at r.t. [510].

lustrous colourless leaflets [510]; m.p. 72° [510].

6 Aromatic Hydroxyketones Derived from 1,3-Diphenylpropane

1-[2,4-Dihydroxy-5-(3-phenylpropyl)phenyl]-1-butanone

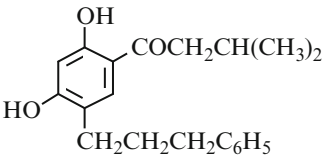
$C_{19}H_{22}O_3$ mol. wt. 298.38



Synthesis
-Obtained by treatment of a 2,4-dihydroxy-diphenylpropane (*sym*) dibutyrate and 2,4-dihydroxydiphenylpropane (*sym*) mixture with aluminium chloride in nitrobenzene at 50° for 3–4 h [3326].
m.p. 78° [3326].

1-[2,4-Dihydroxy-5-(3-phenylpropyl)phenyl]-3-methyl-1-butanone

$C_{20}H_{24}O_3$ mol. wt. 312.41



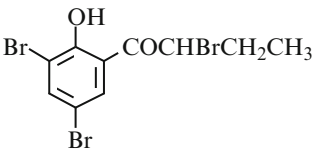
Synthesis
-Preparation by Fries rearrangement of 2,4-dihydroxy-diphenylpropane diisovalerate in the presence of 2,4-dihydroxydiphenylpropane and aluminium chloride in nitrobenzene [3326].
m.p. 105° [3326].

7 Aromatic Hydroxyketones Derived from Various Halogenated 1-Butanoic Acid

7.1 From 2-Bromo-1-Butanoic Acid

2-Bromo-1-(3,5-dibromo-2-hydroxyphenyl)-1-butanone

[238074-77-6] $C_{10}H_9Br_3O_2$ mol. wt. 400.89

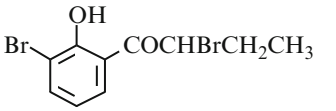


Syntheses
-Obtained by reaction of bromine with 3,5-dibromo-2-hydroxybutyrophenone in refluxing acetic acid (89 %) [375].
-Also refer to: [998].

yellow crystals [375];
m.p. 135–136° [375]; ^{1}H NMR [375], IR [375].

2-Bromo-1-(3-bromo-2-hydroxyphenyl)-1-butanone

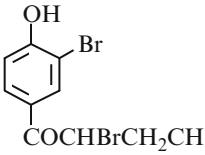
[727687-90-3] $C_{10}H_{10}Br_2O_2$ mol. wt. 322.00



Synthesis
-Refer to: [375].

2-Bromo-1-(3-bromo-4-hydroxyphenyl)-1-butanone

$C_{10}H_{10}Br_2O_2$ mol. wt. 322.00



Synthesis
-Refer to: [441].
Methyl ether (2S) [306972-94-1]
$C_{11}H_{12}Br_2O_2$ mol. wt. 336.02

-Preparation of nonracemic α-bromoketones by stereoselective bromination of aryl alkyl tartrate acetals followed by hydrolysis (50 %, 98 % ee) [441].

m.p. 82–83° [441];
^{1}H NMR [441], ^{13}C NMR [441], IR [441], MS [441].

2-Bromo-1-(3-hydroxyphenyl)-1-butanone

[90841-48-8] $C_{10}H_{11}BrO_2$ mol. wt. 243.10

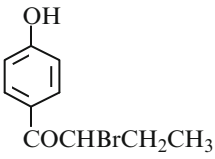
Synthesis
-Refer to: [3002].
m.p. 59.1° [3002].

Methyl ether [91335-45-4] $C_{11}H_{13}BrO_2$ mol. wt. 257.13

m.p. 35° [3002].

2-Bromo-1-(4-hydroxyphenyl)-1-butanone

[53903-58-5] $C_{10}H_{11}BrO_2$ mol. wt. 243.10



Syntheses
-Refer to: [3002, 3471].
m.p. 86.5–87.5° [3002].

Methyl ether [881-43-6] $C_{11}H_{13}BrO_2$ mol. wt. 257.13

-Obtained by treatment of 1-(4-methoxyphenyl)-1-butanone with bromine,
*in glacial acetic acid below 20°, the solution poured into ice water after disappearance of the bromine colour (88 %) [3062];
*in ethyl ether and glacial acetic acid at r.t. (80 %) [1114].
-Obtained by reaction of 2-bromobutanoyl chloride with anisole in the presence of aluminium chloride in 1,2-dichloroethane and the solution was cooled with an ice bath between 45 min and 90 min (43 %) [3308].
-Also refer to: [580, 1000, 1630, 2157, 2158, 2375, 2888, 2987, 3241, 3383, 3472].

colourless oil [3308]; m.p. 51° [3062], 50–52° [2157], 45–46° [1114]; ^{1}H NMR [1114, 2157, 3308], ^{13}C NMR [2157], IR [3308], MS [1114, 3308].

Methyl ether (2*S*) [306972-91-8] $C_{11}H_{13}BrO_2$ mol. wt. 257.13

-Preparation of nonracemic α-bromoketones by stereoselective bromination of aryl alkyl tartrate acetals followed by hydrolysis (65 %, 92 % ee) [441].

m.p. 51–53° [441]; ^{1}H NMR [441], ^{13}C NMR [441], IR [441], MS [441].

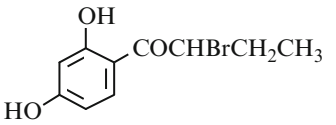
Benzyl ether [35081-43-3] $C_{17}H_{17}BrO_2$ mol. wt. 333.22

-Obtained by irradiation with UV lamp of solution of 4-benzyloxybutyrophenone and bromine in methylene chloride for 15 h between 15 and 18° (59 %) [556].

m.p. 60° [556].

2-Bromo-1-(2,4-dihydroxyphenyl)-1-butanone

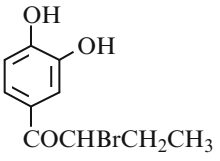
$C_{10}H_{11}BrO_3$ mol. wt. 259.10



Synthesis
-Obtained by reaction of α-bromobutyronitrile with resorcinol (Houben-Hoesch reaction) [1700].
m.p. 114–115° [1700].

2-Bromo-1-(3,4-dihydroxyphenyl)-1-butanone

$C_{10}H_{11}BrO_3$ mol. wt. 259.10



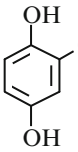
Synthesis
-Obtained by reaction of α-bromobutyric acid with pyrocatechol in the presence of phosphorus oxychloride on a water bath [934].
m.p. 135° [934].

Dimethyl ether [23474-83-1] $C_{12}H_{15}BrO_3$ mol. wt. 287.15

m.p. 90–91.5° [713].

2-Bromo-1-(2,5-dihydroxyphenyl)-1-butanone

$C_{10}H_{11}BrO_3$ mol. wt. 259.10

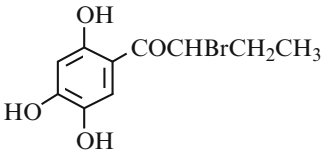


Synthesis
-Refer to: [3271].
Dimethyl ether [93175-38-3]
$C_{12}H_{15}BrO_3$ mol. wt. 287.15

-Obtained by bromination of 2,5-dimethoxybutyrophenone (85 %) [3271].

2-Bromo-1-(2,4,5-trihydroxyphenyl)-1-butanone

$C_{10}H_{11}BrO_4$ mol. wt. 275.10



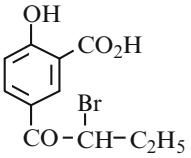
Synthesis
-Refer to: [2696].
Trimethyl ether [90834-07-4]
$C_{13}H_{17}BrO_4$ mol. wt. 317.18

-Obtained by reaction of bromine with 2,4,5-trimethoxybutyrophenone in acetic acid at 35–40°, then at 25° for 40 min [2695].
-Also refer to: [2696].

m.p. 65–65.5° [2695];
^{1}H NMR [2695], IR [2695], MS [2695].

5-(2-Bromo-1-oxobutyl)-2-hydroxybenzoic acid

$C_{11}H_{11}BrO_4$ mol. wt. 287.14



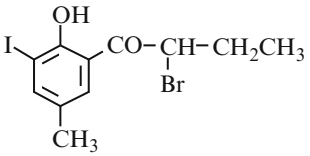
Synthesis
-Refer to: [700].
Methyl ester [24085-13-0]
$C_{12}H_{13}BrO_4$ mol. wt. 301.14

-Obtained by bromination of methyl 5-butyryl-2-hydroxybenzoate at r.t. in chloroform (96 %) [700].
-Also refer to: [434, 1932–1934].

m.p. 83° [700, 1932–1934].

2-Bromo-1-(2-hydroxy-3-iodo-5-methylphenyl)-1-butanone

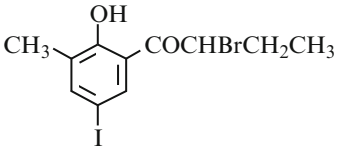
$C_{11}H_{12}BrIO_2$ mol. wt. 383.02



Synthesis
-Obtained by action of bromine in acetic acid on the 2-hydroxy-3-iodo-5-methylphenylbutanone (69 %) [374].
yellow crystals [374]; m.p. 109–110° [374]; IR [374].

2-Bromo-1-(2-hydroxy-5-iodo-3-methylphenyl)-1-butanone

[1186304-76-6] $C_{11}H_{12}BrIO_2$ mol. wt. 383.02

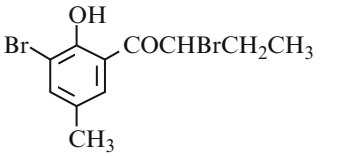


Synthesis
-Obtained by reaction of bromine with 1-(2-hydroxy-5-iodo-3-methylphenyl)-1-butanone in acetic acid (69 %) [374].
yellow crystals [374];

m.p. 109–110° [374];
^{1}H NMR [374], ^{13}C NMR [374], IR [374].

2-Bromo-1-(3-bromo-2-hydroxy-5-methylphenyl)-1-butanone

[396100-57-5] $C_{11}H_{12}Br_2O_2$ mol. wt. 336.02

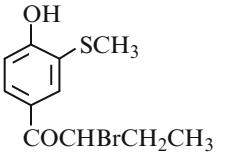


Synthesis
-Obtained by reaction of bromine with 3-bromo-2-hydroxy-5-methylbutyrophenone in refluxing acetic acid (70 %) [375].
yellow crystals [375];

m.p. 117–118° [375]; ^{1}H NMR [375], IR [375].

2-Bromo-1-[4-hydroxy-3-(methylthio)phenyl]-1-butanone

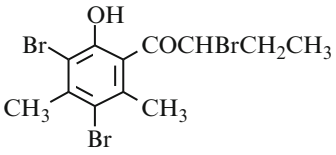
$C_{11}H_{13}BrO_2S$ mol. wt. 289.19



Syntheses
-Preparation by reaction of bromine with 4-hydroxy-3-(methylthio)butyrophenone in chloroform in the presence of calcium carbonate at 25° [2476].
-Also refer to: [2949].

2-Bromo-1-(3,5-dibromo-2-hydroxy-4,6-dimethylphenyl)-1-butanone

$C_{12}H_{13}Br_3O_2$ mol. wt. 428.95



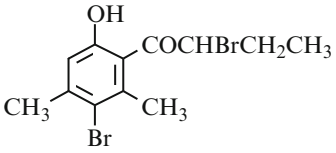
Synthesis

-Obtained by reaction of bromine with 2-hydroxy-4,6-dimethylbutyrophenone in the presence of iron powder or in hot acetic acid [189].

m.p. 124–125° [189].

2-Bromo-1-(3-bromo-6-hydroxy-2,4-dimethylphenyl)-1-butanone

[861310-96-5] $C_{12}H_{14}Br_2O_2$ mol. wt. 350.05



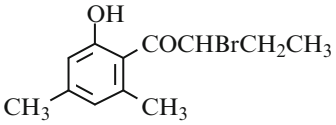
Synthesis

-Obtained by reaction of bromine (2 mol) with 2-hydroxy-4,6-dimethylbutyrophenone in carbon disulfide [189].

m.p. 112.5–113.5° [189].

2-Bromo-1-(2-hydroxy-4,6-dimethylphenyl)-1-butanone

$C_{12}H_{15}BrO_2$ mol. wt. 271.15



Synthesis

-Refer to: [189].

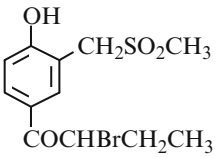
Acetate $C_{14}H_{17}BrO_3$ mol. wt. 313.19

-Obtained by reaction of bromine with 1-(2-hydroxy-4,6-dimethylphenyl) acetate in carbon disulfide [189].

m.p. 36.5–38.5° [189].

2-Bromo-1-[4-hydroxy-3-(methylsulfonylmethyl)phenyl]butanone

$C_{12}H_{15}BrO_4S$ mol. wt. 335.22



Synthesis

-Refer to: [1573].

Benzyl ether [56490-82-5]

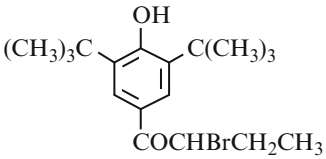
$C_{19}H_{21}BrO_4S$ mol. wt. 425.34

-Obtained by refluxing a mixture of 1-[4-Hydroxy-3-(methylsulfonylmethyl)-phenyl]butanone, PHT,2-pyrrolidinone in THF for 2 h (83 %) [1573].

m.p. 93–96° [1573]; ^{1}H NMR [1573].

2-Bromo-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-butanone

[17055-14-0] $C_{18}H_{27}BrO_2$ mol. wt. 355.32



Syntheses

-Obtained by reaction of 2-bromobutanoyl chloride with 2,6-di-tert-butylphenol in the presence of titanium tetrachloride [1468].

-Also obtained by reaction of bromine with 4-hydroxy-3,5-di-tert-butylbutyrophenone in octane for 30 min at 70° (84 %) [3238, 3239].

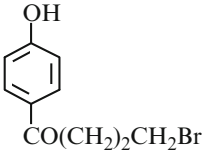
-Also obtained from 4-hydroxy-3,5-di-tert-butylbutyrophenone by reaction with cupric bromide in ethyl acetate-chloroform (80 %) [2773].

m.p. 126–127° [2773], 120–122° [3238, 3239];
^{1}H NMR [2773].

7.2 From 4-Bromo-1-Butanoic Acid

4-Bromo-1-(4-hydroxyphenyl)-1-butanone

$C_{10}H_{11}BrO_2$ mol. wt. 243.10



Synthesis

-Refer to: [3354].

Methyl ether [1023634-25-4]

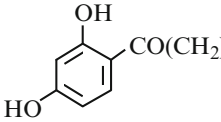
$C_{11}H_{13}BrO_2$ mol. wt. 257.13

-Refer to: [565, 679, 1683, 3354].

^{1}H NMR [565, 3354], ^{13}C NMR [565].

4-Bromo-1-(2,4-dihydroxyphenyl)-1-butanone

[105174-45-6] $C_{10}H_{11}BrO_3$ mol. wt. 259.10



Syntheses

-Obtained by reaction of 4-bromobutyric acid with resorcinol in the presence of aluminium bromide in carbon disulfide (42 %) [1738, 1992].

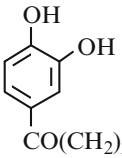
-Also obtained by reaction of 4-bromobutyryl bromide with resorcinol in the presence of aluminium bromide in nitrobenzene (34 %) [1738].

-Also refer to: [3156].

colourless crystals [1738]; m.p. 79–80° [1738];
^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

4-Bromo-1-(3,4-dihydroxyphenyl)-1-butanone

[105174-43-4] $C_{10}H_{11}BrO_3$ mol. wt. 259.10



Syntheses

-Obtained by reaction of 4-bromobutyric acid with pyrocatechol in the presence of aluminium bromide in carbon disulfide (36 %) [1992].

-Also obtained by reaction of 4-bromobutyryl bromide with pyrocatechol in the presence of aluminium bromide in carbon disulfide (36 %) [1738].

colourless powder [1738]; m.p. 98–99° [1738];
^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

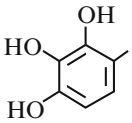
Dimethyl ether [105174-48-9] $C_{12}H_{15}BrO_3$ mol. wt. 287.15

-Obtained by reaction of 4-bromobutyryl bromide with veratrole in the presence of aluminium chloride in carbon disulfide for 30 min at r.t., then 15 min at 40° (59 %) [1738].
-Also obtained by reaction of 4-bromobutyryl chloride with veratrole in the presence of aluminium chloride in methylene chloride for 3 h at 0° (75 %) [3236].
-Also refer to: [492, 3237].

pale yellow crystals [1738]; white needles [3236];
m.p. 96–97° [1738, 3236];
^{1}H NMR [1738, 3236], IR [1738], UV [1738], MS [1738].

4-Bromo-1-(2,3,4-trihydroxyphenyl)-1-butanone

[105174-47-8] $C_{10}H_{11}BrO_4$ mol. wt. 275.10



Synthesis

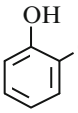
-Obtained by reaction of 4-bromobutyryl bromide with pyrogallol in the presence of aluminium in carbon disulfide at r.t. for 24 h (45 %) [1738].

colourless needles [1738]; m.p. 101° [1738];
^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

7.3 From 2-Chloro-1-Butanoic Acid

2-Chloro-1-(2-hydroxyphenyl)-1-butanone

[103040-41-1] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



Syntheses

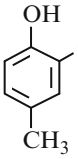
-Obtained by refluxing 3-chloro-3-ethyl-2,4-chromandione (b.p.$_{2.5}$ 135°; m.p. 53°) in a carbon tetrachloride/water mixture until carbon dioxide evolution ceased [1043].

-Also refer to: [1044].

b.p.$_{0.5}$ 110° [1043, 1044].

2-Chloro-1-(2-hydroxy-5-methylphenyl)-1-butanone

[871882-61-0] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



Synthesis

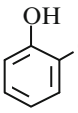
-Preparation by reaction of α-chlorobutyryl bromide with p-cresol methyl ether in the presence of aluminium chloride in carbon disulfide at r.t. for 5–6 h (80 %) [188].

b.p.$_{12}$ 159–160° [188]; m.p. 61–62° [188].

7.4 From 3-Chloro-1-Butanoic Acid

3-Chloro-1-(2-hydroxyphenyl)-1-butanone

[129218-86-6] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



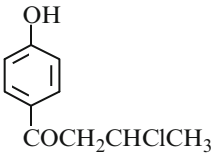
Synthesis

-Obtained by treatment of phenyl 3-butenoate with aluminium chloride between 80 and 130° for 1 h (38 %) [95].

^{1}H NMR [95], IR [95], MS [95].

3-Chloro-1-(4-hydroxyphenyl)-1-butanone

$C_{10}H_{11}ClO_2$ mol. wt. 198.65



Synthesis

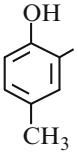
-Refer to: [1846].

Methyl ether [654643-45-5] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

-Refer to: [1846].

3-Chloro-1-(2-hydroxy-5-methylphenyl)-1-butanone

[871882-79-0] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



Syntheses

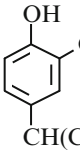
-Preparation condensation of β-chlorobutyryl chloride (oil; b.p.$_{21}$ 51–53°) with 4-methylanisole in the presence of aluminium chloride in carbon disulfide [193].

-Also refer to: [183].

oil [193]; b.p.$_{20}$ 167–170° [183, 193]; m.p. 66–67° [183].

3-Chloro-1-[2-hydroxy-5-(1-methylethyl)phenyl]-1-butanone

$C_{13}H_{17}ClO_2$ mol. wt. 240.73



Synthesis

-Refer to: [1455].

Methyl ether [188405-38-1]

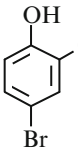
$C_{14}H_{19}ClO_2$ mol. wt. 254.76

-Refer to: [1455].

7.5 From 4-Chloro-1-Butanoic Acid

1-(5-Bromo-2-hydroxyphenyl)-4-chloro-1-butanone

[69639-79-8] $C_{10}H_{10}BrClO_2$ mol. wt. 277.54



Syntheses

-Refer to: [623, 2022].

m.p. 49° [125]; IR [125], MS [125].

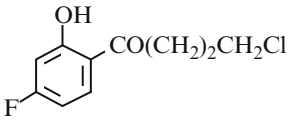
Methyl ether [69639-78-7] $C_{11}H_{12}BrClO_2$ mol. wt. 291.57

-Refer to: [623, 2022].

^{1}H NMR [125], IR [125], MS [125].

4-Chloro-1-(4-fluoro-2-hydroxyphenyl)-1-butanone

[61053-78-9] $C_{10}H_{10}ClFO_2$ mol. wt. 216.64



Syntheses
-Refer to: [2634–2636, 2710, 2984].
b.p.$_{1.1}$ 128–131° [2710, 2984].

Acetate $C_{12}H_{12}ClFO_3$ mol. wt. 258.68
O-Acetyloxime (1*E*) [313369-23-2] $C_{14}H_{15}ClFNO_4$ mol. wt. 315.73

-Refer to: [2634, 2635].

Oxime [313544-35-3] $C_{10}H_{11}ClFNO_2$ mol. wt. 231.65

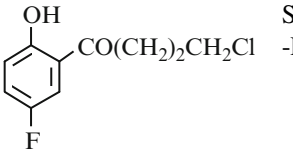
-Refer to: [2636].

Oxime (1*E*) [85485-53-6] $C_{10}H_{11}ClFNO_2$ mol. wt. 231.65

-Refer to: [2634, 2635].

4-Chloro-1-(5-fluoro-2-hydroxyphenyl)-1-butanone

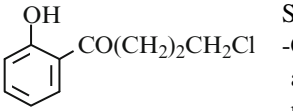
[79214-31-6] $C_{10}H_{10}ClFO_2$ mol. wt. 216.64



Synthesis
-Refer to: [2623].

4-Chloro-1-(2-hydroxyphenyl)-1-butanone

[313369-21-0] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



Syntheses
-Obtained by reaction of 4-chlorobutyryl chloride with anisole in the presence of aluminium chloride in nitroethane at r.t. for 18 h [2185].
-Also refer to: [2459, 2634–2636].

^{1}H NMR [2459], MS [2459].

Oxime [313544-36-4] $C_{10}H_{12}ClNO_2$ mol. wt. 213.66

-Refer to: [2636].

Oxime (1*E*) [313369-22-1] $C_{10}H_{12}ClNO_2$ mol. wt. 213.66

-Refer to: [2634, 2635].

Acetate $C_{12}H_{13}ClO_3$ mol. wt. 240.68

O-Acetyloxime [313369-24-3] $C_{14}H_{16}ClNO_4$ mol. wt. 297.74

-Refer to: [2634, 2635].

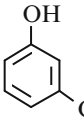
Methyl ether [40877-17-6] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

-Refer to: [2459, 2775, 2776, 2815].

^{1}H NMR [2459], MS [2459], UV [2815].

4-Chloro-1-(3-hydroxyphenyl)-1-butanone

$C_{10}H_{11}ClO_2$ mol. wt. 198.65



Synthesis
-Refer to: [3286].

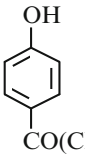
Methyl ether [258882-48-3]
$C_{11}H_{13}ClO_2$ mol. wt. 212.68

-Refer to: [2460 (61 %), 2782, 3286].

colourless oil [2460];
^{1}H NMR [2460, 2782], MS [2460, 2782].

4-Chloro-1-(4-hydroxyphenyl)-1-butanone

[7150-55-2] $C_{10}H_{11}ClO_2$ mol. wt. 198.65



Syntheses
-Obtained by reaction of 4-chlorobutyryl chloride with phenol in the presence of aluminium chloride in nitrobenzene at 40° for 3 h (50 %) [1581].

-Also obtained by Fries rearrangement of phenyl 4-chloro-butyrate in the presence of aluminium chloride in nitrobenzene for 18 h at r.t. (34 %) [3189].
-Also refer to: [111, 253, 299, 300, 711, 712, 968, 1492, 1498, 1580, 1868, 1886, 1949, 2319, 2385–2387, 2815, 2894, 2895, 3134, 3210].

m.p. 115–117° [1581], 114–115.2° [1492, 1498, 3189];
^{1}H NMR [1581], UV [2815], MS [1581, 1886].

N.B.: Reported m.p. 113–116.5° in Aldrich Catalogue 1986–1987.

Acetate $C_{12}H_{13}ClO_3$ mol. wt. 240.68

-Prepared by acetylation of 4′-hydroxy compound (50 %) [3189].

m.p. 30–31.5° [3189].

Methyl ether [40877-19-8] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

-Obtained by reaction of anisole with 4-chlorobutanoyl chloride,
*in the presence of aluminium chloride [2850], (71 %) [3189];
*in the presence of Si-Fe catalyst at 25° (48 %) [427].
-Also obtained by reaction of 4-methoxyphenylmagnesium bromide with 4-chlorobutyronitrile (32 %) [3044].
-Also obtained by cross coupling reaction of 4-chlorobutyryl chloride with $(4\text{-}CH_3OC_6H_5)_3Bi$ in the presence of Pd(o) as catalyst (66 %) [2565].
-Also refer to: [253, 456, 609, 668, 711, 712, 830, 1120, 1340, 1387, 1490–1497, 1710–1713, 1845, 1859, 1886, 2009, 2023, 2565, 2754, 2815, 2847, 2894, 2895, 3164, 3229, 3244, 3285–3287, 3389, 3390, 3422].

pale red liquid [3044];
$b.p._{0.8–0.9}$ 152–154° [1845], $b.p._{.2}$ 159–163° [3189], $b.p._{3–4}$ 162–165° [2754], $b.p._{.6}$ 175° [1496], $b.p._{.5}$ 175° [1490–1495, 1497];
m.p. 31–32° [2754], 31° [3164], 28.5–30° [3189];
^{1}H NMR [1340, 2565, 3044, 3164, 3422],
^{13}C NMR [2565, 3044, 3422],
IR [2565, 3044, 3164], UV [2815], MS [2565].

USE: For preparation of acylaminothiazoles as inhibitors of 15-lipoxygenase [3285]; For preparation of imidazolyl inhibitors of 15-lipoxygenase [3287]; For preparation of piperidine derivatives as NMDA receptor antagonists [3389].

2,4-Dinitrophenylhydrazone of the methyl ether

[75349-76-7] $C_{17}H_{17}ClN_4O_5$ mol. wt. 392.80

m.p. 153–154° [2754].

Ethyl ether [75343-08-7] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

-Obtained by reaction of phenetole with 4-chlorobutanoyl chloride in the presence of aluminium chloride (70 %) [3189].
-Also refer to: [40, 809, 1492, 2754, 2815].

m.p. 51–52° [2754], 50.4–51.8° [1491, 1492, 1497, 3189];
UV [2815].

2,4-Dinitrophenylhydrazone of the ethyl ether

[75343-28-1] $C_{18}H_{19}ClN_4O_5$ mol. wt. 406.83

m.p. 151–153° [2754].

Propyl ether [92019-28-8] $C_{13}H_{17}ClO_2$ mol. wt. 240.73

-Obtained by reaction of phenyl propyl ether with 4-chlorobutanoyl chloride in the presence of aluminium chloride (47 %) [3189].
-Also refer to: [1492, 1498].

b.p.$_5$ 183–185° [3189], b.p.$_6$ 183° [1492, 1498]; m.p. 29.5–32° [3189].

Butyl ether [92317-86-7] $C_{14}H_{19}ClO_2$ mol. wt. 254.76

-Obtained by reaction of phenyl butyl ether with 4-chlorobutanoyl chloride in the presence of aluminium chloride (66 %) [3189].
-Also refer to: [1492, 1498].

m.p. 36.8–38° [1492, 1498, 3189].

Benzyl ether $C_{17}H_{17}ClO_2$ mol. wt. 288.77

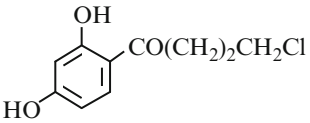
Refer to: [1868].

Phenyl ether [22620-38-8] $C_{16}H_{15}ClO_2$ mol. wt. 274.75

-Refer to: [2009, 2905].

4-Chloro-1-(2,4-dihydroxyphenyl)-1-butanone

[105174-49-0] $C_{10}H_{11}ClO_3$ mol. wt. 214.65



Synthesis
-Obtained by reaction of 4-chlorobutyryl chloride with resorcinol in the presence of aluminium chloride in carbon disulfide at r.t. for 24 h (37 %) [1738].

yellow crystals [1738]; m.p. 92–93° [1738];
^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

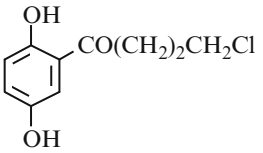
Dimethyl ether [80269-97-2] $C_{12}H_{15}ClO_3$ mol. wt. 242.70

-Obtained by reaction of 4-chlorobutyryl chloride with resorcinol dimethyl ether in the presence of aluminium chloride in nitrobenzene at 0°, then at r.t. for 36 h (50 %) [3189].
-Also refer to: [2009, 2010].

b.p.$_4$ 150–190° [1494]; m.p. 61–62° [1494], 61–62.5° [3189]; UV [2815].

4-Chloro-1-(2,5-dihydroxyphenyl)-1-butanone

$C_{10}H_{11}ClO_3$ mol. wt. 214.65



Synthesis
-Refer to: [3189].

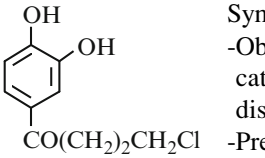
Dimethyl ether [91767-62-3]
$C_{12}H_{15}ClO_3$ mol. wt. 242.70

-Obtained by reaction of 4-chlorobutyryl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in nitrobenzene at 0°, then at r.t. for 36 h (42 %) [3189].
-Also refer to: [1491, 1494, 1497, 3209].

b.p.$_{.4}$ 150–190° [1491, 1494, 1497, 3189];
m.p. 27–30° [1491, 1497, 3189].

4-Chloro-1-(3,4-dihydroxyphenyl)-1-butanone

[105133-00-4] $C_{10}H_{11}ClO_3$ mol. wt. 214.65



Syntheses
-Obtained by reaction of 4-chlorobutyryl chloride with pyrocatechol in the presence of aluminium chloride in carbon disulfide at r.t. for 30 min, then at 40° for 1 h (40 %) [1738].
-Preparation [1948] using the general procedure [1738].

colourless crystals [1738]; m.p. 100–101° [1738];
^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

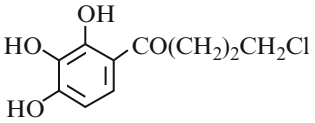
Dimethyl ether [57010-67-0] $C_{12}H_{15}ClO_3$ mol. wt. 242.70

-Obtained by reaction of 4-chlorobutyryl chloride with pyrocatechol dimethyl ether in the presence of aluminium chloride in nitrobenzene at 0°, then at r.t. for 36 h (57 %) [3189].
-Also refer to: [1492, 1498, 2560, 2815, 3164].

m.p. 92–93° [1492, 1498, 3189], 91–92° [2560], 90–92° [3164];
^{1}H NMR [3164], IR [3164], UV [2815].

4-Chloro-1-(2,3,4-trihydroxyphenyl)-1-butanone

[105174-51-4] $C_{10}H_{11}ClO_4$ mol. wt. 230.65



Synthesis
-Obtained by reaction of 4-chlorobutyryl chloride with pyrogallol in the presence of aluminium chloride in carbon disulfide at r.t. for 3 h (32 %) [1738].

yellow crystals [1738]; m.p. 99–100° [1738];
^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

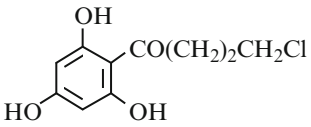
Trimethyl ether [92019-50-6] $C_{13}H_{17}ClO_4$ mol. wt. 272.73

-Obtained by reaction of 4-chlorobutyryl chloride with pyrogallol trimethyl ether in the presence of aluminium chloride in nitrobenzene at 0°, then at r.t. for 36 h (12 %) [3189].
-Also refer to: [1494].

m.p. 83.8–85.4° [1494, 3189].

4-Chloro-1-(2,4,6-trihydroxyphenyl)-1-butanone

$C_{10}H_{11}ClO_4$ mol. wt. 230.65



Synthesis
-Refer to: [3282].
Trimethyl ether [80904-51-4]
$C_{13}H_{17}ClO_4$ mol. wt. 272.73

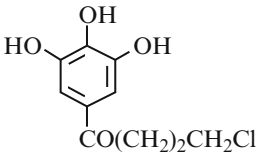
-Refer to: [1812, 2338, 3282].

m.p. 48° [1812]; HPLC [2338].

USE: Preparation of buflomedil by amination of the above trimethyl ether with pyrrolidine in cyclohexane in the presence of sodium iodide [3282].

4-Chloro-1-(3,4,5-trihydroxyphenyl)-1-butanone

$C_{10}H_{11}ClO_4$ mol. wt. 230.65



Synthesis
-Refer to: [3188].
Trimethyl ether [17766-59-5]
$C_{13}H_{17}ClO_4$ mol. wt. 272.73

-Obtained by heating of α-(3,4,5-trimethoxybenzoyl)-γ-butyrolactone with concentrated hydrochloric acid on a steam bath for 3 h. After cooling, fused zinc chloride was added and heating was continued for 2 h (85 %) [2465].
-Also refer to: [3188].

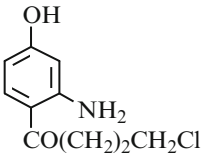
m.p. 80–82° [2465].

2,4-Dinitrophenylhydrazone of the trimethyl ether $C_{19}H_{21}ClN_4O_7$ mol. wt. 452.71

m.p. 139–140° [2465].

1-(2-Amino-4-hydroxyphenyl)-4-chloro-1-butanone

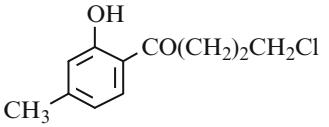
[313545-13-0] $C_{10}H_{12}ClNO_2$ mol. wt. 213.66



Synthesis
-Refer to: [2636].

4-Chloro-1-(2-hydroxy-4-methylphenyl)-1-butanone

[113425-32-4] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

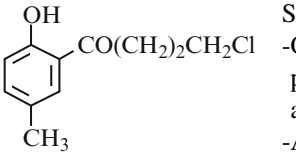


Syntheses
-Obtained by reaction of 4-chlorobutyryl chloride with m-cresol in the presence of aluminium chloride in nitrobenzene at 40° for 3 h (60 %) [1581].
-Also refer to: [1580].

m.p. 95–97° [1581]; ^{1}H NMR [1581], MS [1581].

4-Chloro-1-(2-hydroxy-5-methylphenyl)-1-butanone

[51317-85-2] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

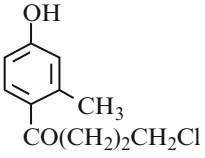


Syntheses
-Obtained by reaction of 4-chlorobutyric acid with p-cresol in the presence of boron trifluoride in autoclave at 70° for 2 h (83 %) [2311].
-Also obtained by reaction of 4-chlorobutyryl chloride with 4-methylanisole in the presence of aluminium chloride in nitroethane at r.t. for 18 h [2185].
-Also obtained by Fries rearrangement of 4-methylphenyl 4-chlorobutyrate with aluminium chloride in nitrobenzene at 60–70° for 8 h (67 %) [2559].
-Also refer to: [1127].

b.p.$_{0.3}$ 135–136° [2559], b.p.$_1$ 149–152° [1127];
m.p. 42° [1127, 2311], 39–41° [2185], 36–38° [2559].

4-Chloro-1-(4-hydroxy-2-methylphenyl)-1-butanone

$C_{11}H_{13}ClO_2$ mol. wt. 212.68



Syntheses
-Refer to: [3082, 3244].

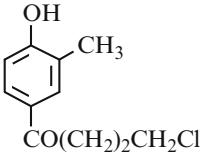
Methyl ether [838822-54-1]
$C_{12}H_{15}ClO_2$ mol. wt. 226.70
-Refer to: [3082, 3244].

^{1}H NMR [3244].

USE: Preparation of heterocycle-containing styrene derivatives as tyrosine kinase inhibitors for prevention/treatment of cancers, etc., [3082].

4-Chloro-1-(4-hydroxy-3-methylphenyl)-1-butanone

[113425-30-2] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



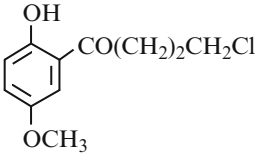
Syntheses
-Obtained by reaction of 4-chlorobutyryl chloride with o-cresol [2675] in the presence of aluminium chloride in nitrobenzene at 40° for 3 h (60 %) [1581].
-Also refer to: [1580, 1847].

m.p. 99° [2675]; 95–97° [1581];
^{1}H NMR [1581, 2675], ^{13}C NMR [2675], IR [2675], MS [1581].

USE: Coordination complexes as catalyst in polycarbonate manuf. [1847]; Preparation of highly active and recyclable catalytic system for CO_2/Propylene oxide copolymn. for prepn. of polycarbonates with high mol. wt. [2675].

4-Chloro-1-(2-hydroxy-5-methoxyphenyl)-1-butanone

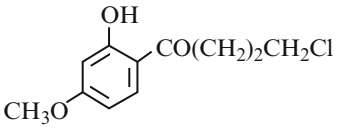
[173055-18-0] $C_{11}H_{13}ClO_3$ mol. wt. 228.68



Synthesis
-Refer to: [2623].

4-Chloro-1-(2-hydroxy-4-methoxyphenyl)-1-butanone

[65242-00-4] $C_{11}H_{13}ClO_3$ mol. wt. 228.68

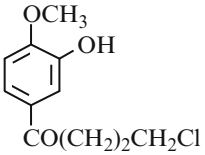


Synthesis
-Obtained by reaction of 4-chlorobutanoic acid with m-methoxyphenol in the presence of 40 % boron trifluoride etherate at 90° for 45 min (37 %) [821].

colourless needles [821]; m.p. 37–39° [821];
^{1}H NMR [821], IR [821], UV [821], MS [821].

4-Chloro-1-(3-hydroxy-4-methoxyphenyl)-1-butanone

$C_{11}H_{13}ClO_3$ mol. wt. 228.68



Synthesis
-Refer to: [1738].

4-Chlorobutyrate $C_{15}H_{18}Cl_2O_4$ mol. wt. 333.21

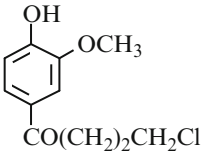
-Obtained by reaction of 4-chlorobutyric acid with guaiacol in the presence of phosphorous oxychloride for 3 h at 80° (51 %) [1738].
-Also obtained by reaction of 4-chlorobutyryl chloride with guaiacol in the presence of aluminium chloride in carbon disulfide for 1 h at 0°, then at r.t. for 5 h (43 %) [1738].

colourless crystals [1738]; m.p. 67° [1738];
^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

N.B.: Or its 4-(4-chlorobutyryloxy)-3-methoxy isomer below; non precised.

4-Chloro-1-(4-hydroxy-3-methoxyphenyl)-1-butanone

$C_{11}H_{13}ClO_3$ mol. wt. 228.68



Synthesis
-Refer to: [1738].
4-Chlorobutyrate $C_{15}H_{18}Cl_2O_4$ mol. wt. 333.21
-Obtained by reaction of 4-chlorobutyric acid with guaiacol in the presence of phosphorous oxychloride for 3 h at 80° (51 %) [1738].

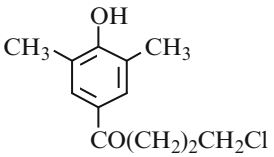
-Also obtained by reaction of 4-chlorobutyryl chloride with guaiacol in the presence of aluminium chloride in carbon disulfide for 1 hat 0°, then at r.t. for 5 h (43 %) [1738].

colourless crystals [1738]; m.p. 67° [1738];
^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

N.B.: Or its 3-(4-chlorobutyryloxy-)-4-methoxy isomer above; non precised.

4-Chloro-1-(4-hydroxy-3,5-dimethylphenyl)-1-butanone

[113425-31-3] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

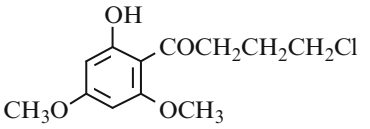


Syntheses
-Obtained by reaction of 4-chlorobutyryl chloride with 2,6-dimethylphenol in the presence of aluminium chloride in nitrobenzene at 40° for 3 h (60 %) [1581].
-Also refer to: [1580].

m.p. 83–85° [1581]; ^{1}H NMR [1581], MS [1581].

4-Chloro-1-(2-hydroxy-4,6-dimethoxyphenyl)-1-butanone

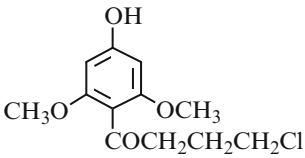
[121079-06-9] $C_{12}H_{15}ClO_4$ mol. wt. 258.70



Synthesis
-Refer to: [2338].
HPLC [2338].

4-Chloro-1-(4-hydroxy-2,6-dimethoxyphenyl)-1-butanone

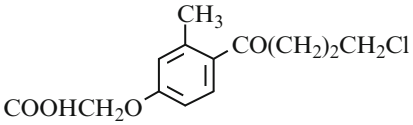
[185835-74-9] $C_{12}H_{15}ClO_4$ mol. wt. 258.70



Synthesis
-Refer to: [2338].
HPLC [2338].

4-(4-Chlorobutyryl)-3-methylphenoxyacetic acid

[1148-02-3] $C_{13}H_{15}ClO_4$ mol. wt. 270.71

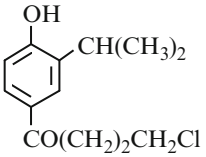


Syntheses
-Refer to: [2047, 2048, 2766, 2767].

m.p. 86.5–88° [2047, 2048, 2766, 2767].

4-Chloro-1-[4-hydroxy-3-(1-methylethyl)phenyl]-1-butanone

[1080021-89-1] $C_{13}H_{17}ClO_2$ mol. wt. 240.73

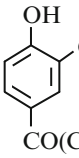


Syntheses
-Obtained by Friedel-Crafts acylation of 2-isopropylphenol using 4-chlorobutyryl chloride [2675].
-Also refer to: [1847].
m.p. 78° [2979];
^{1}H NMR [2675, 2979], ^{13}C NMR [2675, 2979], IR [2675, 2979].

USE: Coordination complexes as catalyst in polycarbonate manuf. [1847]; Preparation of highly active and recyclable catalytic system for CO_2/Propylene oxide copolymn. for prepn. of polycarbonates with high mol. wt. [2675].

4-Chloro-1-[3-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-butanone

[1080021-90-4] $C_{14}H_{19}ClO_2$ mol. wt. 254.76



Syntheses
-Obtained by Friedel-Crafts acylation of 2-tert-butylphenol using 4-chlorobutyryl chloride [2675].
-Also refer to: [1847].
m.p. 121° [2675];

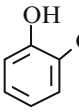
^{1}H NMR [2675], ^{13}C NMR [2675], IR [2675].

USE: Coordination complexes as catalyst in polycarbonate manuf. [1847]; Preparation of highly active and recyclable catalytic system for CO_2/Propylene oxide copolymn. for prepn. of polycarbonates with high mol. wt. [2675].

7.6 From Fluoro-1-Butanoic Acid

2,2,3,3,4,4,4-Heptafluoro-1-(2-hydroxyphenyl)-1-butanone

$C_{10}H_5F_7O_2$ mol. wt. 290.14



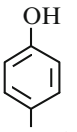
Synthesis
-Refer to: [1848].
Methyl ether [217474-49-2]
$C_{11}H_7F_7O_2$ mol. wt. 304.16

-Obtained by refluxing a mixture of 2-(nonafluorobutyl)anisole in acetic acid with hydrobromic acid and aluminium oxide under nitrogen atmosphere during 16 days (43 %) [1848].

oil [1848];
^{1}H NMR [1848], ^{19}F NMR [1848], MS [1848]; GC [1848].

2,2,3,3,4,4,4-Heptafluoro-1-(4-hydroxyphenyl)-1-butanone

[217474-50-5] $C_{10}H_5F_7O_2$ mol. wt. 290.14



Syntheses
-Obtained by refluxing a mixture of 4-(nonafluorobutyl)-anisole in acetic acid with hydrobromic acid and aluminium oxide under nitrogen atmosphere during 20 h (9 %) [1848].
-Also refer to: [3377].

m.p. 62–64° [1848];
^{1}H NMR [1848], ^{19}F NMR [1848], MS [1848]; GC [1848].

Methyl ether [117482-22-1] $C_{11}H_7F_7O_2$ mol. wt. 304.16

-Preparation: An NMP solution containing $Pd(OAc)_2$, tributylphosphine, heptafluorobutyrate and 4-methoxyboronic acid in a 25 ml Schlenk tube was heated under argon at 80° for 4 h (87 %) [1577].
-Obtained by refluxing a mixture of 4-(nonafluorobutyl)anisole in acetic acid with hydrobromic acid and aluminium oxide under nitrogen atmosphere during 20 h (65 %) [1848].
-Also refer to: [1458].

colourless oil [1577]; oil [1848];
^{1}H NMR [1577, 1848], ^{13}C NMR [1577],
^{19}F NMR [1577, 1848], MS [1577, 1848];
GC-MS [1577]; GC [1848].

O-[(Trifluoromethyl)sulfonyl]oxime of the methyl ether

[749924-46-7] $C_{12}H_7F_{10}NO_4S$ mol. wt. 451.24

yellow crystals [3377]; ^{1}H NMR [3377], ^{19}F NMR [3377].

USE: As latent acids for photoresist [3377].

Phenyl ether $C_{16}H_{10}F_7O_2$ mol. wt. 367.24 [3377].

O-[(Trifluoromethyl)sulfonyl]oxime of the phenyl ether

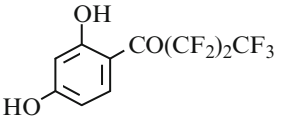
[749924-49-0] $C_{17}H_9F_{10}NO_4S$ mol. wt. 513.31

m.p. 40–42° [3377]; ^{1}H NMR [3377], ^{19}F NMR [3377].

USE: As latent acids for photoresist [3377].

2,2,3,3,4,4,4-Heptafluoro-1-(2,4-dihydroxyphenyl)-1-butanone

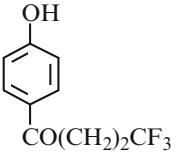
[65240-03-1] $C_{10}H_5F_7O_3$ mol. wt. 306.14



Syntheses
-Refer to: [450, 2996].
m.p. 90° [450].

4,4,4-Trifluoro-1-(4-hydroxyphenyl)-1-butanone

$C_{10}H_9F_3O_2$ mol. wt. 218.18



Synthesis
-Refer to: [698].

Methyl ether

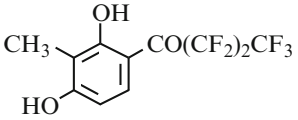
$C_{11}H_{11}F_3O_2$ mol. wt. 232.20

-Obtained by reaction of 4-chloroanisole with 4,4,4-trifluorobutanal in the presence of $Pd(dba)_2$ (2 mol%), Pd phosphine (6 mol%), 4 Å MS and pyrrolidine in DMA at 140° for 4 h (54 %) [698].

^{1}H NMR [698], ^{13}C NMR [698], IR [698], MS [698].

2,2,3,3,4,4,4-Heptafluoro-1-(2,4-dihydroxy-3-methylphenyl)-1-butanone

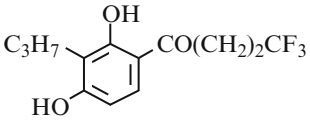
[65240-04-2] $C_{11}H_7F_7O_3$ mol. wt. 320.16



Synthesis
-Refer to: [450].
m.p. 75° [450].

1-(2,4-Dihydroxy-3-propylphenyl)-4,4,4-trifluoro-1-butanone

[194981-87-8] $C_{13}H_{15}F_3O_3$ mol. wt. 276.26

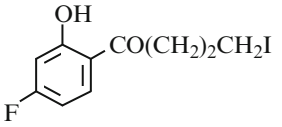


Syntheses
-Refer to: [20, 307].
^{1}H NMR [21].

7.7 From 4-Iodo-1-Butanoic Acid

4-Iodo-1-(2-hydroxy-4-fluorophenyl)-1-butanone

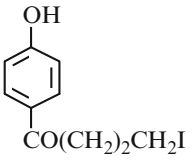
$C_{10}H_{10}FIO_2$ mol. wt. 308.09



Synthesis
-Refer to: [3187].
m.p. 41.4° [3187].

1-(4-Hydroxyphenyl)-4-iodo-1-butanone

$C_{10}H_{11}IO_2$ mol. wt. 290.10



Syntheses
-Obtained by treatment of 1-(4-hydroxyphenyl)-4-chloro-1-butanone with sodium iodide in methyl ethyl ketone at 90° [3134].
-Also refer to: [3212].
m.p. 96–97° [3134]; MS [3134].

Methyl ether [215667-87-1] $C_{11}H_{13}IO_2$ mol. wt. 304.13

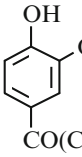
-Obtained *via* the cerium ammonium nitrate mediated oxidative coupling of 2-(4-methoxy-phenyl)cyclobutanol and sodium iodide in 20 % H_2O/DME at 0° (67 %) [565].
-Preparation from 4-chloro-1-(4-methoxyphenyl)-1-butanone (75 %) [1120].
-Also refer to: [1122, 1928, 3081, 3212].

m.p. 43° [1120];
^{1}H NMR [565, 1120], ^{13}C NMR [565, 1120], IR [1120],
MS [1120, 1928].

USE: Nickel-catalyzed cross-coupling of 4-iodo-1-(4-methoxyphenyl)-1-butanone with n-butyl-magnesium chloride in DMA at −35° for 30 min (68 %) [3212].

1-(3,4-Dihydroxyphenyl)-4-iodo-1-butanone

[105174-61-6] $C_{10}H_{11}IO_3$ mol. wt. 306.10



Synthesis
-Obtained by reaction of sodium iodide with 4-chloro-1-(3,4-dihydroxyphenyl)-1-butanone in boiling acetone for 24 h (56 %) [1738].
m.p. 131° [1738];

^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

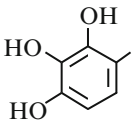
Dimethyl ether [105174-55-8] $C_{12}H_{15}IO_3$ mol. wt. 334.15

-Obtained by reaction of sodium iodide with 4-chloro-1-(3,4-dimethoxyphenyl)-1-butanone in boiling acetone for 24 h (39 %) [1738].

m.p. 93° [1738];
^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

4-Iodo-1-(2,3,4-trihydroxyphenyl)-1-butanone

[105174-58-1] $C_{10}H_{11}IO_4$ mol. wt. 322.10



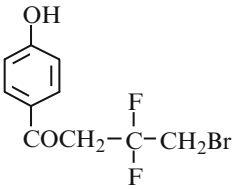
Synthesis
-Obtained by reaction of sodium iodide with 4-bromo-1-(2,3,4-trihydroxyphenyl)-1-butanone in acetone at r.t. for 12 h (65 %) [1738].
m.p. 114° [1738];

^{1}H NMR [1738], IR [1738], UV [1738], MS [1738].

7.8 From Various Halogeno-1-Butanoic Acid

4-Bromo-3,3-difluoro-1-(4-hydroxyphenyl)-1-butanone

$C_{10}H_9BrF_2O_2$ mol. wt. 279.08



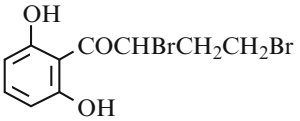
Synthesis
-Refer to: [3354].
Methyl ether [1023272-24-3]
$C_{11}H_{11}BrF_2O_2$ mol. wt. 293.11
-Obtained by treatment of 4-methoxyphenyl difluorocyclopropyl ketone with N-pentylpyridinium bromide at 70° for 10 h under nitrogen,

*in trifluoroacetic acid (74 %) [3354];
*in trifluoromethanesulfonic acid (76 %) [3354].

^{1}H NMR [3354], ^{13}C NMR [3354], ^{19}F NMR [3354].

2,4-Dibromo-1-(2,6-dihydroxyphenyl)-1-butanone

$C_{10}H_{10}Br_2O_3$ mol. wt. 338.00



Synthesis
-Refer to: [272].
Dimethyl ether [753013-71-7]
$C_{12}H_{14}Br_2O_3$ mol. wt. 366.05

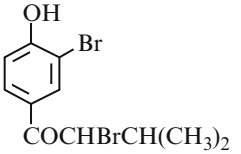
-Refer to: [272].

m.p. 99–100° [272]; MS [272].

USE: Preparation of hydroxycoumaranone derivs. as uPA receptor antagonists for treatment of cancers [272].

2-Bromo-1-(3-bromo-4-hydroxyphenyl)-3-methyl-1-butanone

$C_{11}H_{12}Br_2O_2$ mol. wt. 336.02



Synthesis
-Refer to: [441].
Methyl ether (2S) [306972-95-2]
$C_{12}H_{14}Br_2O_2$ mol. wt. 350.05

-Preparation of nonracemic α-bromoketones by stereoselective bromination of aryl alkyl tartrate acetals followed by hydrolysis (70 %, 71 % ee) [441].

pale brown oil [441]; ^{1}H NMR [441], IR [441], MS [441].

2,3-Dibromo-1-(2-hydroxy-5-methylphenyl)-1-butanone

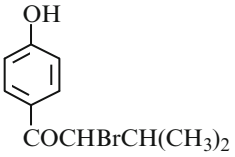
$C_{11}H_{12}Br_2O_2$ mol. wt. 336.02

Synthesis
-Refer to: [183].

Acetate $C_{13}H_{14}Br_2O_3$ mol. wt. 378.06
-Refer to: [183]; m.p. 79.5–80.5° [183].

2-Bromo-1-(4-hydroxyphenyl)-3-methyl-1-butanone

[412051-38-8] $C_{11}H_{13}BrO_2$ mol. wt. 257.13



Syntheses
-Refer to: [881–884, 1114].
^{1}H NMR [881].

USE: For preparation of benzoxathiin derivatives as estrogen receptor modulators [882, 883].

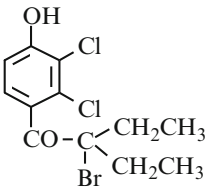
Methyl ether [35446-28-7] $C_{12}H_{15}BrO_2$ mol. wt. 271.15

-Obtained by treatment of 1-(4-methoxyphenyl)-4-methyl-1-pentanone with bromine in ethyl ether and glacial acetic acid at r.t. (93 %) [1114].
-Also refer to: [143, 896, 3231 (89 %)].

oil [1114]; m.p. 73° [3231];
^{1}H NMR [896, 1114, 3231], IR [3231], MS [896, 1114].

2-Bromo-1-(2,3-dichloro-4-hydroxyphenyl)-2-ethyl-1-butanone

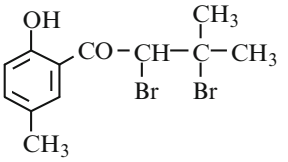
[4091-11-6] $C_{12}H_{13}BrCl_2O_2$ mol. wt. 340.04



Syntheses
-Obtained by reaction of bromine with 1-(2,3-dichloro-4-hydroxyphenyl)-2-ethyl-1-butanone in acetic acid at r.t. for 15 min [2060].
-Also refer to: [2054, 2058, 2059, 2061].
m.p. 122.5–123.5° [2054, 2058–2061].

2,3-Dibromo-1-(2-hydroxy-5-methylphenyl)-3-methyl-1-butanone

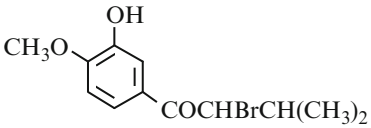
$C_{12}H_{14}Br_2O_2$ mol. wt. 350.05



Synthesis
-Obtained by reaction of bromine with isobutenyl-p-cresyl-ketone (oil; b.p. 277–278°) in carbon disulfide [193].
m.p. 70–71° [193].

2-Bromo-1-(3-hydroxy-4-methoxyphenyl)-3-methyl-1-butanone

[99783-83-2] $C_{12}H_{15}BrO_3$ mol. wt. 287.15

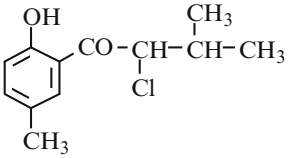


Synthesis
-Obtained by treatment of 3-hydroxy-4-methoxy-isovalerophenone with cupric bromide in refluxing an ethyl acetate/chloroform mixture for 2 h (79 %) [144].

oil [144]; ^{1}H NMR [144].

2-Chloro-1-(2-hydroxy-5-methylphenyl)-3-methyl-1-butanone

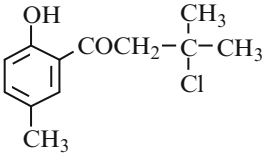
[871886-71-4] $C_{12}H_{15}ClO_2$ mol. wt. 226.70



Synthesis
-Obtained by reaction of α-chloroisovaleryl bromide with p-cresol methyl ether in the presence of aluminium chloride in carbon disulfide at r.t. [188].
m.p. 75–76° [188].

3-Chloro-1-(2-hydroxy-5-methylphenyl)-3-methyl-1-butanone

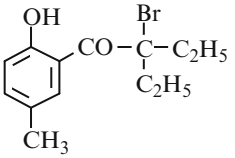
$C_{12}H_{15}ClO_2$ mol. wt. 226.70



Syntheses
-Obtained by reaction of hydrogen chloride with isobutenyl-p-cresyl-ketone (oil; b.p. 277–278°) in acetic acid [193].
-Also refer to: [192] (**II**).
m.p. 53–55° [193].

2-Bromo-2-ethyl-1-(2-hydroxy-5-methylphenyl)-1-butanone

$C_{13}H_{17}BrO_2$ mol. wt. 285.18

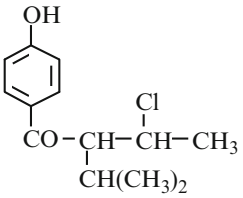


Synthesis
-Preparation by reaction of bromodiethylacetyl bromide with 4-methylanisole in the presence of aluminium chloride in carbon disulfide on a water bath for 6 h (almost quantitative yield) [194].

b.p.$_{14}$ 175° [194]; $n_D^{20} = 1.565$ [194]; $d_{20} = 1.307$ [194].

3-Chloro-1-(4-hydroxyphenyl)-2-(1-methylethyl)-1-butanone

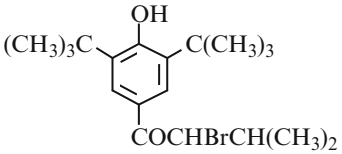
$C_{13}H_{17}ClO_2$ mol. wt. 240.73



Synthesis
-Refer to: [2767].
b.p.$_{0.5}$ 156–167° [2767]; m.p. 75–77° [2767].

2-Bromo-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-methyl-1-butanone

[17055-16-2] $C_{19}H_{29}BrO_2$ mol. wt. 369.34



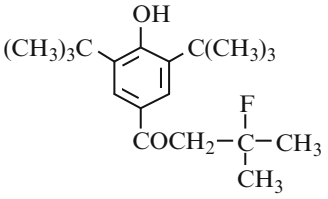
Syntheses
-Obtained by reaction of 2-bromoisopentanoyl chloride with 2,6-di-tert-butylphenol in the presence of titanium tetrachloride [1468].
-Also obtained by reaction of bromine with 4-hydroxy-3,5-di-tert-butylisovalerophenone in octane for 30 min at 70° (79 %) [3239].

-Also refer to: [3238].

m.p. 113–115° [3238, 3239].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-fluoro-3-methyl-1-butanone

[174635-34-8] $C_{19}H_{29}FO_2$ mol. wt. 308.4



Synthesis
-Refer to: [2482].
m.p. 94° [1499].

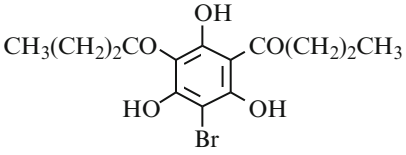
BIOLOGICAL ACTIVITY: As antiinflammatory and analgesic agent [2482].

Chapter 2
Butanones: Polyketones

1 Aromatic Hydroxyketones Derived from 1-Butanoic Acid

1,1′-(5-Bromo-2,4,6-trihydroxy-1,3-phenylene)bis-1-butanone

[2999-16-8] $C_{14}H_{17}BrO_5$ mol. wt. 345.19



Syntheses

-Obtained by reaction of butyryl chloride with 2-bromophloroglucinol in the presence of boron trifluoride etherate (72–78 %) [3391].

-Also refer to: [457, 2911].

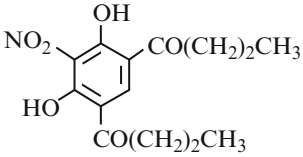
m.p. 146–148° [3391], 102–104° [457, 2911].

N.B.: One of the reported melting point is obviously wrong.

BIOLOGICAL ACTIVITY: Antischistosomal [3391].

1,1′-(4,6-Dihydroxy-5-nitro-1,3-phenylene)bis-1-butanone

[107522-52-1] $C_{14}H_{17}NO_6$ mol. wt. 295.29



Syntheses

-Obtained by Fries rearrangement of 2-nitroresorcinol dibutyrate (1 mol) with aluminium chloride (3.3 mol),

*without solvent at 100–110° for 3 h (33 %) [105];

*in nitrobenzene at 100–110° for 3 h (13 %) or at 25–28° for 70 h (13 %) [105].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_2

-Also obtained by reaction of butyric anhydride with 2-nitroresorcinol in the presence of aluminium chloride (3.3 mol) in nitrobenzene at 120–130° (56 %) [105].

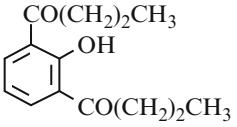
m.p. 154° [105].

Diacetate [107778-29-0] $C_{18}H_{21}NO_8$ mol. wt. 379.37

-Refer to: [105]; m.p. 95° [105].

1,1′-(2-Hydroxy-1,3-phenylene)bis-1-butanone

[205067-94-3] $C_{14}H_{18}O_3$ mol. wt. 234.30



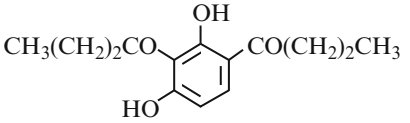
Synthesis

-Refer to: [3450].

N.B.: Resonance-assisted intramolecular hydrogen bonding [3450].

1,1′-(2,4-Dihydroxy-1,3-phenylene)bis-1-butanone

[2999-22-6] $C_{14}H_{18}O_4$ mol. wt. 250.29



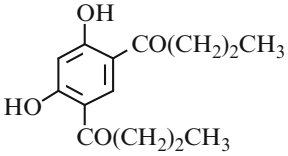
Syntheses

-Obtained by Fries rearrangement of resorcinol dibutyrate with aluminium chloride, *at 130–135° for 4 h [2651]; *at 180–185° for 90 min (50 %) [855].

b.p.$_{20}$ 190° [855, 2651]; m.p. 67° [855].

1,1′-(4,6-Dihydroxy-1,3-phenylene)bis-1-butanone

[2999-21-5] $C_{14}H_{18}O_4$ mol. wt. 250.29



Syntheses

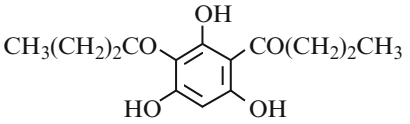
-Obtained by Fries rearrangement of resorcinol dibutyrate with zinc chloride at 130° (40–50 %) [2651].

-Also obtained from 2,4-dihydroxyacetophenone (5 %) [385].

m.p. 64–65° [2651], 64° [385].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-butanone

[3098-40-6] $C_{14}H_{18}O_5$ mol. wt. 266.29



Syntheses

-Obtained by reaction of acrylic acid with phlorobutyrophenone in the presence of phosphorous pentoxide in methanesulfonic acid for 30 min at 70° under nitrogen atmosphere [1026].

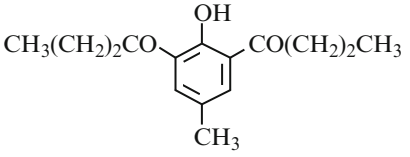
-Also obtained by reaction of butyryl chloride,
*with phlorobutyrophenone in the presence of aluminium chloride in boiling carbon disulfide and nitrobenzene mixture for 2 h [1026];
*phloroglucinol in the presence of aluminium chloride in nitrobenzene for 3 days at r.t. (5–10 %) [421].
-Also obtained by reaction of butyric acid with phloroglucinol in the presence of boron trifluoride etherate [3019].
-Also refer to: [3033, 3391].

m.p. 180° [2646], 179–180° [1608, 1610, 2616, 2618], 135–137° [421], 126–128° [3391];
^{1}H NMR [421, 3019], ^{13}C NMR [1026, 3019], IR [421, 1026, 3019], UV [3019], MS [421].

BIOLOGICAL ACTIVITY: Antagonist both thromboxane A_2 and Leukotriene D_4 [3019]; Inhibitory effects of treatment with this acylphenol on TPA Induced EBV-EA Activation [3033].

1,1′-(2-Hydroxy-5-methyl-1,3-phenylene)bis-1-butanone

[88580-91-0] $C_{15}H_{20}O_3$ mol. wt. 248.32



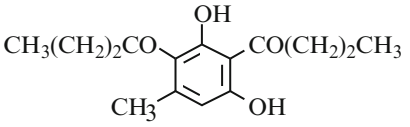
Synthesis
-Obtained by reaction of butyryl chloride with p-cresol in the presence of aluminium chloride in nitrobenzene (40 %) [1979].
m.p. 46° [1979];

^{1}H NMR [1979], IR [1979], UV [1979].

USE: For preparation of phenoxo-bridged macrocyclic dizinc (II) complex [2130].

1,1′-(2,6-Dihydroxy-4-methyl-1,3-phenylene)bis-1-butanone

[875854-88-9] $C_{15}H_{20}O_4$ mol. wt. 264.32

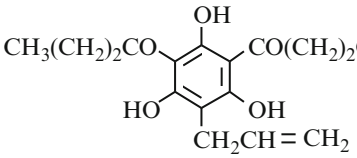


Syntheses
-Obtained by Fries rearrangement of orcinol dibutyrate in the presence of aluminium chloride (3 mol) at 140–150° for 90 min (33 %) [855].
-Also obtained by treatment of 2,6-dihydroxy-4-methylbutyrophenone with butyric anhydride in the presence of aluminium chloride in nitrobenzene [854].

m.p. 67° [854, 855].

1,1′-[2,4,6-Trihydroxy-5-(2-propenyl)-1,3-phenylene]bis-1-butanone
2,4-Dibutyryl-6-(propen-2-yl)phloroglucinol (**21**) [1026]

$C_{17}H_{22}O_5$ mol. wt. 306.36

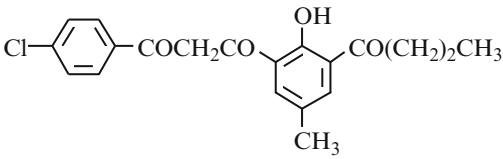


Synthesis
-Also obtained by reaction of butyryl chloride with 2-butyryl-4-(propen-2-yl) phloroglucinol in the presence of aluminium chloride in boiling carbon disulfide and nitrobenzene mixture for 2 h [1026].

IR [1026], MS [1026].

3-[2-(4-Chlorobenzoyl)acetyl]-2-hydroxy-5-methyl-1-butanone
α-4-Chlorobenzoyl-2-hydroxy-5-methyl-3-butyrylacetophenone

[213622-31-2] $C_{20}H_{19}ClO_4$ mol. wt. 358.82

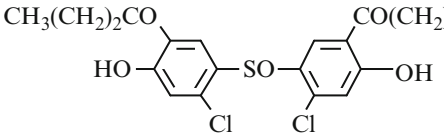


Synthesis
-Obtained by treatment of 1-[3-acetyl-2-(4-chlorobenzoyloxy)-5-methyl-phenyl]-1-butanone with powdered KOH in pyridine (Baker-Venkataraman rearrangement) (81 %) [344].

m.p. 126–127° [344]; ^{1}H NMR [344], IR [344].

1,1′-[Sulfonylbis(6-chloro-4-hydroxy-3,1-phenylene)]bis-1-butanone

[50444-95-6] $C_{20}H_{20}Cl_2O_5S$ mol. wt. 443.35



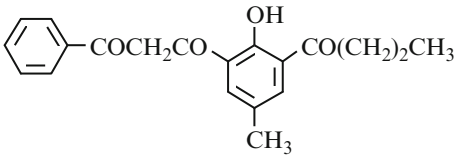
Synthesis
-Obtained by treatment of 4-chloro-2-hydroxybutyrophenone with thionyl chloride in the presence of aluminium chloride in carbon disulfide (52 %) [2430].

m.p. 227° [2430]; ^{1}H NMR [2430], IR [2430].

USE: Antifungal [2430].

3-(2-Benzoylacetyl)-2-hydroxy-5-methyl-1-butanone
α-Benzoyl-2-hydroxy-5-methyl-3-butyrylacetophenone

[213622-30-1] $C_{20}H_{20}O_4$ mol. wt. 324.38

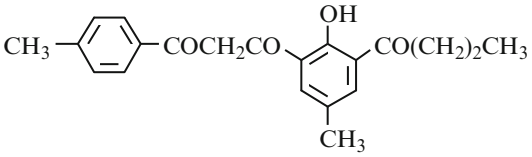


Synthesis
-Obtained by treatment of 1-[3-acetyl-2-(benzoyloxy)-5-methylphenyl]-1-butanone with powdered KOH in pyridine (Baker-Venkataraman rearrangement) (80 %) [344].

m.p. 115–116° [344]; ^{1}H NMR [344], IR [344].

3-[2-(4-Methylbenzoyl)acetyl]-2-hydroxy-5-methyl-1-butanone
α-4-Methylbenzoyl-2-hydroxy-5-methyl-3-butyrylacetophenone

[213622-32-3] $C_{21}H_{22}O_4$ mol. wt. 338.40

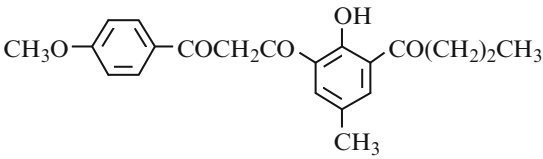


Synthesis
-Obtained by treatment of 1-[3-acetyl-2-(4-methylbenzoyloxy)-5-methyl-phenyl]-1-butanone with powdered KOH in pyridine (Baker-Venkataraman rearrangement) (82 %) [344].

m.p. 134–135° [344]; ^{1}H NMR [344], IR [344].

3-[2-(4-Methoxybenzoyl)acetyl]-2-hydroxy-5-methyl-1-butanone
α-4-Methoxybenzoyl-2-hydroxy-5-methyl-3-butyrylacetophenone

[213622-33-4] $C_{21}H_{22}O_5$ mol. wt. 354.40

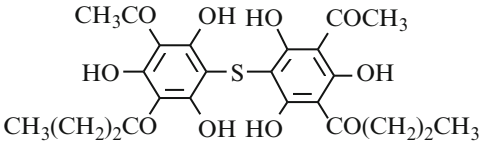


Synthesis
-Obtained by treatment of 1-[3-acetyl-2-(4-methoxybenzoyloxy)-5-methyl-phenyl]-1-butanone with powdered KOH in pyridine (Baker-Venkataraman rearrangement) (78 %) [344].

m.p. 118–119° [344]; ^{1}H NMR [344], IR [344].

1,1′-Thiobis[2,4,6-trihydroxy-3-(1-oxoethyl)-5,1-phenylene]bis-1-butanone

$C_{24}H_{26}O_{10}S$ mol. wt. 506.53

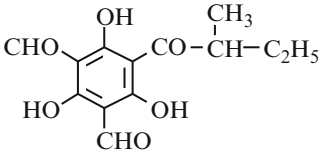


Synthesis
-Refer to: [3391].
m.p. 173–175° [3391].

2 Aromatic Hydroxyketones Derived from 2-Methyl-1-Butanoic Acid

2,4,6-Trihydroxy-5-(2-methyl-1-oxobutyl)-1,3-benzenedicarboxaldehyde

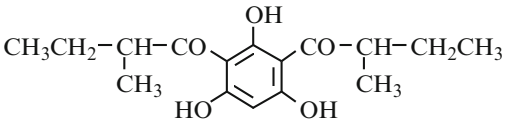
$C_{13}H_{14}O_6$ mol. wt. 266.25



Isolation from natural sources
-From the leaf essential oil of *Eucalyptus apodophylla* (Myrtaceae) [2046].
MS [2046]; GC-MS [2046].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-2-methyl-1-butanone

[139409-36-2] $C_{16}H_{22}O_5$ mol. wt. 294.35



Synthesis
-Obtained by reaction of 2-methyl-butanoic acid with phloroglucinol in the presence of boron trifluoride etherate [3019].

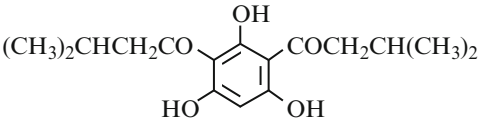
^{1}H NMR [3019], ^{13}C NMR [3019], IR [3019], UV [3019],

BIOLOGICAL ACTIVITY: Antagonist both thromboxane A_2 and Leukotriene D_4 [3019].

3 Aromatic Hydroxyketones Derived from 3-Methyl-1-Butanoic Acid

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-3-methyl-1-butanone
2′,4′,6′-Trihydroxy-3′-isovalerylisovalerophenone

[2999-10-2] $C_{16}H_{22}O_5$ mol. wt. 294.35



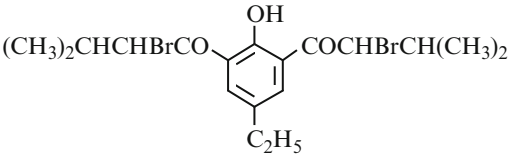
Syntheses
-Obtained by reaction of isovaleryl chloride with phloroglucinol in the presence of aluminium chloride (30 %) [621].
in nitrobenzene at 0° for 3 days (10 %) (**IX**) [898].
-Also obtained by reaction of isovaleric acid with phloroglucinol in the presence of boron trifluoride etherate [3019], (32 %) [2042], at 100° for 2 h (67 %) [338].
-Also obtained by reaction of isovaleric acid with phloroglucinol in the presence of titanium tetrachloride [3033].
-Also refer to: [337, 962, 1983, 2684, 2911].

cream coloured solid [338]; yellow prisms [2042];
m.p. 117–118° [2042], 114–115° [898], 113–114° [2911];
^{1}H NMR [338, 898, 2042, 3019], ^{13}C NMR [3019], IR [2042, 3019], UV [898, 3019], MS [338, 898].

BIOLOGICAL ACTIVITY: S-Euglobals: Biomimetic synthesis, antileishmanial, antimalarial, and antimicrobial activities [336]; Antagonist both thromboxane A_2 and Leukotriene D_4 [3019]; Effects on transpiration and stomatal closure [3408]; Inhibitory effects of treatment with this acylphenol on TPA Induced EBV-EA Activation [3033]; Industrial bactericidal and fungicidal agent, algicide and biofouling inhibitor [962]; For the prevention and treatment of bone and cartilage diseases [2684].

1,1′-(5-Ethyl-2-hydroxy-1,3-phenylene)bis-2-bromo-3-methyl-1-butanone

$C_{18}H_{24}Br_2O_3$ mol. wt. 448.19



Synthesis
-Obtained by treatment of 1,1′-(5-ethyl-2-hydroxy-1,3-phenylene)bis-3-methyl-1-butanone with cupric bromide in ethyl acetate/chloroform for 2.5 h at r.t. under nitrogen (97 %) [403].

oil [403]; IR [403].

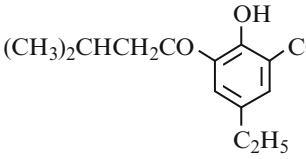
Methyl ether [412340-39-7] $C_{19}H_{26}Br_2O_3$ mol. wt. 462.22

-Obtained by treatment of 4-ethyl-2,6-diisovalerylanisole in chloroform with a suspension of cupric bromide in ethyl acetate at reflux for 2.5 h (97 %) [403].

cognac coloured oil [403]; IR [403].

1,1′-(5-Ethyl-2-hydroxy-1,3-phenylene)bis-3-methyl-1-butanone

[77346-71-5] $C_{18}H_{26}O_3$ mol. wt. 290.40



Synthesis

-Obtained by Fries rearrangement of 4-ethyl-2-isovalerylphenyl 3-isovalerate in the presence of aluminium chloride at 150–160° (28 %) [403].

yellow oil [403]; b.p.$_{0.2}$ 115–125° [403]; ^{1}H NMR [403], IR [403].

Methyl ether [77346-72-6] $C_{19}H_{28}O_3$ mol. wt. 304.43

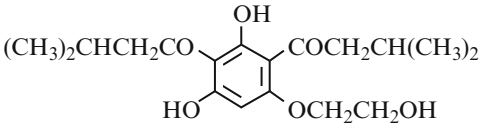
-Obtained by reaction of methyl iodide with the title diketone in the presence of potassium carbonate in acetone at r.t. for 20 h (95 %) [403].

-Preparation by treatment of 4-ethyl-2,6-diisovalerylphenol with methyl iodide in the presence of potassium carbonate in acetone at r.t. for 20 h (95 %) [403].

pale yellow oil [403]; b.p.$_{0.3}$ 110–115° [403]; ^{1}H NMR [403], IR [403].

1,1′-[2,4-Dihydroxy-6-(2-hydroxyethoxy)-1,3-phenylene]bis-3-methyl-1-butanone

[1103524-25-9] $C_{18}H_{26}O_6$ mol. wt. 338.40

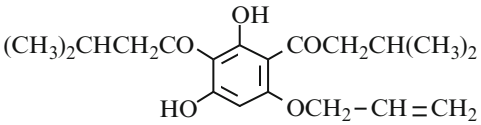


Synthesis

-Obtained by reaction of 2-bromoethanol with 2,4-diisovalerylphloroglucinol in the presence of potassium carbonate in acetone at r.t. for 10 h (50 %) [338].

1,1′-[2,4-Dihydroxy-6-(2-propen-1-yloxy)-1,3-phenylene]bis-3-methyl-1-butanone

[918814-60-5] $C_{19}H_{26}O_5$ mol. wt. 334.41



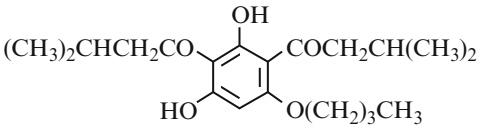
Synthesis
-Obtained by Friedel-Crafts acylation of phloroglucinol mono-allyl ether with isopentanoyl chloride in the presence of titanium tetrachloride (10 %) [337].

yellow sticky solid [337];
^{1}H NMR [337], ^{13}C NMR [337], IR [337], UV [337], MS [337].

BIOLOGICAL ACTIVITY: *In vitro* antileishmanial activity [337]; Cytotoxicity [337].

1,1′-(4-Butoxy-2,6-dihydroxy-1,3-phenylene)bis-3-methyl-1-butanone

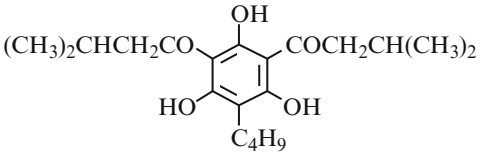
[1103524-21-5] $C_{20}H_{30}O_5$ mol. wt. 350.46



Synthesis
-Obtained by treatment of 2,4-diisovaleryl-phloroglucinol with 1-bromobutane (4 equiv.) in the presence of potassium carbonate in acetone at r.t. for 10 h (10 %) [338].

1,1′-(5-Butyl-2,4,6-trihydroxy-1,3-phenylene)bis-3-methyl-1-butanone

[1103524-22-6] $C_{20}H_{30}O_5$ mol. wt. 350.46

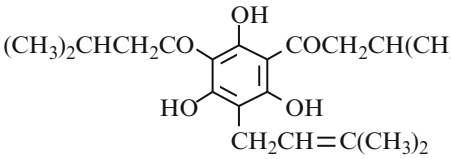


Synthesis
-Obtained by reaction of butyl bromide with 2,4,6-trihydroxy-3-isovaleryliso-valerophenone in the presence of sodium methoxide in refluxing methanol for 2 h (60 %) [338].

yellow oil [338]; ^{1}H NMR [338], MS [338].

1,1′-[2,4,6-Trihydroxy-5-(3-methyl-2-butenyl)-1,3-phenylene]bis-3-methyl-1-butanone

[216301-02-9] $C_{21}H_{30}O_5$ mol. wt. 362.47

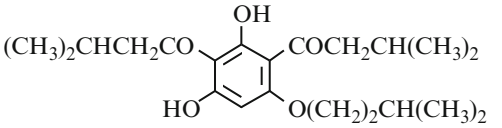


Synthesis
-Refer to: [2684].

BIOLOGICAL ACTIVITY: For the prevention and treatment of bone and cartilage diseases [2684].

1,1′-[2,4-Dihydroxy-6-(3-methylbutoxy)-1,3-phenylene]bis-3-methyl-1-butanone

[918814-65-0] $C_{21}H_{32}O_5$ mol. wt. 364.48



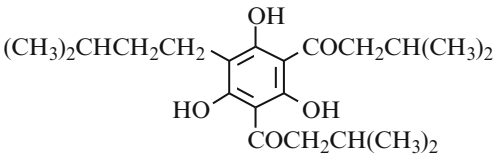
Synthesis
-Obtained by Friedel-Crafts acylation of phloroglucinol monoisopentyl ether with isopentanoyl chloride in the presence of titanium tetrachloride (17 %) [337].

yellow solid [337]; m.p. 65–67° [337];
^{1}H NMR [337], ^{13}C NMR [337], IR [337], UV [337], MS [337].

BIOLOGICAL ACTIVITY: Antiprotozoal and antimicrobial [337].

1,1′-[2,4,6-Trihydroxy-5-(3-methylbutyl)-1,3-phenylene]bis-3-methyl-1-butanone

[26104-02-9] $C_{21}H_{32}O_5$ mol. wt. 364.48

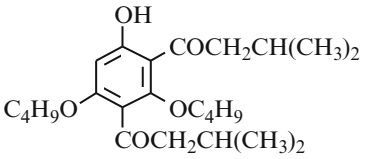


Synthesis
-Obtained by reaction of isovaleryl chloride with 2-isopentylphloroglucinol in the presence of aluminium chloride in nitrobenzene at 0° for 3 days (1 %) (**XIV**) [898].

m.p. 109.5–111° [898]; ^{1}H NMR [898], UV [898], MS [898].

1,1′-(2,4-Dibutoxy-6-hydroxy-1,3-phenylene)bis-3-methyl-1-butanone

[1103524-20-4] $C_{24}H_{38}O_5$ mol. wt. 406.56

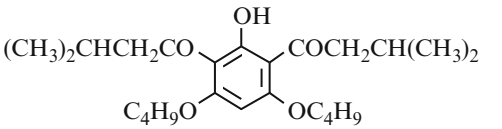


Synthesis
-Obtained by reaction of n-butyl bromide with 2,4-diisovaleroylphloroglucinol in the presence of potassium carbonate in acetone at r.t. for 10 h (15 %) [338].

BIOLOGICAL ACTIVITY: A new class of GPR40 (FFAR1) agonists [338].

1,1′-(4,6-Dibutoxy-2-hydroxy-1,3-phenylene)bis-3-methyl-1-butanone

[1103524-19-1] $C_{24}H_{38}O_5$ mol. wt. 406.56



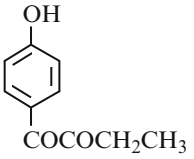
Synthesis
-Obtained by reaction of n-butyl bromide with 2,4-diisovaleroylphloroglucinol in the presence of potassium carbonate in acetone at r.t. for 10 h (25 %) [338].

BIOLOGICAL ACTIVITY: A new class of GPR40 (FFAR1) agonists [338].

4 Aromatic Hydroxy-1,2-Butanediones

1-(4-Hydroxyphenyl)-1,2-butanedione

$C_{10}H_{10}O_3$ mol. wt. 178.19



Synthesis
-Refer to: [2165].

Methyl ether [10201-46-4]
$C_{11}H_{12}O_3$ mol. wt. 192.21

-Obtained by treatment of 1-(4-methoxyphenyl)-1-propyne with PdI_2 (2 mol%) in dimethyl sulfoxide at 140° for 1.5 h (58 %) [2165].
-Also refer to: [1114, 1405, 2986, 3217, 3230, 3232, 3307].

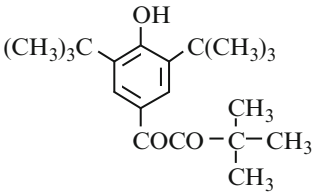
b.p.$_{0.2}$ 120–123° [3307], b.p.$_1$ 155° [1405], b.p.$_{25}$ 168–170° [3232];
^{1}H NMR [3232], IR [3232]; $n_D^{20} = 1.5480$ [3307].

Dioxime of the methyl ether [10262-13-2] $C_{11}H_{14}N_2O_3$ mol. wt. 222.24

m.p. 207–208° [3307].

1-[3,5-(1,1-Dimethylethyl)-4-hydroxyphenyl]-3,3-dimethyl-1,2-butanedione

[96251-01-3] $C_{20}H_{30}O_3$ mol. wt. 318.46



Syntheses
-Obtained by oxygenation of 1-[3,5-(dimethylethyl)-4-hydroxyphenyl]-3,3-dimethyl-1-butyne with Co(Salpr) in methylene chloride at 0° (56 %) [2290].
-Also refer to: [2007, 2289].

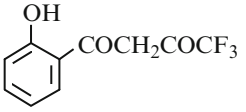
colourless prisms [2290]; m.p. 136–137° [2289, 2290];
^{1}H NMR [2007, 2289, 2290], ^{13}C NMR [2007],
IR [2289, 2290], UV [2290].

5 Aromatic Hydroxy-1,3-Butanediones

5.1 Unsubstituted Aromatic Ring

1-(2-Hydroxyphenyl)-4,4,4-trifluoro-1,3-butanedione

$C_{10}H_7F_3O_3$ mol. wt. 232.16



Synthesis
-Obtained by treatment of o-hydroxyacetophenone trifluoroacetate with base (pyridine/potassium hydroxide) (Baker-Venkataraman rearrangement) [1564].

Methyl ether [15191-69-2] $C_{11}H_9F_3O_3$ mol. wt. 246.19

b.p. 262° [2902]; m.p. 36–38° [1086];
^{1}H NMR [2902], ^{13}C NMR [2902], MS [1086].

2-Bromo-1-(4-hydroxyphenyl)-1,3-butanedione

$C_{10}H_9BrO_3$ mol. wt. 257.08

Synthesis
-Refer to: [1094].
Methyl ether [91065-87-1]
$C_{11}H_{11}BrO_3$ mol. wt. 271.11
-Obtained by treatment of the sodium or copper salts of 1-(4-methoxyphenyl)-1,3-butanedione with bromine in cooled carbon tetrachloride [1094].

-Also refer to: [2628].

Dirty white [1094]; m.p. 39° [1094].

2-Chloro-1-(2-hydroxyphenyl)-1,3-butanedione

$C_{10}H_9ClO_3$ mol. wt. 212.63

Synthesis
-Refer to: [3400].

Methyl ether [1001024-95-8]
$C_{11}H_{11}ClO_3$ mol. wt. 226.66
-Obtained by reaction of N-chlorosuccinimide with 1-(2-hydroxyphenyl)-1,3-butanedione in refluxing carbon tetrachloride for 4 h at 75–80° (47 %) [3400].

yellow oil [3400];
^{1}H NMR [3400], ^{13}C NMR [3400], MS [3400]; GC-MS [3400].

1-(2-Hydroxyphenyl)-1,3-butanedione

[16636-62-7] $C_{10}H_{10}O_3$ mol. wt. 178.19

Syntheses
-Obtained by adding a solution of 2-hydroxyacetophenone in ethyl acetate to a suspension of pulverized sodium in ether [168, 947, (65 %) 3325].
-Also obtained by treatment of o-acetoxyacetophenone with metallic sodium in refluxing benzene for 3 h (poor yield) [3234].
-Also refer to: [383, 919, 1108, 1564, 3400].

colourless needles [3325]; pale yellow plates [3234];
m.p. 110° [1110], 102° [3234], 101° [234], 98° [1109], 90.5–91.5° [3325];
^{1}H NMR [919, 2288, 2807, 3459], ^{13}C NMR [3459], UV [3317], MS [2968].

Methyl ether [56290-53-0] $C_{11}H_{12}O_3$ mol. wt. 192.21

-Obtained by reaction of 2-methoxybenzoyl chloride with acetone in the presence of LDA (1.5 equiv.) in tetrahydrofuran (37 %) [3400].
-Also obtained from 2-methoxyacetophenone [2677].
-Also obtained from methyl 2-methoxybenzoate and acetone [383].
-Also refer to: [168, 942, 1011, 1207, 1413, 1856, 2313, 2526, 2628, 2935, 3259, 3459, 3463].

b.p.$_{20}$ 173–174° [2677];
m.p. 37° [2677], 36–37° [383], 36° [942];
^{1}H NMR [3459], ^{13}C NMR [3459].

Copper (II) salt $C_{22}H_{22}O_6Cu$ mol. wt. 445.96

m.p. 153° [2313].

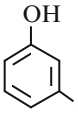
Ethyl ether [60159-70-8] $C_{12}H_{14}O_3$ mol. wt. 206.24

-Obtained by reaction of 2-ethoxyacetophenone with ethyl acetate in the presence of sodium ethoxide [3083].

m.p. 58° [328], 57–58° [3083], 54–56° [101]; ^{1}H NMR [101], IR [101], UV [3083].

1-(3-Hydroxyphenyl)-1,3-butanedione

$C_{10}H_{10}O_3$ mol. wt. 178.19



Synthesis
-Refer to: [3384].

Methyl ether [29681-99-0]
$C_{11}H_{12}O_3$ mol. wt. 192.21

-Obtained by reaction of 3-methoxyacetophenone with ethyl acetate in the presence of sodium ethoxide [3083].
-Also obtained by Claisen condensation between ethyl acetate and m-methoxyacetophenone in the presence of sodium amide [313].
-Also refer to: [34, 168, 314, 316, 1192, 1193, 1206, 1214, 2628, 2935, 3384].

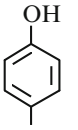
b.p.$_1$ 115° [313], b.p. 280–283° [3083];
UV [313, 314, 316, 3083];
pK [313]; $n_D^{25} = 1.5930$ [313].

Cu salt $C_{22}H_{22}O_6Cu$ mol. wt. 445.96

-Refer to: [313]; m.p. 150° [313].

1-(4-Hydroxyphenyl)-1,3-butanedione

[51944-08-2] $C_{10}H_{10}O_3$ mol. wt. 178.19



Syntheses
-Obtained by treatment of p-acetoxyacetophenone in acetic anhydride with boron trifluoride-acetic acid complex for 2.5 h (78 %) [1538].
-Also obtained by treatment of its acetate with sodium hydroxide in refluxing dilute methanol for 35 min [1538].
-Also refer to: [45, 294, 675, 774, 1292, 1433, 3384].

m.p. 114–116° [1433], 112–112.5° [1538], 112° [675];
^{1}H NMR [1433], IR [1433], UV [1433].

Be salt $C_{20}H_{18}O_6Be$ mol. wt. 363.37

-Refer to: [1538 (84 %)].

m.p. 255° [1538].

Cu salt $C_{20}H_{18}O_6Cu$ mol. wt. 417.91

-Refer to: [1538 (99 %)].

m.p. 280–282° [1538].

Mg salt $C_{20}H_{18}O_6Mg$ mol. wt. 378.66

-Refer to: [1538].

m.p. >300° [1538].

Zn salt $C_{20}H_{18}O_6Zn$ mol. wt. 419.75

-Refer to: [1538].

m.p. >300° [1538].

Acetate [91963-55-2] $C_{12}H_{12}O_4$ mol. wt. 220.23

-Obtained by action of acetic anhydride with p-hydroxybenzoylacetone in the presence of aqueous sodium hydroxide [1538].

m.p. 70–70.5° [1538], 70° [675].

Cu salt of the acetate $C_{24}H_{22}O_8Cu$ mol. wt. 501.20

m.p. 248° [1538].

Methyl ether [4023-80-7] $C_{11}H_{12}O_3$ mol. wt. 192.21

-Obtained by reaction of 4-methoxyacetophenone with ethyl acetate in the presence of sodium ethoxide [327, 3083].
-Also obtained by Claisen condensation between ethyl acetate and p-methoxyacetophenone in the presence of sodium amide [313].
-Obtained [2072] according to [2676].
-Also refer to: [45, 237, 294, 295, 314–316, 327, 330, 575, 612, 629, 630, 697, 744, 745, 774, 800, 819, 904, 960, 1015, 1031, 1072, 1094, 1141, 1190, 1191, 1207, 1214, 1220, 1241, 1275, 1292, 1350, 1433, 1920, 1952, 1959, 1976, 2230, 2502, 2525, 2853, 2872, 2897, 2898, 3257, 3359, 3360, 3384, 3446].

m.p. 57–58° [1433], 57° [612], 56.5° [2525], 55° [295],
54.5° [327, 1920], 54° [237, 1275, 1338, 1350, 2502], 53–54° [330], 53° [313],
52–54° [3083], 52–53° [1072, 1241], 51–53° [629], 48–51° [2230],
48–49° [2072];

^{1}H NMR [819, 1220, 1241, 1433, 1920, 2230], ^{13}C NMR [745, 1220, 2230], IR [819, 1031, 1241, 1433, 1920, 2230], UV [313, 314, 316, 1031, 1433, 1920, 3083],
MS [697, 1015, 1959, 2230].

Na salt $C_{11}H_{11}O_3Na$ mol. wt. 215.20

-Refer to: [1094 (58 %)].

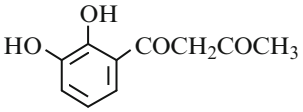
Cu salt $C_{22}H_{22}O_6Cu$ mol. wt. 445.96

-Refer to: [313, 1094 (60 %), 1920].

m.p. 229° [313], 220° [1920].

1-(2,3-Dihydroxyphenyl)-1,3-butanedione

$C_{10}H_{10}O_4$ mol. wt. 194.19



Synthesis
-Refer to: [48].
Dimethyl ether [65547-52-6]
$C_{12}H_{14}O_4$ mol. wt. 222.24

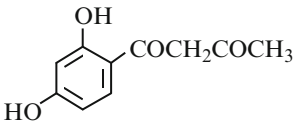
-Preparation from 2,3-dimethoxyacetophenone on Claisen condensation with ethyl acetate in the presence of pulverized sodium [48].
N.B.: Ratio of the keto and enol forms 1:3.

-Refer to: [48].

light yellow liquid [48]; ^{1}H NMR [48].

1-(2,4-Dihydroxyphenyl)-1,3-butanedione

$C_{10}H_{10}O_4$ mol. wt. 194.19



Synthesis
-Refer to: [48].
Dimethyl ether [65547-54-8]
$C_{12}H_{14}O_4$ mol. wt. 222.24

-Preparation from 2,4-dimethoxyacetophenone (68 %) [2677].
-Preparation from 2,4-dimethoxyacetophenone on Claisen condensation with ethyl acetate in the presence of pulverized sodium [48, 3313].
-Preparation from 2,4-dimethoxybenzoyl chloride (75 %) [2914].
-Also refer to: [276, 1193, 1206, 2780].
N.B.: Ratio of the keto and enol forms 1:2 [48].

yellow glistening needles [48];
m.p. 68–69° [48], 67–68° [2914], 58.5° [2677];
^{1}H NMR [48, 2914], ^{13}C NMR [2914], IR [2914].

BIOLOGICAL ACTIVITY: As bronchodilatator [3313].

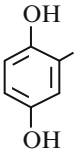
Diethyl ether $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of 2,4-diethoxyacetophenone with ethyl acetate in the presence of sodium [3083].
-Also refer to: [382, 1740].

m.p. 90° [382, 3083]; UV [3083].

1-(2,5-Dihydroxyphenyl)-1,3-butanedione

$C_{10}H_{10}O_4$ mol. wt. 194.19



Synthesis
-Refer to: [3313].
Dimethyl ether [65547-50-4]
$C_{12}H_{14}O_4$ mol. wt. 222.24

-Preparation from 2,5-dimethoxyacetophenone on Claisen condensation with ethyl acetate in the presence of pulverized sodium (49 %) [48, 3313].
N.B.: Ratio of the keto and enol forms 1:2.
-Also refer to: [48, 168, 1206, 3312].

light yellow liquid [48]; $b.p._{\cdot 0.1}$ 97° [3312]; ^1H NMR [48];
$n_D^{25} = 1.5893$ [3312].

BIOLOGICAL ACTIVITY: As bronchodilatator [3313].

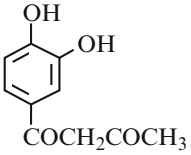
Diethyl ether $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of 2,5-diethoxyacetophenone with ethyl acetate in the presence of sodium [3083].
-Also refer to: [752].

m.p. 60° [752], 58–59° [3083]; UV [3083].

1-(3,4-Dihydroxyphenyl)-1,3-butanedione

$C_{10}H_{10}O_4$ mol. wt. 194.19



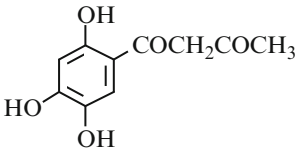
Synthesis
-Refer to: [3083].
Dimethyl ether [13298-49-2]
$C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by reaction of 3,4-dimethoxyacetophenone with ethyl acetate in the presence of sodium [3083].

$b.p._{\cdot 0.05}$ 132° [1338]; m.p. 71–72° [3083], 69–71° [464], 62° [1338];
IR [464], UV [464, 3083], MS [1959].

1-(2,4,5-Trihydroxyphenyl)-1,3-butanedione

$C_{10}H_{10}O_5$ mol. wt. 210.19



Synthesis
-Refer to: [834].
Trimethyl ether [62406-99-9]
$C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained by gently heating a mixture of 2,4,5-trimethoxyacetophenone, sodium sand and ethyl acetate until a vigorous reaction set in, then to heat the mixture at reflux for 2 h (76 %) [834].
N.B.: Ratio of the keto and enol forms 1:9
-Also refer to: [48].

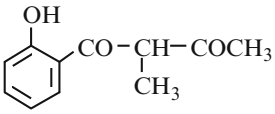
pale yellow plates [834]; m.p. 89° [834];
^{1}H NMR [48, 834], IR [834].

Na salt $C_{13}H_{15}O_5Na$ mol. wt. 274.25

m.p. 201° (d) [834].

1-(2-Hydroxyphenyl)-2-methyl-1,3-butanedione

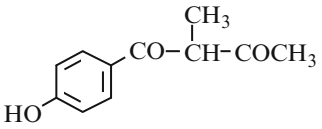
[35115-14-1] $C_{11}H_{12}O_3$ mol. wt. 192.21



Synthesis
-Obtained by treatment of 2,3-dimethylchromone with dilute alkali [1126].
b.p.$_7$ 130° [2288]; ^{1}H NMR [2288].

1-(4-Hydroxyphenyl)-2-methyl-1,3-butanedione

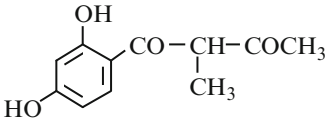
[91142-94-8] $C_{11}H_{12}O_3$ mol. wt. 192.21



Synthesis
-Refer to: [675].
m.p. 59–60° [675].

1-(2,4-Dihydroxyphenyl)-2-methyl-1,3-butanedione

$C_{11}H_{12}O_4$ mol. wt. 208.21



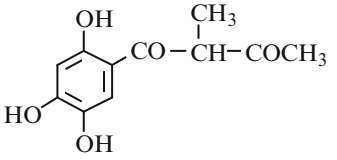
Synthesis
-Refer to: [1740].
Diethyl ether $C_{15}H_{20}O_4$ mol. wt. 264.32

-Obtained by reaction of ethyl acetate with 2,4-diethoxypropiophenone in the presence of pulverized sodium [1740].

m.p. 72.5° [1740].

1-(2,4,5-Trihydroxyphenyl)-2-methyl-1,3-butanedione

$C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis
-Refer to: [834].
Trimethyl ether [62407-00-5]
$C_{14}H_{18}O_5$ mol. wt. 266.29

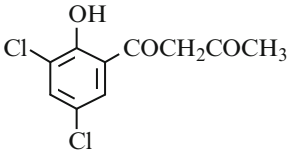
-Obtained by adding 1-(2,4,5-trihydroxyphenyl)-1,3-butanedione in THF to 50 % sodium hydride dispersion in oil. After isolation of the sodium salt, this one was warmed with methyl iodide for 4 h (64 %) [834].

pale yellow plates [834]; m.p. 114.5° [834];
^{1}H NMR [834], IR [834].

5.2 Substituted Aromatic Ring

1-(3,5-Dichloro-2-hydroxyphenyl)-1,3-butanedione

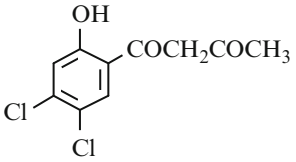
$C_{10}H_8Cl_2O_3$ mol. wt. 247.08



Synthesis
-Obtained by treatment of 3,5-dichloro-2-hydroxyacetophenone with ethyl acetate and sodium metal [947].

1-(4,5-Dichloro-2-hydroxyphenyl)-1,3-butanedione

[111477-92-0] $C_{10}H_8Cl_2O_3$ mol. wt. 247.08

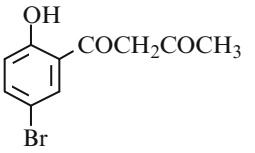


Syntheses
-Obtained by treatment of 4,5-dichloro-2-hydroxyacetophenone with ethyl acetate and sodium metal [947].
-Also refer to: [1889, 2472].

m.p. 134–135° [1889, 2472].

1-(5-Bromo-2-hydroxyphenyl)-1,3-butanedione

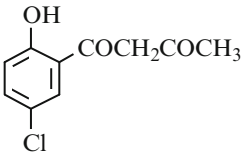
$C_{10}H_9BrO_3$ mol. wt. 257.08



Syntheses
-Obtained by treatment of 5-bromo-2-hydroxyacetophenone with ethyl acetate and sodium metal [947].
-Also refer to: [1564].

1-(5-Chloro-2-hydroxyphenyl)-1,3-butanedione

[65897-66-7] $C_{10}H_9ClO_3$ mol. wt. 212.63



Syntheses
-Obtained by treatment of 5-chloro-2-hydroxyacetophenone with ethyl acetate and sodium metal [947].
-Also refer to: [1109, 1110, 1564, 2691, 3324, 3325].

pale yellow crystals [3324];
m.p. 121° [1109], 118° [1110], 113–114° [2691], 110–111° [3324, 3325];
^{1}H NMR [2691], ^{13}C NMR [2691], IR [2691].

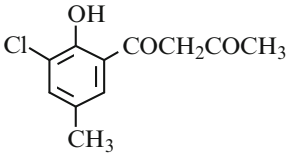
Methyl ether [861349-33-9] $C_{11}H_{11}ClO_3$ mol. wt. 226.66

-Obtained by treatment of 5-chloro-2-methoxyacetophenone with ethyl acetate in the presence of sodium [3324].

m.p. 76.5–77.5° [3324].

1-(3-Chloro-2-hydroxy-5-methylphenyl)-1,3-butanedione

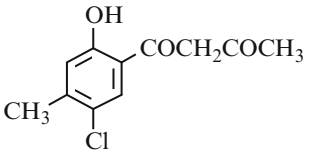
$C_{11}H_{11}ClO_3$ mol. wt. 226.66



Synthesis
-Obtained by treatment of 3-chloro-2-hydroxy-5-methyl-acetophenone with ethyl acetate and sodium metal [947].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1,3-butanedione

[152153-24-7] $C_{11}H_{11}ClO_3$ mol. wt. 226.66

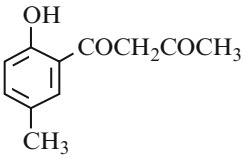


Syntheses
-Obtained by treatment of 5-chloro-2-hydroxy-4-methyl-acetophenone with ethyl acetate and sodium metal [947].
-Also refer to: [3324, 3325].

pale yellow crystals [3324]; m.p. 115.5–116.5° [3324, 3325].

1-(2-Hydroxy-5-methylphenyl)-1,3-butanedione

[16636-64-9] $C_{11}H_{12}O_3$ mol. wt. 192.21



Syntheses
-Obtained by adding a solution of 2-hydroxy-5-methylacetophenone in ethyl acetate to a suspension of pulverized sodium in ether, [(64 %) 235, 947, (60 %) 3325].
-Also refer to: [268, 919, 1108–1110, 1011, 2745, 2746, 3324].

colourless needles [3325]; compact prisms [235];
m.p. 112° [1110], 110° [1108], 102° [1109], 99° [235], 94.5–96° [3324, 3325], 94–96° [268]; ^{1}H NMR [919].

Dioxime [56686-34-1] $C_{11}H_{14}N_2O_3$ mol. wt. 222.24

m.p. 122–123° [268, 1011]; ^{1}H NMR [268].

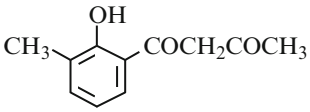
Methyl ether [56290-52-9] $C_{12}H_{14}O_3$ mol. wt. 206.24

-Obtained by condensation of ethyl acetate with 2-methoxy-5-methylacetophenone [193].
-Also refer to: [942, 1338].

b.p.$_{0.1}$ 115° [942, 1338], b.p.$_{15}$ 182–183° [193]; $n_D^{17.9} = 1.5758$ [193].

1-(2-Hydroxy-3-methylphenyl)-1,3-butanedione

[58218-17-0] $C_{11}H_{12}O_3$ mol. wt. 192.21



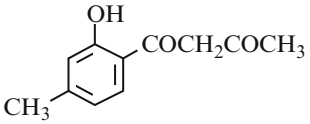
Synthesis
-Refer to: [3325].
m.p. 85–86° [3325], 84–85° [268].

Dioxime [56686-30-7] $C_{11}H_{14}N_2O_3$ mol. wt. 222.24

m.p. 150–151° [3325], 148–149° [268]; ^{1}H NMR [268].

1-(2-Hydroxy-4-methylphenyl)-1,3-butanedione

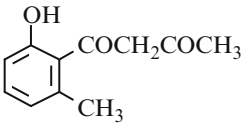
[58218-16-9] $C_{11}H_{12}O_3$ mol. wt. 192.21



Synthesis
-Refer to: [3325].
m.p. 76–77° [3325].

1-(2-Hydroxy-6-methylphenyl)-1,3-butanedione

$C_{11}H_{12}O_3$ mol. wt. 192.21

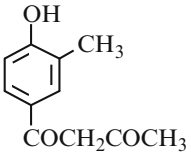


Synthesis
-Obtained by adding a solution of 2-hydroxy-6-methylacetophenone in ethyl acetate to a suspension of pulverized sodium in ether (85–90 %) [3325].

colourless needles [3325]; m.p. 85–86° [3325].

1-(4-Hydroxy-3-methylphenyl)-1,3-butanedione

[92016-84-7] $C_{11}H_{12}O_3$ mol. wt. 192.21



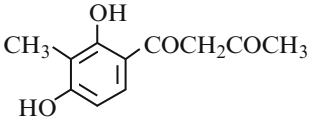
Synthesis
-Preparation from 4-acetoxy-3-methylacetophenone [1538].
m.p. 95–96° [1538].

Copper salt $C_{22}H_{22}O_6Cu$ mol. wt. 445.96

m.p. 280–282° [1538].

1-(2,4-Dihydroxy-3-methylphenyl)-1,3-butanedione

$C_{11}H_{12}O_4$ mol. wt. 208.21



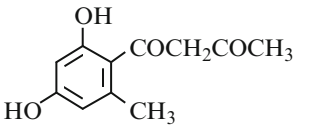
Synthesis
-Refer to: [55].
Dimethyl ether [124259-63-8]
$C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by treatment of 2,4-dimethoxy-3-methylacetophenone with ethyl acetate and sodium metal (65 %) [55].

oil [55]; ^{1}H NMR [55].

1-(2,4-Dihydroxy-6-methylphenyl)-1,3-butanedione

$C_{11}H_{12}O_4$ mol. wt. 208.21



Synthesis
-Refer to: [55].
Dimethyl ether [53270-35-2]
$C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by deacetalisation of 1-(2,4-dimethoxy-6-methylphenyl)-2-(2-methyl-1,3-dioxolan-2-yl)ethanone (m.p. 54°) with concentrated hydrochloric acid in dilute acetone (95 %) [1330].

-Also obtained by decarboxylation of 5-(2,4-dimethoxy-6-methylphenyl)-3,5-dioxo-1-pentanoic acid on heating [2974] in refluxing chloroform for 5 h in a stream nitrogen (95 %) [1330].
-Also obtained by refluxing a mixture of 2,4-dimethoxy-6-methylacetophenone, ethyl acetate and sodium metal [2974] for 1 h (115–120°) (88 %) [47], (68 %) [55], (62 %) [2813].
-Also refer to: [1168].

yellow needles [47];
m.p. 77–78° [1168], 74–76° [47, 55, 2813], 72–73° [454, 1330, 2974], 65–66.5° [1259];
^{1}H NMR [47, 55, 454, 1330, 2974], IR [454, 1330, 2974], UV [1330, 2974], MS [454, 1330, 2974].

N.B.: In the paper [55], this compound is called by error 3-(**2′,6′**-dimethoxy-**3′**-methylphenyl)-1-methylpropane-1,3-dione.

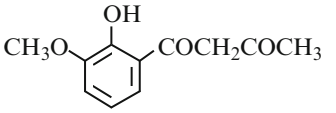
Dibenzyl ether [82883-60-1] $C_{25}H_{24}O_4$ mol. wt. 388.46

-Obtained by deacetalisation of 1-(2,4-dibenzyloxy-6-methylphenyl)-2-(2-methyl-1,3-dioxolan-2-yl)ethanone (m.p. 82–83°) with concentrated hydrochloric acid in dilute acetone (97 %) [454].
-Also refer to: [453, 455].

m.p. 83° [453, 454];
^{1}H NMR [453, 454], IR [453, 454], MS [454].

1-(2-Hydroxy-3-methoxyphenyl)-1,3-butanedione

[65547-78-6] $C_{11}H_{12}O_4$ mol. wt. 208.21

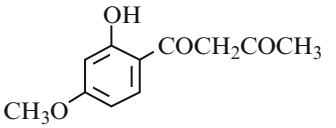


Synthesis
-Obtained by adding a solution of 2-hydroxy-3-methoxy-acetophenone in ethyl acetate to a suspension of pulverized sodium in ether, then to warm at reflux for 3 h (48 %) [48].

yellow small needles [48]; m.p. 66–68° [48]; ^{1}H NMR [48].

1-(2-Hydroxy-4-methoxyphenyl)-1,3-butanedione

[101396-11-6] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Obtained by treatment of 2-acetoxy-4-methoxy-acetophenone with metallic sodium in refluxing benzene for 3 h (poor yield) [3234].
-Also obtained from 7-methoxy-2-methyl-4*H*-1-benzopyran-4-one [1740].

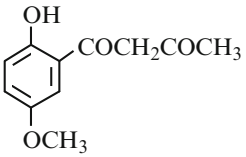
-Also refer to: [234, 276, 2216, 2780].

yellowish brown needles [3234];
m.p. 75° [3234], 71–72° [234], 68° [2216].

Copper salt Refer to: [3234].

1-(2-Hydroxy-5-methoxyphenyl)-1,3-butanedione

[65547-81-1] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Obtained by adding a solution of 2-hydroxy-5-methoxyacetophenone in ethyl acetate to a suspension of pulverized sodium in ether (64 %) [48, 3312, 3313].
-Also obtained by catalytic debenzylation of 2-benzyloxy-4,5-dimethoxybenzoylacetone in the presence of 5 % Pd/C in ethyl acetate (quantitative yield) [48].
-Also obtained by irradiation of 4-methoxyphenyl 3-oxobutanoate with a 125 W medium pressure mercury lamp inside a quartz immersion well in for 6 h at r.t. (25 %) [96].
-Also obtained by treatment of 3-(ethylenedioxy)-1-(2-hydroxy-5-methoxylphenyl)-1-butanone with dilute sulfuric acid in the presence of silica gel [96].
-Also obtained by reaction of 2-hydroxy-5-methoxyacetophenone with ethyl acetate in the presence of sodium hydride [1540].

yellow needles [48];
m.p. 102–104° [3312], 102–103° [48], 101–102° [1540];
^{1}H NMR [48, 96], IR [48].

BIOLOGICAL ACTIVITY: As bronchodilatator [3313].

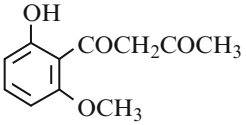
Benzyl ether [65547-83-3] $C_{18}H_{18}O_4$ mol. wt. 298.34

-Obtained by Claisen condensation of 2-benzyloxy-5-methoxyacetophenone (m.p. 44–45°) with ethyl acetate (quantitative yield) [48].

yellowish needles [48]; m.p. 59–60° [48].

1-(2-Hydroxy-6-methoxyphenyl)-1,3-butanedione

[65547-63-9] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Obtained by adding a solution of 2-hydroxy-6-methoxyacetophenone in ethyl acetate to a suspension of pulverized sodium [48], (48 %) [2564].

colourless needles [48, 2564]; m.p. 96–97° [48], 94–95° [2564];
^{1}H NMR [2968], ^{13}C NMR [2968], MS [2968].

Copper salt green crystals [2564];

m.p. 226° [2564].

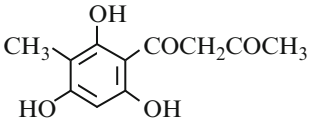
Methyl ether [32085-87-3] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Preparation from 2,6-dimethoxyacetophenone on Claisen condensation with ethyl acetate in the presence of pulverized sodium (57 %) [48].
N.B.: Ratio of the keto and enol forms 1:2.

colourless needles [48]; b.p.$_{5-6}$ 178–180° [240]; m.p. 49–50° [48]; ^{1}H NMR [48].

1-(2,4,6-Trihydroxy-3-methylphenyl)-1,3-butanedione

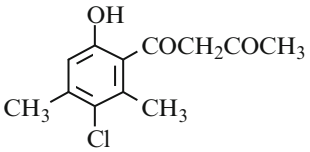
$C_{11}H_{12}O_5$ mol. wt. 224.21



Syntheses
-Refer to: [2178, 2755].

1-(5-Chloro-2-hydroxy-4,6-dimethylphenyl)-1,3-butanedione

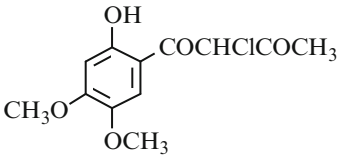
[855242-08-9] $C_{12}H_{13}ClO_3$ mol. wt. 240.69



Synthesis
-Refer to: [24].
m.p. 116–117° [24].

1-(2-Hydroxy-4,5-dimethoxyphenyl)-2-chloro-1,3-butanedione

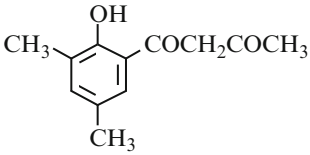
$C_{12}H_{13}ClO_5$ mol. wt. 272.68



Synthesis
-Refer to: [1537].

1-(2-Hydroxy-3,5-dimethylphenyl)-1,3-butanedione

[104516-36-1] $C_{12}H_{14}O_3$ mol. wt. 206.24



Syntheses
-Obtained by adding a solution of 2-hydroxy-3,5-dimethyl-acetophenone in ethyl acetate to a suspension of pulverized sodium in ether (75–80 %) [3325].
-Also refer to: [1016].

colourless needles [3325]; m.p. 116–117° [3325], 85° [1016].

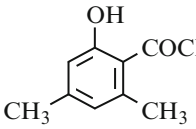
Methyl ether $C_{13}H_{16}O_3$ mol. wt. 220.27

-Obtained by adding a solution of 2-methoxy-3,5-dimethylacetophenone in ethyl acetate to a suspension of pulverized sodium in ether (57 %) [3325].

colourless needles [3325]; m.p. 59–60° [3325].

1-(2-Hydroxy-4,6-dimethylphenyl)-1,3-butanedione

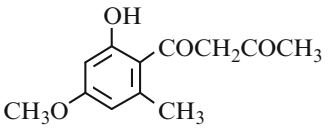
[861778-02-1] $C_{12}H_{14}O_3$ mol. wt. 206.24



Syntheses
-Refer to: [3325].
m.p. 116–117° [3325].

1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1,3-butanedione

[58530-24-8] $C_{12}H_{14}O_4$ mol. wt. 222.24



Syntheses
-Obtained by refluxing a mixture of 2-hydroxy-4-methoxy-6-methylacetophenone, ethyl acetate, ethyl ether and sodium metal for 4 h (65 %) [47].
-Also obtained by decarboxylation of 5-(2-hydroxy-4-methoxy-6-methylphenyl)-3,5-dioxopentanoic acid on heating [2974].
-Also refer to: [53].

yellow needles [47]; m.p. 142–144° [47].

Benzyl ether [68436-75-9] $C_{19}H_{20}O_4$ mol. wt. 312.37

-Obtained by adding a solution of 2-hydroxy-4-methoxy-6-methylacetophenone in ethyl acetate to a suspension of pulverized sodium in ether. The mixture was refluxed on a water bath for 2–3 h (58 %) [53].
N.B.: Ratio of the keto and enol forms 1:5

colourless needles [53]; m.p. 76–77° [53]; ^{1}H NMR [53].

Allyl ether [75160-45-1] $C_{15}H_{18}O_4$ mol. wt. 262.31

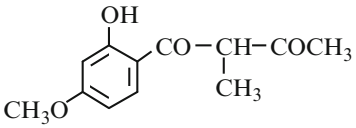
-Obtained by adding a solution of 2-allyloxy-4-methoxy-6-methylacetophenone in ethyl acetate to pulverized sodium in ethyl ether.
Then, the mixture was refluxed on a water bath for 3 h (56 %) [54].

-Refer to: [1127, 2559].

b.p.$_{0.3}$ 135–136° [2559], b.p.$_1$ 149–152° [1127];
light brown needles [54]; m.p. 47–49° [54]; ^{1}H NMR [54].

1-(2-Hydroxy-4-methoxyphenyl)-2-methyl-1,3-butanedione

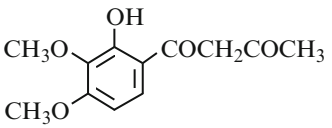
$C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Refer to: [1740].

1-(2-Hydroxy-3,4-dimethoxyphenyl)-1,3-butanedione

[65547-75-3] $C_{12}H_{14}O_5$ mol. wt. 238.24



Synthesis
-Obtained by adding a solution of 2-hydroxy-3,4-dimethoxyacetophenone in ethyl acetate to a suspension of pulverized sodium in ether [48, 3313].

yellow needles [48]; m.p. 107–108° [48], 104–107° [3312]; ^{1}H NMR [48], IR [48].

BIOLOGICAL ACTIVITY: As bronchodilatator [3313].

Methyl ether [65547-48-0] $C_{13}H_{16}O_5$ mol. wt. 252.27

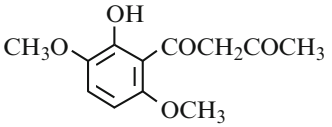
-Preparation from 2,3,4-trimethoxyacetophenone on Claisen condensation with ethyl acetate in the presence of pulverized sodium [48, 3313].
N.B.: Ratio of the keto and enol forms 1:9 [48].

colourless glistening plates [48]; b.p.$_{20}$ 217° [482]; m.p. 65° [384], 64–65° [48], 59–60° [482]; ^{1}H NMR [48].

BIOLOGICAL ACTIVITY: As bronchodilatator [3313].

1-(2-Hydroxy-3,6-dimethoxyphenyl)-1,3-butanedione

[65547-62-8] $C_{12}H_{14}O_5$ mol. wt. 238.24



Syntheses
-Obtained by adding a solution of 2-hydroxy-3,6-dimethoxyacetophenone in ethyl acetate to a suspension of pulverized sodium,
*in ethyl ether (33 %) [48];

*in methanol (65 %) [3206].

yellow needles [48]; m.p. 113–114° [48], 112–114° [3206].

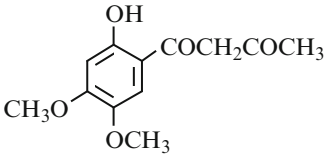
Methyl ether [65547-46-8] $C_{13}H_{16}O_5$ mol. wt. 252.27

-Preparation from 2,3,6-trimethoxyacetophenone on Claisen condensation with ethyl acetate in the presence of pulverized sodium [48].
N.B.: Ratio of the keto and enol forms 1:2.

yellow needles [48]; m.p. 87–89° [48]; ^{1}H NMR [48].

1-(2-Hydroxy-4,5-dimethoxyphenyl)-1,3-butanedione

[65547-68-4] $C_{12}H_{14}O_5$ mol. wt. 238.24



Syntheses
-Obtained by adding a solution of 2-hydroxy-4,5-dimethoxyacetophenone in ethyl acetate to a suspension of pulverized sodium in ether. [48].
-Also obtained by catalytic debenzylation of 2-benzyloxy-4,5-dimethoxybenzoylacetone in the presence of 5 % Pd/C for 6 h (quantitative yield) [48].

yellow needles [48]; b.p.$_{0.01}$ 130° [1537];
m.p. 110–111° [48], 109° [1537];
^{1}H NMR [48].

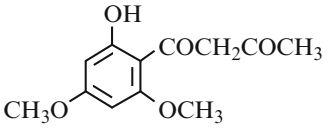
Benzyl ether [65547-70-8] $C_{19}H_{20}O_5$ mol. wt. 328.36

-Obtained by Claisen condensation of 2-benzyloxy-4,5-dimethoxyacetophenone (m.p. 121°) with ethyl acetate (70 %) [48].

yellow needles [48]; m.p. 151° [48].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-1,3-butanedione

[65547-60-6] $C_{12}H_{14}O_5$ mol. wt. 238.24



Syntheses
-Obtained by adding a solution of 2-hydroxy-4,6-dimethoxyacetophenone in ethyl acetate to a suspension of pulverized sodium in ether. Then, the mixture was refluxed for 1.5 h (67 %) [48], (37 %) [3313].

N.B.: Ratio of the keto and enol forms 3:1 [48].

-Also refer to: [2144, 2178].

colourless cubic crystals [48]; white solid [3313];
m.p. 83–85° [3313], 82–83° [48], 82° [1943];
^{1}H NMR [48], IR [48].

BIOLOGICAL ACTIVITY: As bronchodilatator [3313].

Benzyl ether [68436-79-3] $C_{19}H_{20}O_5$ mol. wt. 328.36

-Obtained by adding a solution of 2-hydroxy-4,6-dimethoxyacetophenone in ethyl acetate to a suspension of pulverized sodium in ether. The mixture was refluxed on a water bath for 3 h (48 %) [53].
N.B.: Ratio of the keto and enol forms 4:3 [53].

oil [53]; ^{1}H NMR [53].

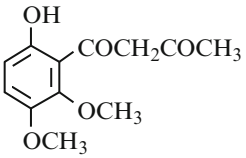
Allyl ether [75160-39-3] $C_{15}H_{18}O_5$ mol. wt. 278.30

-Obtained by adding a solution of 2-allyloxy-4,6-dimethoxyacetophenone in ethyl acetate to pulverized sodium in ethyl ether. Then, the mixture was refluxed on a water bath for 3 h (51 %) [54].

oil [54]; ^{1}H NMR [54].

1-(6-Hydroxy-2,3-dimethoxyphenyl)-1,3-butanedione

[65547-71-9] $C_{12}H_{14}O_5$ mol. wt. 238.24



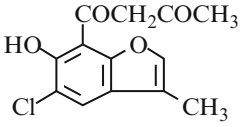
Syntheses
-Obtained by adding a solution of 6-hydroxy-2,3-dimethoxyacetophenone in ethyl acetate to a suspension of pulverized sodium [2564], (49 %) [48].
N.B.: Ratio of the chromanone, enol and keto forms 1:1:3 [48].

liquid [2564]; light yellow needles [48]; m.p. 93–95° [48];
^{1}H NMR [48], IR [48].

Copper salt m.p. 234° [2564].

1-(5-Chloro-6-hydroxy-3-methyl-7-benzofuranyl)-1,3-butanedione

$C_{13}H_{11}ClO_4$ mol. wt. 266.7

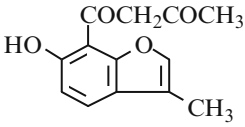


Synthesis
-Obtained by reaction of ethyl acetate with 7-acetyl-5-chloro-6-hydroxy-3-methylcoumarone in the presence of sodium at reflux for 4 h [2828].

m.p. 124° [2828].

1-(6-Hydroxy-3-methyl-7-benzofuranyl)-1,3-butanedione

[100397-26-0] $C_{13}H_{12}O_4$ mol. wt. 232.24



Syntheses

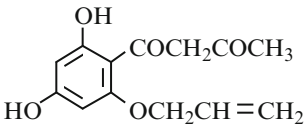
-Obtained by reaction of ethyl acetate with 7-acetyl-6-hydroxy-3-methylcoumarone in the presence of sodium at reflux for 4 h [2828].

-Also obtained by treatment of 7-acetyl-6-acetyloxy-3-methylbenzofuran in pyridine with powdered KOH for 50 min (Baker-Venkataraman rearrangement) (87 %) [2219].
-Also refer to: [1881].

m.p. 105° [2219], 91–92° [1881], 90–91° [2828];
^{1}H NMR [2219], IR [2219].

1-[2,4-Dihydroxy-6-(2-propenyloxy)phenyl]-1,3-butanedione

$C_{13}H_{14}O_5$ mol. wt. 250.25

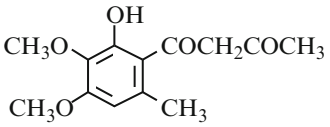


Synthesis

-Refer to: [54].

1-(2-Hydroxy-3,4-dimethoxy-6-methylphenyl)-1,3-butanedione

$C_{13}H_{16}O_5$ mol. wt. 252.27



Synthesis

-Refer to: [52].

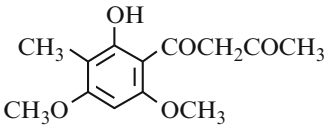
Methyl ether $C_{14}H_{18}O_5$ mol. wt. 266.29

-Obtained by Claisen condensation of 2,3,4-trimethoxy-6-methylacetophenone with ethyl acetate in the presence of pulverized sodium in ethyl ether. Then, the mixture was refluxed for 1.5 h at 115–120° (67 %) [52].

colourless needles [52]; 55–56° [52].

1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-1,3-butanedione

[211751-37-0] $C_{13}H_{16}O_5$ mol. wt. 252.27



Syntheses

-Obtained by reaction of ethyl acetate with 2-hydroxy-4,6-dimethoxy-3-methylacetophenone in the presence of sodium powder, on an boiling water bath for 4 h, then at r.t. overnight (55 %) [2756].

-Also refer to: [2178].

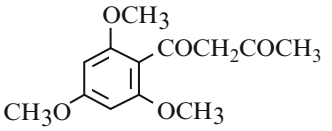
m.p. 116–117° [2756].

Methyl ether $C_{14}H_{18}O_5$ mol. wt. 266.29

m.p. 70–71° [2756].

1-(2,4,6-Trimethoxyphenyl)-1,3-butanedione
(Eugenone)

[480-27-3] $C_{13}H_{16}O_5$ mol. wt. 252.27



Syntheses

-Obtained from 2,4,6-trimethoxyacetophenone on Claisen condensation with ethyl acetate in the presence of pulverized sodium (58 %) [48], (32 %) [2757].

-Obtained by reaction of ethyl acetate with 2,4,6-trimethoxyacetophenone in the presence of sodium sand [3313].

N.B.: Ratio of the keto and enol forms 1:2 [48].

-Also obtained by adding a solution of tritylpotassium in DME to a solution of 2,4,6-trimethoxy-acetophenone in THF and to keep the mixture at r.t. (37 %) [1690].

-From biogenetic-type synthesis of [2137].

-Also refer to: [50, 53, 263, 1519, 1943, 2040, 2178, 3312].

Isolation from natural sources

-From the essential oil of *Pimpinella acuminata* seed (umbelliferone) (0.6 %) [163].

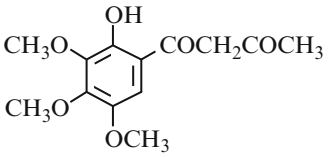
-From the oil of *Eugenia caryophyllata* [2040].

white solid [48]; sublimation 100–105°/0.008 Torr [2040];
m.p. 106° [1943], 102–104° [1690], 101–102° [48], 99–100° [2040], 97–99° [2757], 96–97° [3312, 3313], 94–95° [1519];
^{1}H NMR [48, 1690], IR [1690], UV [1690, 2757],
MS [163, 1690]; GLC [163].

BIOLOGICAL ACTIVITY: As bronchodilatator [3313].

1-(2-Hydroxy-3,4,5-trimethoxyphenyl)-1,3-butanedione

[67231-46-3] $C_{13}H_{16}O_6$ mol. wt. 268.27



Synthesis
-Obtained by Claisen condensation of 2-hydroxy-3,4,5-trimethoxyacetophenone with ethyl acetate in the presence of pulverized sodium in ethyl ether. Then, the mixture was refluxed for 1.5 h at 115–120°, after solvent elimination (34 %) [52].

^{1}H NMR [52].

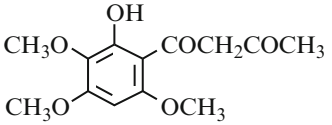
Methyl ether [67231-43-0] $C_{14}H_{18}O_6$ mol. wt. 282.29

-Obtained by Claisen condensation of 2,3,4,5-tetramethoxyacetophenone with ethyl acetate in the presence of pulverized sodium in ethyl ether. Then, the mixture was refluxed for 1.5 h at 115–120°, after solvent elimination [52].

^{1}H NMR [52].

1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1,3-butanedione

[875850-72-9] $C_{13}H_{16}O_6$ mol. wt. 268.27



Syntheses
-Obtained by condensation of 2-hydroxy-3,4,6-trimethoxy-acetophenone with ethyl acetate in the presence of sodium (68 %) [595].
-Also refer to: [52, 3312, 3313].

light fawn-coloured plates [595];
m.p. 123–124° [595], 117–119° [3312].

BIOLOGICAL ACTIVITY: As bronchodilatator [3313].

Methyl ether [67231-33-8] $C_{14}H_{18}O_6$ mol. wt. 282.29

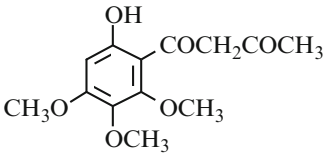
-Obtained by Claisen condensation of 2,3,4,6-tetramethoxyacetophenone with ethyl acetate in the presence of pulverized sodium in ethyl ether. Then, the mixture was heated on a boiling water bath for 3 h (60 %) [52].
-Also refer to: [3312, 3313].

yellow solid [52]; m.p. 76–78° [3312], 55–56° [52];
^{1}H NMR [52].

BIOLOGICAL ACTIVITY: As bronchodilatator [3313].

1-(2-Hydroxy-4,5,6-trimethoxyphenyl)-1,3-butanedione

$C_{13}H_{16}O_6$ mol. wt. 268.27

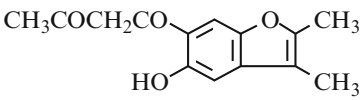


Synthesis
-Obtained by condensation of 2-hydroxy-4,5,6-trimethoxy-acetophenone with ethyl acetate in the presence of sodium (68 %) [595].

pale cream-coloured glistening plates [595];
m.p. 141–142° [595].

1-(5-Hydroxy-2,3-dimethyl-6-benzofuranyl)-1,3-butanedione

$C_{14}H_{14}O_4$ mol. wt. 246.26

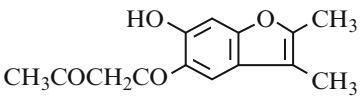


Synthesis
-Obtained by Claisen condensation of ethyl acetate with 6-acetyl-5-hydroxy-2,3-dimethylbenzofuran in the presence of sodium (25.5 %) [2662].

m.p. 151° [2662].

1-(6-Hydroxy-2,3-dimethyl-5-benzofuranyl)-1,3-butanedione

[4196-61-6] $C_{14}H_{14}O_4$ mol. wt. 246.26

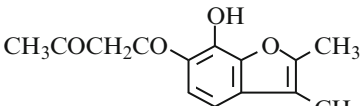


Synthesis
-Obtained by Claisen condensation of ethyl acetate with 5-acetyl-6-hydroxy-2,3-dimethyl-benzofuran in the presence of sodium (14.5 %) [2662].

m.p. 163–164° [2662].

1-(7-Hydroxy-2,3-dimethyl-6-benzofuranyl)-1,3-butanedione

[4349-54-6] $C_{14}H_{14}O_4$ mol. wt. 246.26

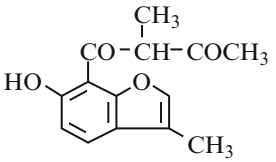


Synthesis
-Obtained by Claisen condensation of ethyl acetate with 6-acetyl-7-hydroxy-2,3-dimethylbenzofuran in the presence of sodium (7 %) [2662].

m.p. 141–142° [2662].

1-(6-Hydroxy-3-methyl-7-benzofuranyl)-2-methyl-1,3-butanedione

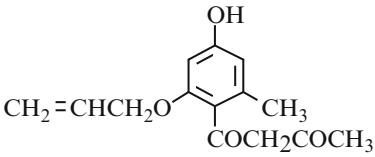
$C_{14}H_{14}O_4$ mol. wt. 246.26



Synthesis
-Obtained by reaction of ethyl acetate with 6-hydroxy-3-methyl-7-propionylcoumarone in the presence of sodium at reflux for 6 h [2828].
m.p. 96° [2828].

1-[4-Hydroxy-2-methyl-6-(2-propenyloxy)phenyl]-1,3-butanedione

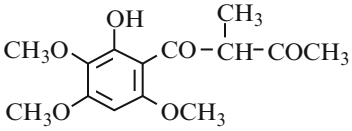
$C_{14}H_{16}O_4$ mol. wt. 248.28



Synthesis
-Refer to: [54].

1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-2-methyl-1,3-butanedione

[854460-42-7] $C_{14}H_{18}O_6$ mol. wt. 282.29

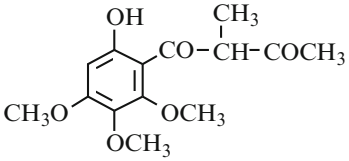


Synthesis
-Obtained by adding powder sodium to a solution of 2-hydroxy-3,4,6-trimethoxypropiophenone in ethyl acetate and ethyl ether. When the initial reaction was over, the mixture was heated under reflux for 4 h (62 %) [2177].

colourless rectangular prisms [2177]; m.p. 133–134° [2177].

1-(2-Hydroxy-4,5,6-trimethoxyphenyl)-2-methyl-1,3-butanedione

$C_{14}H_{18}O_6$ mol. wt. 282.29

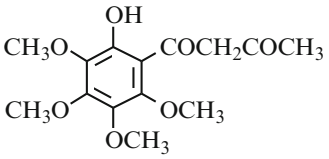


Synthesis
-Obtained by adding powder sodium to a solution of 2-hydroxy-4,5,6-trimethoxypropiophenone in ethyl acetate and ethyl ether. When the initial reaction was over, the mixture was heated under reflux for 4 h (25 %) [2177].

colourless rectangular prisms [2177]; m.p. 204–206° [2177].

1-(2-Hydroxy-3,4,5,6-tetramethoxyphenyl)-1,3-butanedione

[67231-48-5] $C_{14}H_{18}O_7$ mol. wt. 298.29



Synthesis

-Obtained by Claisen condensation of 2-hydroxy-3,4,5,6-tetramethoxyacetophenone with ethyl acetate in the presence of pulverized sodium in ethyl ether. Then, the mixture was refluxed for 1.5 h at 115–120°, after solvent elimination (43 %) [52].

^{1}H NMR [52], IR [52].

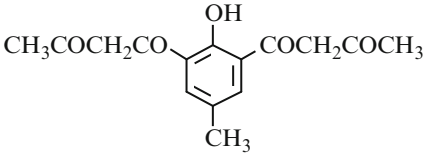
Methyl ether [67231-44-1] $C_{15}H_{20}O_7$ mol. wt. 312.32

-Obtained by Claisen condensation of 2,3,4,5,6-pentamethoxyacetophenone with ethyl acetate in the presence of pulverized sodium in ethyl ether. Then, the mixture was refluxed for 1.5 h at 115–120°, after solvent elimination (61 %) [52].

m.p. 70–71° [52].

1-(2-Hydroxy-5-methylphenyl)-1,3-bis-1,3-butanedione

$C_{15}H_{16}O_5$ mol. wt. 276.29



Syntheses

-Obtained by reaction of ethyl acetate with 2,6-diacetyl-4-methylphenol in the presence of sodium at r.t. for a few min. This was gently heated at 100°, then refluxed for 2 h (15 %) [230].

-Also obtained [931] by conversion of 2,6-diacetyl-4-methylphenol by slightly modification of the procedure [230].

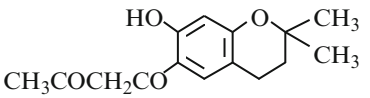
bright yellow powder [230]; m.p. 129° [230].

Copper (II) complex $C_{30}H_{28}O_{10}Cu$ mol. wt. 612.09

-Preparation by treatment of tetraketone with cupric acetate in refluxing ethanol for 1 h (70 %) [230].

1-(3,4-Dihydro-7-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1,3-butanedione

[83805-59-8] $C_{15}H_{18}O_4$ mol. wt. 262.31



Syntheses

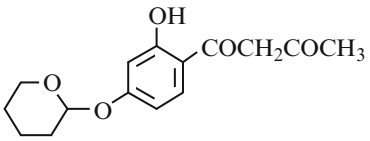
-Obtained by refluxing a mixture of 6-acetyl-3,4-dihydro-7-hydroxy-2,2-dimethyl-2*H*-1-benzo-pyran, ethyl acetate and sodium metal for 4 h (75 %) [51].

-Also refer to: [2518, 3223 (15 %)].

m.p. 108–109° [51, 2518], 107° [3223];
^{1}H NMR [51, 2518, 3223], IR [3223].

1-[2-Hydroxy-4-(2-tetrahydropyranyl)oxyphenyl]-1,3-butanedione

$C_{15}H_{18}O_5$ mol. wt. 278.30



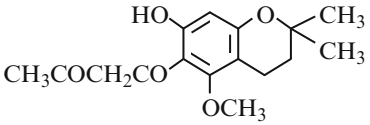
Synthesis

-Preparation by reaction of ethyl acetate with resacetophenone 4-tetrahydropyranyl ether in the presence of powdered sodium at r.t. for 12 h (75 %) [1100].

m.p. 97–98° [2786].

1-(3,4-Dihydro-7-hydroxy-5-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1,3-butanedione

[83805-67-8] $C_{16}H_{20}O_5$ mol. wt. 292.33



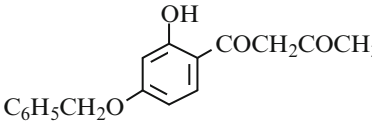
Synthesis

-Obtained by refluxing a mixture of 6-acetyl-3,4-dihydro-7-hydroxy-5-methoxy-2,2-dimethyl-2*H*-1-benzopyran, ethyl acetate and sodium metal for 3 h (70 %) [51].

m.p. 104–105° [51]; ^{1}H NMR [51].

1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1,3-butanedione

[34128-24-0] $C_{17}H_{16}O_4$ mol. wt. 284.31



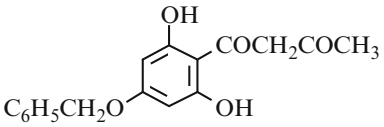
Synthesis

-Obtained by refluxing for 3 h a mixture of 4-benzyloxy-2-hydroxyacetophenone, ethyl acetate and sodium metal (46 %) [51].

shining needles [51]; m.p. 120–121° [51]; ^{1}H NMR [51].

1-[2,6-Dihydroxy-4-(phenylmethoxy)phenyl]-1,3-butanedione

[52751-45-8] $C_{17}H_{16}O_5$ mol. wt. 300.31

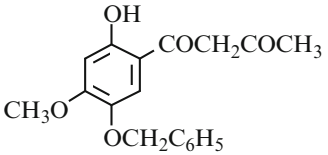


Synthesis
-Obtained (by-product) by refluxing benzyl chloride and 4-acetyloxy-2,6-dihydroxy-acetophenone for 24 h (0.5 %) [67].

m.p. 162–164° [67]; ^{1}H NMR [67], UV [67].

1-[2-Hydroxy-4-methoxy-5-(phenylmethoxy)phenyl]-1,3-butanedione

[101790-57-2] $C_{18}H_{18}O_5$ mol. wt. 314.34

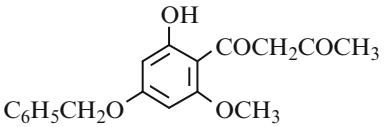


Syntheses
-Preparation by treatment of 2-acetoxy-5-benzoyloxy-4-methoxyacetophenone with sodium hydride in refluxing pyridine for 15 min (70 %) [835].
-Also obtained by reaction of ethyl acetate with 2-hydroxy-4-methoxy-5-benzyloxyacetophenone in the presence of sodium at reflux for 6 h (52 %) [835].

m.p. 124° [835].

1-[2-Hydroxy-6-methoxy-4-(phenylmethoxy)phenyl]-1,3-butanedione

[83805-61-2] $C_{18}H_{18}O_5$ mol. wt. 314.34

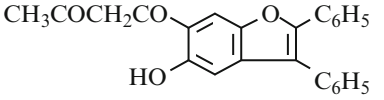


Synthesis
-Obtained by refluxing for 3 h a mixture of 4-benzyloxy-2-hydroxy-6-methoxy-acetophenone, ethyl acetate and sodium metal (52 %) [51].

m.p. 135–136° [51]; ^{1}H NMR [51].

1-(5-Hydroxy-2,3-diphenyl-6-benzofuranyl)-1,3-butanedione

[2035-55-4] $C_{24}H_{18}O_4$ mol. wt. 370.40



Synthesis
-Obtained by reaction of 6-acetyl-5-hydroxy-2,3-diphenylbenzofuran with ethyl acetate in the presence of sodium at reflux for 1 h (82 %) [2200].

m.p. 159° [2200].

Methyl ether [78481-50-2] $C_{25}H_{20}O_4$ mol. wt. 384.43

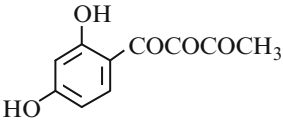
-Refer to: [2–4].

m.p. 158° [3, 4];
^{1}H NMR [3, 4], IR [3], MS [3, 4].

6 Aromatic Hydroxy-1,2,3-Butanetrione

1-(2,4-Dihydroxyphenyl)-1,2,3-butanetrione

$C_{10}H_8O_5$ mol. wt. 208.17



Synthesis
-Refer to: [2677].

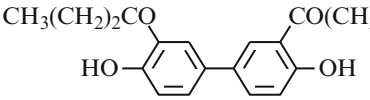
Dimethyl ether $C_{12}H_{12}O_5$ mol. wt. 236.22

-Refer to: [2677]; m.p. 97° [2677].

7 Aromatic Hydroxyketones Derived from Diphenyle

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)bis-1-butanone

[103509-18-8] $C_{20}H_{22}O_4$ mol. wt. 326.39

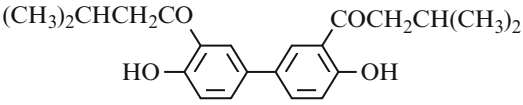


Syntheses
-Preparation by Fries rearrangement of 4,4′-biphenyl dibutanoate with aluminium chloride,
*in the presence of sodium chloride at 140° (93 %) [2091];
*in refluxing chlorobenzene for 24 h (89 %) [2377].
-Also refer to: [2365].

m.p. 125–126° [2377]; IR [2377].

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)bis-3-methyl-1-butanone

$C_{22}H_{26}O_4$ mol. wt. 354.45



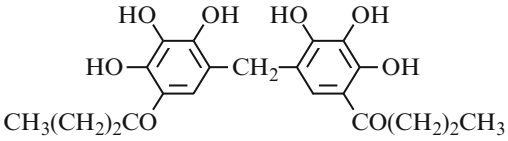
Synthesis
-Preparation by Fries rearrangement of 4,4′-biphenyl diisovalerate with aluminium chloride in the presence of sodium chloride at 140° (99 %) [2091].

m.p. 94–95° [2091].

8 Aromatic Hydroxyketones Derived from Diphenylmethane

1,1′-[Methylenebis(2,3,4-trihydroxy-5,1-phenylene)]bis-1-butanone

$C_{21}H_{24}O_8$ mol. wt. 404.42



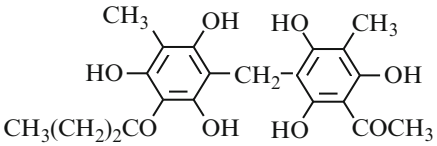
Synthesis

-Obtained by treatment of 4-butyroyl-pyrogallol with 35 % aqueous solution of formaldehyde in refluxing ethanol for 10 min [506].

m.p. 181–182° [506].

3-[(3-Acetyl-2,4,6-trihydroxy-5-methylphenyl)methyl]-(2,4,6-trihydroxy-5-methyl-3-ylphenyl)-1-butanone

$C_{21}H_{24}O_8$ mol. wt. 404.42



Synthesis

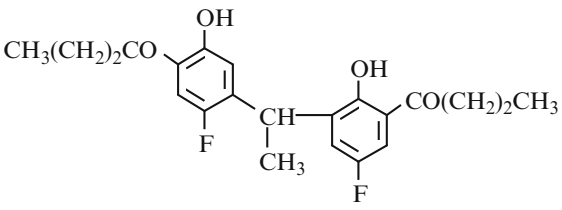
-Obtained by reaction of paraformaldehyde with a mixture (1:1) of 3-methylphlorobutyro-phenone and 3-methylphloroacetophenone in dilute ethanol in the presence of concentrated sulfuric acid (10 drops) at r.t. for 48 h [2034].

pale yellow needles [2034]; m.p. 246–248° [2034].

1-(4-Butyryl-2-fluoro-5-hydroxyphenyl)-1-(3-butyryl-5-fluoro-2-hydroxyphenyl)ethane

3′,4‴-Ethylidenebis[5′-fluoro-2′-hydroxybutyrophenone] (Sadtler)

[100697-01-6] $C_{22}H_{24}F_2O_4$ mol. wt. 390.43



Synthesis

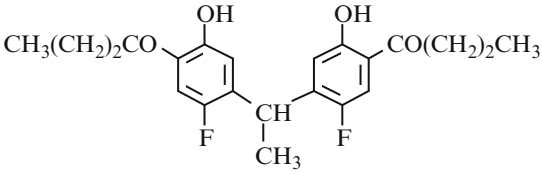
-Obtained by Fries rearrangement (by-product) of p-fluorophenyl butyrate with aluminium chloride in 1,2-dichloroethane at 100° for 2 h (1–2 %) (**5**) [1998].

N.B.: In tar of the industrial preparation from 500 kg of the ester (Sanofi industries, Aramon, Fr.).

m.p. 93° (Sadtler standard N° 38634M) [1998];
^{1}H NMR (Sadtler standard N° 38634M) [1998],
IR (Sadtler standard N° 65683K) [1998], UV [1998], MS [1998].

1,1′-[Ethylidenebis(2-fluoro-5-hydroxy-4,1-phenylene)]bis-1-butanone
Bis(butyryl-4-fluoro-2-hydroxy-5-phenyl)-1,1-ethane [1998]
4′,4‴-Ethylidenebis[5′-fluoro-2′-hydroxybutyrophenone] (Sadtler)

[100696-99-9] $C_{22}H_{24}F_2O_4$ mol. wt. 390.43



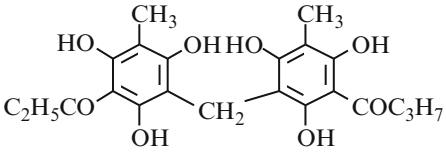
Synthesis
-Obtained by Fries rearrangement (by-product) of p-fluorophenyl butyrate with aluminium chloride in 1,2-dichloroethane at 100° for 2 h (6–8 %) (**3**) [1998].

N.B.: In tar of the industrial preparation from 500 kg of the ester (Sanofi industries, Aramon, Fr.).

m.p. 114° [1998];
^{1}H NMR (Sadtler standard N° 38501M) [1998],
IR (Sadtler standard N° 65539K) [1998], UV [1998], MS [1998].

1-[3-(5-methyl-3-propionyl-2,4,6-trihydroxyphenylmethyl)-2,4,6-trihydroxy-5-methyl-phenyl]-1-butanone
(Abbreviatin PB)

[84633-06-7] $C_{22}H_{26}O_8$ mol. wt. 418.44

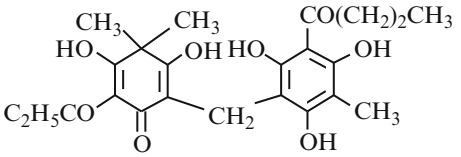


Isolation from natural sources
-From *Dryopteris abbreviata* (DC.) NEWMAN (Aspidiaceae) [724].
pale yellow powder [724];
m.p. 206–208° [724];

^{1}H NMR [724], IR [724], UV [724], MS [724]; TLC [724]; HPLC [724].

3,5-Dihydroxy-4,4-dimethyl-2-(1-oxopropyl)-6-[[2,4,6-trihydroxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,5-cyclohexadien-1-one
(Flavaspidic Acid PB)

[3773-25-9] $C_{23}H_{28}O_8$ mol. wt. 432.48



Isolation from natural sources
-From *Dryopteris abbreviata* (DC.) NEWMAN (Aspidiaceae) [724].
-From rhizomes of *Dryopteris crassirhizoma* (Dryopteridaceae) [1852, 2208].

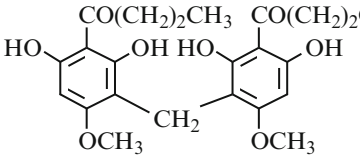
-Also refer to: [2447].

pale yellow powder [724];
m.p. 170–171° [2447], 156–158° [724], 148° [1852];
^{1}H NMR [724, 2208], IR [724], UV [724, 1852],
MS [724]; TLC [724]; HPLC [724].

BIOLOGICAL ACTIVITY: Antioxidant [1852]; Inhibition of enzyme [2208].

1,1′-[Methylenebis(2,4-dihydroxy-6-methoxy-3,1-phenylene)]bis-1-butanone
(Methylene-bis-desaspidinol) (Methylene-bis-desaspidinol-BB)

[32190-32-2] $C_{23}H_{28}O_8$ mol. wt. 432.48



Syntheses
-Preparation by reaction of formaldehyde with desaspidinol [2446, 2450].
-Also obtained (by-product) from phloraspin [2444].

-Also obtained (by-product) from desaspidin [2450].
-Also refer to: [1914, 2451].

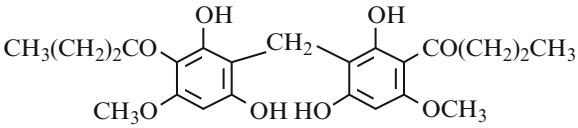
Isolation from natural sources

-From *Dryopteris austriaca* [2446].
-Also refer to: [3302].

m.p. 176–179° [3302], 174–175° [2446, 2451];
^{1}H NMR [2451], MS [1914].

1,1′-[Methylenebis(2,6-dihydroxy-4-methoxy-3,1-phenylene)]bis-1-butanone

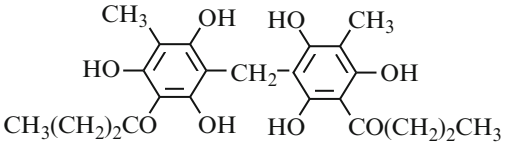
$C_{23}H_{28}O_8$ mol. wt. 432.48



Isolation from natural sources
-From the roots of *Dryopteris championii* [3480].

1,1′-[Methylenebis(2,4,6-trihydroxy-5-methyl-3,1-phenylene)]bis-1-butanone *(Abbreviatin BB)*

[4069-49-2] $C_{23}H_{28}O_8$ mol. wt. 432.48



Synthesis
-Obtained by reaction of *para*-formaldehyde with 3-methylphlorobutyrophenone in dilute methanol in the presence of concentrated sulfuric acid (10 drops) at r.t. for 24 h [2034].

-Also refer to: [725, 1610, 1913, 2208, 2451].

Isolation from natural sources

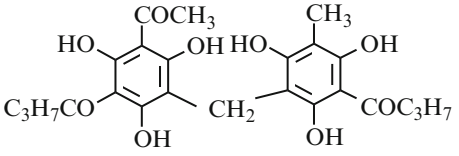
-From *Dryopteris abbreviata* (DC.) NEWMAN (Aspidiaceae) [724, 725].
-From *Dryopteris filix-mas* var. rigidiformis [3302].
-From *Dryopteris athamantica* [3302].
-From *Dryopteris crassirhizoma* (Dryopteridaceae) [2208].

pale yellow needles [725, 2034];
m.p. 213–215° [2451], 212° [1610, 2034], 211–212° [3302], 200–202° [725];
^{1}H NMR [724, 725, 2208], ^{13}C NMR [1913], IR [725], UV [725], MS [725, 2208].

BIOLOGICAL ACTIVITY: Ecotoxicology [2208]; Fatty acid synthase inhibition [2208].

1-[3-(3-Acetyl-5-butyryl-2,4,6-trihydroxyphenylmethyl)-2,4,6-trihydroxy-5-methyl-phenyl]-1-butanone

[68223-50-7] $C_{24}H_{28}O_9$ mol. wt. 460.48

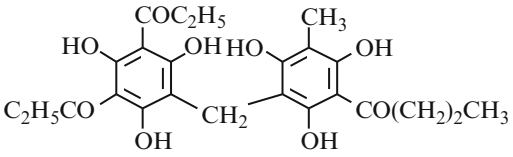


Synthesis
-Obtained by condensation of acylphloroglucinol derivatives [1571].
m.p. 193–195° [1571].

BIOLOGICAL ACTIVITY: Antimalarial [1571].

1-[3-[(3,5-Dipropionyl)-2,4,6-trihydroxyphenylmethyl]-2,4,6-trihydroxy-5-methyl-phenyl]-1-butanone

[68223-39-2] $C_{24}H_{28}O_9$ mol. wt. 460.48

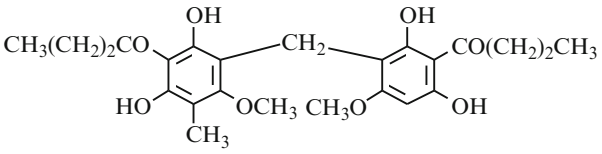


Synthesis
-Obtained by condensation of acylphloroglucinol derivatives [1571].
m.p. 220–221° [1571]

BIOLOGICAL ACTIVITY: Antimalarial [1571].

1-[3-(3-Butyryl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl-2,6-dihydroxy-4-methoxyphenyl]-1-butanone
(Phloraspidinol-BB, Phloraspidinol)

[1509-10-0] $C_{24}H_{30}O_8$ mol. wt. 446.50



Syntheses
-Obtained by reaction of 4 % formaldehyde with a mixture of aspidinol* and desaspidinol* in the presence of 1 % potassium hydroxide for 1 min at r.t., then acidification with dilute hydrochloric acid [2446].
*Aspidinol: 2,6-dihydroxy-4-methoxy-3-methylbutyrophenone.
*Desaspidinol: 2,6-dihydroxy-4-methoxybutyrophenone.
-Also refer to: [1914, 3301].

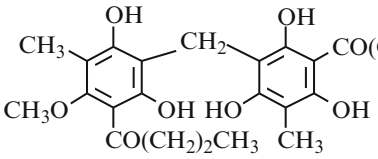
Isolation from natural sources

-From *Dryopteris austriaca* (ferns) [2446, 2451].
-From *Dryopteris athamantica* [3302].
-From *Dryopteris arwanda* [3302].

m.p. 193–194° [2446, 2451, 3302], 190–192° [3301];
^{1}H NMR [3301], MS [1914].

1-[3-[[2,6-Dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxy-5-methylphenyl]-1-butanone
(Aemulin BB)

[56226-93-8] $C_{24}H_{30}O_8$ mol. wt. 446.50

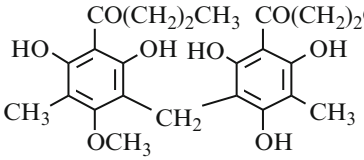


Isolation from natural sources
-From the roots of *Dryopteris championii* [3480].
-From *Dryopteris annula* [3301].

m.p. 90–91° [3301]; ^{1}H NMR [3301], MS [3301].

1-[3-[[2,4-Dihydroxy-6-methoxy-5-methyl-3-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxy-5-methylphenyl]-1-butanone
(Margaspidin) (Margaspidin BB)

[1867-82-9] $C_{24}H_{30}O_8$ mol. wt. 446.50



Syntheses
-Obtained by treatment of a 2,4,6-trihydroxy-3,5-dimethylbutyrophenone and 2,6-dihydroxy-4-methoxy-3-methylbutyrophenone mixture with bis(sulfonium ylide) in the presence of silver oxide (84 %) [2414].
-Also prepared by treatment of a 3-methyl-2,4,6-trihydroxybutyrophenone and aspidinol mixture with 4 % formaldehyde in the presence of 1 % aqueous sodium hydroxide [2443].
-Also refer to: [80, 206, 438, 1914].

Isolation from natural sources

-From *Dryopteris marginata* (Wall.) CHRIST (Aspidiaceae) [2527].
-From *Dryopteris arwanda* [3302].
-From *Dryopteris annula* [3301].
-From *Dryopteris marginalis* [2451].
-From *Dryopteris bissetiana* (Aspidiaceae) [1332].

yellow crystals [2443];
m.p. 189–191° [1332], 179–181° [3301], 178–180° [2443, 2451, 3302], 175–176° [2527], 175° [2527];
^{1}H NMR [1332, 3301], ^{13}C NMR [206], UV [1332, 2443], MS [1914, 2527].

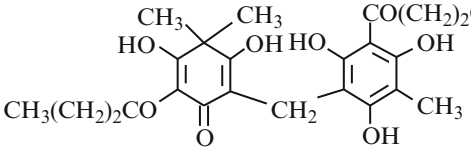
BIOLOGICAL ACTIVITY: Dihydrofolate reductase inhibition screening using protein flexibility and species specificity in structure-based drug discovery [438]; Anthelmintic [2414].

3,5-Dihydroxy-4,4-dimethyl-2-(1-oxobutyl)-6-[[2,4,6-trihydroxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,5-cyclohexadien-1-one

3′[(5-Butyryl-2,4-dihydroxy-3,3-dimethyl-6-oxo-1,4-cyclohexadien-1-yl)methyl]-5′-methyl-phlorobutyrophenone.

(Flavapidic Acid) (Polystichocitrin) (Toxifren)

[114-42-1] $C_{24}H_{30}O_8$ mol. wt. 446.50



Syntheses

-Refer to: [35, 70, 2033, 2617].

Isolation from natural sources

-From the rhizomes of male fern [388, 389].

-From *Dryopteris* ferns [959].

(α-form) orthorhombic crystals;

m.p. 157–158.5° [36], 157–158° [2033], 156° [959, 2449, 2451, 3102], 154° [2618], 93° [2618], 92° [959, 2033], 90° [36];

m.p. 92°, solidifies again at 110° and melts again at 156° [959, 3102];

^{1}H NMR [3302], IR [3302].

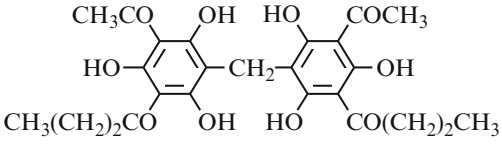
(β-form) monoclinic crystals; X-ray data [959].

BIOLOGICAL ACTIVITY: Anthelmintic [70]; Toxicity [70];

LD_{50} [3102].

1,1′-[Methylenebis(2,4,6-trihydroxy-3-acetyl-5,1-phenylene)]bis-1-butanone

[68223-37-0] $C_{25}H_{28}O_{10}$ mol. wt. 488.49



Syntheses

-Preparation by condensation of two molecules of acylphloroglucinol with formaldehyde or methoxymethyl acetate [3391].

-Also refer to: [1571].

m.p. 166–168° [1571], 156–158° [3391].

Hexamethyl ether $C_{31}H_{40}O_{10}$ mol. wt. 572.65

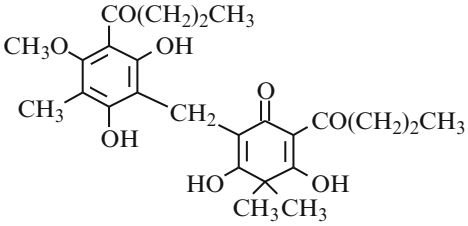
-Preparation by condensation of two molecules of acylphloroglucinol with formaldehyde or methoxymethyl acetate [3391].

m.p. 113–115° [3391].

2-[[2,6-Dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-3,5-dihydroxy-4,4-dimethyl-6-(1-oxobutyl)-2,5-cyclohexadien-1-one
still named

3′-[(5-Butyryl-2,4-dihydroxy-3,3-dimethyl-6-oxo-1,4-cyclohexadien-1-yl)methyl]-2′,4′-dihydroxy-6′-methoxy-5′-methyl-1-butanone
(Aspidin BB) [3102], *(Polystichin)* [3102], *(para-Aspidin)* [2408, 2445].

[584-28-1] $C_{25}H_{32}O_8$ mol. wt. 460.52



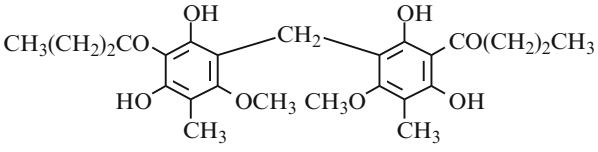
Syntheses
-Obtained by adding formaldehyde to a solution of 3-butyrylfilicinic acid and aspidinol in aqueous potassium hydroxide. The mixture was kept at r.t. for 15 min [2445].
-Also refer to: [36].

Isolation from natural sources
-From *Hypericum uliginosum* HBK (**XX**) [2408].
-From *Dryopteris austriaca* (Jacq.) Woynar (Polypodiaceae) [36, 2445, 3102].

m.p. 123–125° [3300], 124–125° [2445, 3102], 122–124° [3302], 121–123° [36, 387, 390, 2617];
UV [2445, 3102], Ms [1914].

1,1′-[Methylenebis(2,6-dihydroxy-4-methoxy-5-methyl-3,1-phenylene)]bis-1-butanone
(Methylene-bis-aspidinol)

[5377-72-0] $C_{25}H_{32}O_8$ mol. wt. 460.52



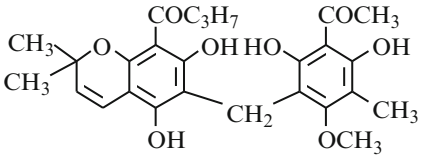
Isolation from natural sources
-Obtained from the leaves and twigs of *Calyptranthes pallens* (Myrtaceae) [1898].
-Also obtained from the rhizomes of *Ctenitis apiciflora* (Aspidiaceae) [3295].
-Also obtained from the rhizomes of *Ctenitis nidus* (Aspidiaceae) [3295].
-Also obtained from the from genus *Dryopteris marginalis* [3297].
-Also refer to: [245].

yellow needles [1898];
m.p. 188–190° [3297], 187–190° [3295], 186–187° [1898];
^{1}H NMR [1898], ^{13}C NMR [1898], IR [1898], UV [1898], MS [1898, 3295].

BIOLOGICAL ACTIVITY: Cytotoxicity [1898].

1-[6-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-1-butanone
(Butyrylmallotochromene)

[116979-51-2] $C_{26}H_{30}O_8$ mol. wt. 470.52

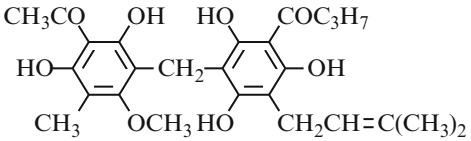


Isolation from natural sources
-From *Mallotus japonicus* (Euphorbiaceae) [136].

BIOLOGICAL ACTIVITY: Anti-HSV-1 [136]; Cytotoxicity [136].

3-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-2,4,6-trihydroxy-5-[(3,3-dimethylallyl)phenyl]-1-butanone
(Butyrylmallotojaponin)

[96853-73-5] $C_{26}H_{32}O_8$ mol. wt. 472.54



Isolation from natural sources
-From the fruits of *Mallotus japonicus* (Euphorbiaceae) [1746].
-From the pericarps of *Mallotus japonicus* (Euphorbiaceae) [136, 138, 139].

Yellow needles [1746]; m.p. 157–158° [1746];
^{1}H NMR [1746], ^{13}C NMR [1746], IR [1746], MS [1746].

BIOLOGICAL ACTIVITY: Anti-HSV-1 [136]; Cytotoxicity [136, 139].

Pentaacetate $C_{36}H_{42}O_{13}$ mol. wt. 682.72

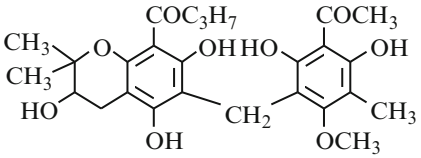
-Obtained by reaction of acetic anhydride with the title ketone in the presence of pyridine at r.t. for 24 h [1746].

^{1}H NMR [1746], MS [1746]; HPLC [1746].

BIOLOGICAL ACTIVITY: Cytotoxicity [139].

1-[6-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-3,4-dihydro-3,5,7-trihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-1-butanone
(Butyrylmallotochromanol)

[129399-52-6] $C_{26}H_{32}O_9$ mol. wt. 488.53

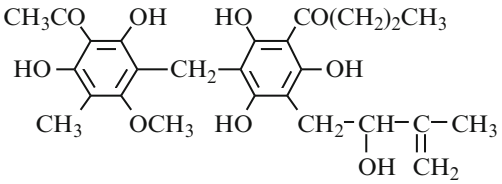


Isolation from natural sources
-From *Mallotus japonicus* (Euphorbiaceae) [136].

BIOLOGICAL ACTIVITY: Anti-HSV-1 [136]; Cytotoxicity [136].

1-[3-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-2,4,6-trihydroxy-5-(2-hydroxy-3-methyl-3-butenyl)phenyl]-1-butanone
(Mallotolerin) (Butyrylmallotolerin)

[102904-17-6] $C_{26}H_{32}O_9$ mol. wt. 488.53



Syntheses
-Refer to: [1359, 1360, 1541, 2453, 2788].

Isolation from natural sources
-From in pericarps of *Mallotus japonicus* (Euphoebiaceae) [136–138, 1462, 2232].

yellow needles [138]; m.p. 197–198° [138];
^{1}H NMR [138], ^{13}C NMR [137], IR [138], UV [138], MS [138].

USE: Biocompatible, biostable coating of medical surfaces composed of polysulfone and hydrophilic polymers [1359].

BIOLOGICAL ACTIVITY: Expandable medical device comprising gemcitabine for treatment and prevention of cardiovascular diseases [2453]; Anti-HSV-1 [136]; Cytotoxicity [136–138].

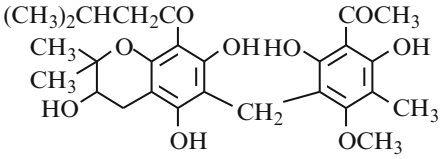
Hexaacetate $C_{38}H_{44}O_{15}$ mol. wt. 744.23

-Obtained by reaction of acetic anhydride with mallotolerin in the presence of pyridine at r.t. [138].

colourless oil [138]; ^{1}H NMR [138].

1-[6-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-3,4-dihydro-3,5,7-trihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-3-methyl-1-butanone

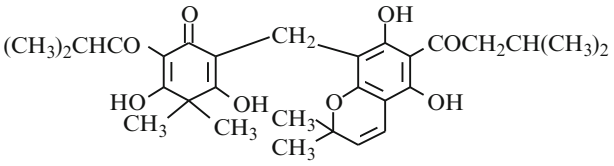
[406463-68-1] $C_{27}H_{34}O_9$ mol. wt. 502.55



Isolation from natural sources
-From the pericarps of *Mallotus japonicus* (Euphorbiaceae) [1461].

2-(5,7-Dihydroxy-6-isovaleryl-2,2-dimethyl-2*H*-chromen-8-ylmethyl)-3,5-dihydroxy-6-isobutyryl-4,4-dimethyl-2,5-cyclohexadiene-1-one
(Isouliginosin B-iBiV)

[72935-11-6] $C_{29}H_{36}O_8$ mol. wt. 512.60

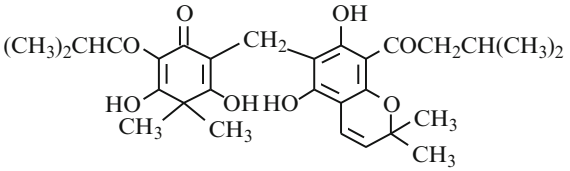


Synthesis
-Obtained by treatment of uliginosin A-iBiV with DDQ (13 %) [2041].

yellow prisms [2041]; m.p. 150–151° [2041];
^{1}H NMR [2041], IR [2041], MS [2041].

2-(5,7-Dihydroxy-8-isovaleryl-2,2-dimethyl-2*H*-chromen-6-ylmethyl)-3,5-dihydroxy-6-isobutyryl-4,4-dimethyl-2,5-cyclohexadiene-1-one
(Uliginosin B-iBiV)

[72935-10-5] $C_{29}H_{36}O_8$ mol. wt. 512.60

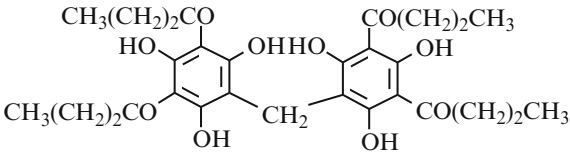


Synthesis
-Obtained by treatment of uliginosin A-iBiV with DDQ (26 %) [2041].

yellow prisms [2041]; m.p. 143–145° [2041];
^{1}H NMR [2041], IR [2041], MS [2041].

1,1′-[Methylenebis(2,4,6-trihydroxy-3,5-phenylene)]bis-1-butanone

[68223-30-3] $C_{29}H_{36}O_{10}$ mol. wt. 544.61



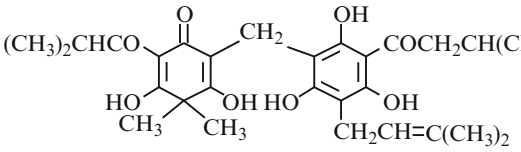
Synthesis
-Preparation by condensation of 40 % formaldehyde with 3,5-dibutyrylphloroglucinol (65 %) [3391].

-Also refer to: [1571].

m.p. 178.5–179.5° [1571], 174–176° [3391].

Uliginosin A-iBiV

[69299-76-9] $C_{29}H_{38}O_8$ mol. wt. 514.62

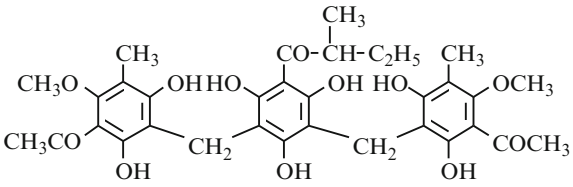


Syntheses
-Obtained by treatment of a mixture of albaspidin-iBiB and 2′,4′,6′-trihydroxy-3′-(3-methyl-2-butenyl)-isovalerophenone with sodium hydride in refluxing methanol for 1.5 h (59 %) [2042].
-Also refer to: [2041].

m.p. 140.5–142° [2042]; ^{1}H NMR [2042], IR [2042], MS [2042].

1-[3,5-Bis[[2,6-dihydroxy-4-methoxy-3-methyl-5-(1-acetyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone
(Agrimol E)

[55576-68-6] $C_{33}H_{38}O_{12}$ mol. wt. 626.66



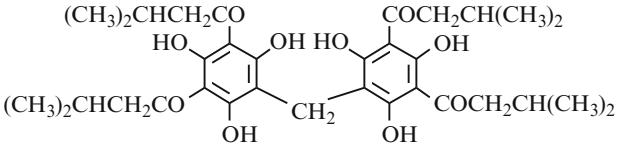
Syntheses
-Refer to: [1866] (Chinese paper).

Isolation from natural sources
-From the Chinese herb medicine *Agrimonia pilosa* [632, 2860] (Chinese paper).

m.p. 240–242° [2860], 239–241° [1866];
^{1}H NMR [632], IR [632, 1866], UV [632], MS [632].

1,1′,1″,1‴-[Methylenebis(2,4,6-trihydroxy-5,1,3-benzenetriyl)]bis-3-methyl-1-butanone
Methylene-bis-(3,5-diisopentanoyl-2,4,6-trihydroxybenzene)

[68223-33-6] $C_{33}H_{44}O_{10}$ mol. wt. 600.71



Syntheses
-Obtained by reaction of formaldehyde with 2,4-diisovalerylphloroglucinol in methylene chloride at 60° for 8–10 h (85 %) [338].

-Also obtained by irradiation of a 2,4-bis(isovaleryl)phloroglucinol and formaldehyde mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (38 %) [621].
-Also refer to: [1571].

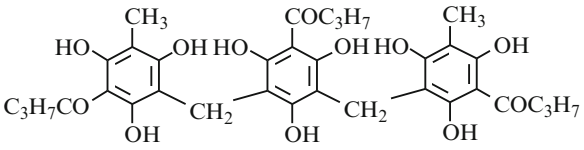
yellow solid [621];
m.p. 165–167° [1571], 158–160° [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621],
MS [621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

-Also refer to: [338].

1-[3,5-Bis[[2,4,6-trihydroxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-1-butanone
(Trisabbreviatin BBB)

[84633-05-6] $C_{34}H_{40}O_{12}$ mol. wt. 640.68

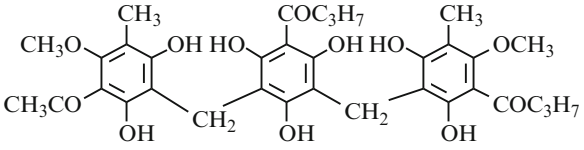


Isolation from natural sources
-From *Dryopteris abbreviata* (DC.) NEWMAN (Aspidiaceae) [724].

pale yellow powder [724];
^{1}H NMR [724], IR [724], UV [724], MS [724];
TLC [724]; HPLC [724].

1-[3-[(3-Acetyl-2,6-dihydroxy-4-methoxy-5-methylphenyl)methyl]-5-[[2,6-dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-1-butanone
(Agrimol F)

[121693-16-1] $C_{34}H_{40}O_{12}$ mol. wt. 640.68



Isolation from natural sources
-From *Hypericum japonicum* Thunb. and *Agromonia pilosa* Ledb. [3372].

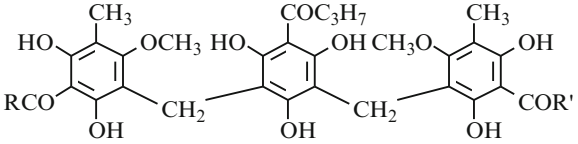
BIOLOGICAL ACTIVITY: Antimicrobial activity of, for *Staphylococcus aureus* [3372].

Trisaspidinol (A mixture of 3 homologous)

BBB ($R = R' = C_3H_7$) [49582-13-0] $C_{36}H_{44}O_{12}$ mol. wt. 668.74

PBB ($R = C_2H_5$, $R' = C_3H_7$) [49582-14-1] $C_{35}H_{42}O_{12}$ mol. wt. 654.71

PBP ($R = R' = C_2H_5$) [49582-15-2] $C_{34}H_{40}O_{12}$ mol. wt. 640.68

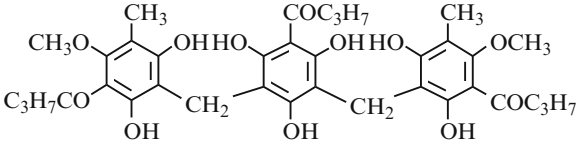


Isolation from natural sources
-From *Dryopteris inaequalis* [3297, 3300].

m.p. 170–172° [3297].

1,1′-[[2,4,6-Trihydroxy-5-(1-oxobutyl)-1,3-phenylene]bis[methylene-(2,4-dihydroxy-6-methoxy-5-methyl-3,1-phenylene)]]bis-1-butanone
(Agrimol C)

[55785-59-6] $C_{36}H_{44}O_{12}$ mol. wt. 668.73



Isolation from natural sources
-From *Agrimol pilosa*, ledeb. [2860].
-From *Hypericum japonicum* Thunb. and *Agromonia pilosa* Ledb. [3372].

m.p. 180–182° [2860];
^{1}H NMR [2860], IR [2860], UV [2860], MS [2860].

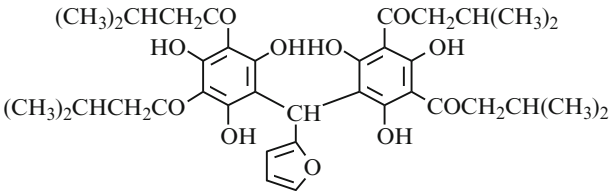
BIOLOGICAL ACTIVITY: Antimicrobial activity of, for *Staphylococcus aureus* [3372].

Heptaacetyl derivative $C_{50}H_{58}O_{19}$ mol. wt. 962.95

-Refer to: [2860].

1-[3-Isopentanoyl-5-[(3,5-diisopentanoyl-2,4,6-trihydroxyphenyl)furan-2-yl-methyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{37}H_{46}O_{11}$ mol. wt. 666.77



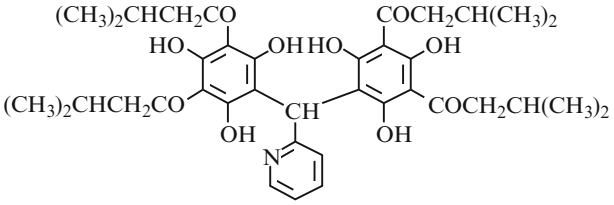
Synthesis
-Obtained by irradiation of a 2,4-bis(isovaleryl) phloro-glucinol in chloroform, p-TsCl and furfural mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (48 %) [621].

yellow oil [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621], MS [621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

1-[3-Isopentanoyl-5-[(3,5-diisopentanoyl-2,4,6-trihydroxyphenyl)pyridin-2-yl-methyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{38}H_{47}NO_{10}$ mol. wt. 677.80



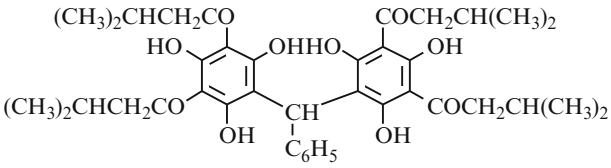
Synthesis
-Obtained by irradiation of a 2,4-bis(isovaleryl) phloro-glucinol in chloroform, p-TsCl and 2-formyl-pyridine mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (46 %) [621].

yellow solid [621]; m.p. 190–192° [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621], MS [621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

1-[3-Isopentanoyl-5-[(3,5-diisopentanoyl-2,4,6-trihydroxyphenyl) phenylmethyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{39}H_{48}O_{10}$ mol. wt. 676.80



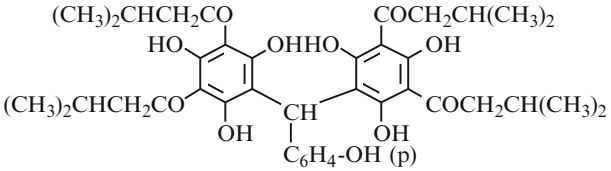
Synthesis
-Obtained by irradiation of a 2,4-bis(isovaleryl) phloro-glucinol in chloroform, p-TsCl and benzaldehyde mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (43 %) [621].

yellow solid [621];
m.p. 180–182° [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621], MS [621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

1-[3-Isopentanoyl-5-[(3,5-diisopentanoyl-2,4,6-trihydroxyphenyl)-(4-hydroxyphenyl)-methyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{39}H_{48}O_{11}$ mol. wt. 692.80



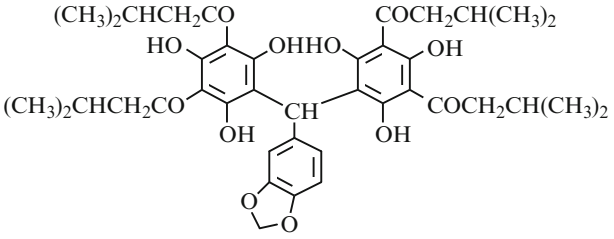
Synthesis
-Obtained by irradiation of a 2,4-bis(isovaleryl) phloro-glucinol in chloroform, p-TsCl and 4-hydroxy-benzaldehyde mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (50 %) [621].

brown oil [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621], MS [621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

1-[3-Isopentanoyl-5-[(3,5-diisopentanoyl-2,4,6-trihydroxyphenyl)-3,4-methylenedioxy-phenylmethyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{40}H_{48}O_{12}$ mol. wt. 720.81



Synthesis

-Obtained by irradiation of a 2,4-bis(isovaleryl) phloro-glucinol in chloroform, p-TsCl and piperonal (3,4-methylene-dioxybenzaldehyde) mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (45 %) [621].

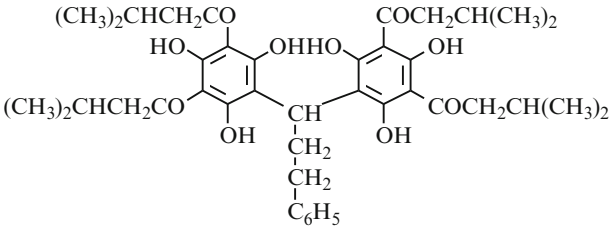
-Also refer to: [620 (41 %)].

yellow crystalline solid [621]; yellow solid [620];
m.p. 186–188° [620], 172–174° [621];
^{1}H NMR [620, 621], ^{13}C NMR [620, 621], IR [621], UV [621], MS [620, 621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

1-[3-Isopentanoyl-5-[(3,5-diisopentanoyl-2,4,6-trihydroxyphenyl) phenylethylmethyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{41}H_{52}O_{10}$ mol. wt. 704.86



Synthesis

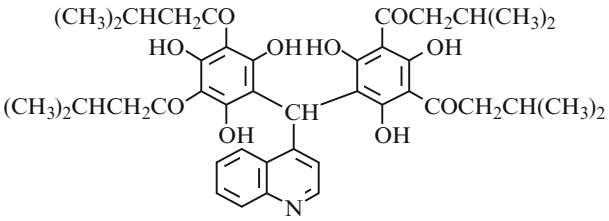
-Obtained by irradiation of a 2,4-bis(isovaleryl) phloro-glucinol and hydrocinna-maldehyde (also named 3-phenyl-propionaldehyde) mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (32 %) [621].

yellow solid [621];
m.p. 138–140° [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621], MS [621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

1-[3-Isopentanoyl-5-[(3,5-diisopentanoyl-2,4,6-trihydroxyphenyl)quinolin-4-yl-methyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{42}H_{49}NO_{10}$ mol. wt. 727.85



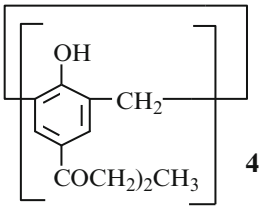
Synthesis
-Obtained by irradiation of a 2,4-bis(isovaleryl) phloro-glucinol in chloroform, p-TsCl and 4-quinoline-carboxaldehyde mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (48 %) [621].

cream coloured solid [621]; m.p. 200–202° [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621], MS [621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

5,11,17,23-Tetrabutyryl-25,26,27,28-tetrahydroxycalix[4]arene

$C_{44}H_{48}O_8$ mol. wt. 704.86

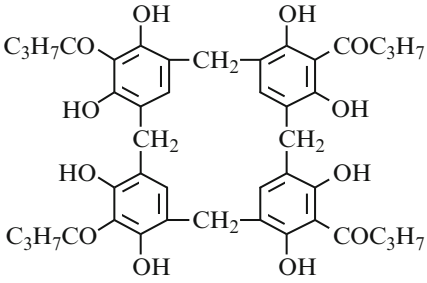


4

Synthesis
-Obtained by Fries rearrangement of 25,26,27,28-tetra-(butyryloxy)calix[4]arene (**7**) with aluminium chloride in nitrobenzene at r.t. overnight (74 %) (**12**) [2293].
m.p. 230–232° [2293];
^{1}H NMR [2293], IR [2293].

Calix[4]resorcinarene

$C_{44}H_{48}O_{12}$ mol. wt. 768.86



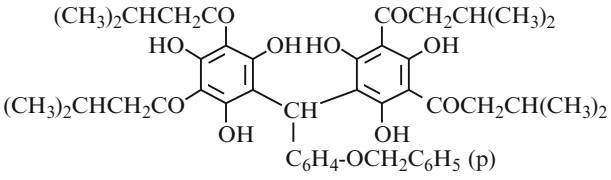
Synthesis
-Obtained by reaction of 2-butyrylresorcinol with 95 % *para*-formaldehyde in the presence of potassium tert-butoxide in THF at 60° for 24 h under an argon atmosphere (58 %) [1732].
yellow needles [1732];
m.p. 256–259° (d) [1732];
^{1}H NMR [1732], ^{13}C NMR [1732], IR [1732], MS [1732].

Monohydrate $C_{44}H_{48}O_{12}$, H_2O mol. wt. 786.87

MS [1732].

1-[3-Isopentanoyl-5-[(3,5-diisopentanoyl-2,4,6-trihydroxyphenyl)-4-benzyloxyphenyl-methyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{46}H_{54}O_{11}$ mol. wt. 782.93



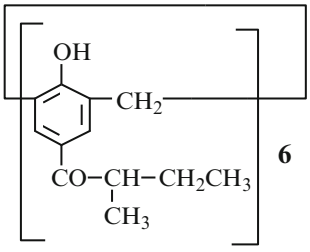
Synthesis
-Obtained by irradiation of a 2,4-bis(isovaleryl) phloro-glucinol in chloroform, p-TsCl and 4-benzyl-oxyoxybenzaldehyde mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (42 %) [621].

brown crystals [621]; m.p. 152–154° [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621], MS [621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

5,11,17,23,29,35-Hexakis(2-methylbutanoyl)-37,38,39,40,41,42-hexahydroxycalix[6]arene

$C_{72}H_{84}O_{12}$ mol. wt. 1141.43



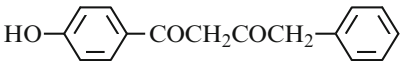
Synthesis
-Obtained by Fries rearrangement of 37,38,39,40,41,42-hexakis[(2-methylbutanoyl)oxy]-calix[6]arene (**2b**) with aluminium chloride in chlorobenzene at 45–50° for 17 h under a nitrogen atmosphere (34 %) (**3b**) [135].

m.p. >360° [135];
^{1}H NMR [135], IR [135].

9 Aromatic Hydroxyketones Derived from 1,3-Butanedioic Acid

1-(2-Hydroxyphenyl)-4-phenyl-1,3-butanedione

[16850-82-1] $C_{16}H_{14}O_3$ mol. wt. 254.29

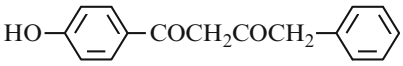


Synthesis
-Refer to: [301, 302, 916].

m.p. 107–108° [302, 916]; ^{1}H NMR [916], ^{13}C NMR [916], MS [916].

1-(4-Hydroxyphenyl)-4-phenyl-1,3-butanedione

$C_{16}H_{14}O_3$ mol. wt. 254.29



Synthesis
-Refer to: [3083].

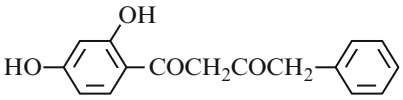
Methyl ether [54103-37-6] $C_{17}H_{16}O_3$ mol. wt. 268.31

-Obtained by reaction of 4-methoxyacetophenone with ethyl phenylacetate in the presence of sodium [3083].

m.p. 75–76° [3083]; UV [3083].

1-(2,4-Dihydroxyphenyl)-4-phenyl-1,3-butanedione

$C_{16}H_{14}O_4$ mol. wt. 270.28



Synthesis
-Refer to: [3083].

Dimethyl ether [859080-81-2] $C_{18}H_{18}O_4$ mol. wt. 298.34

m.p. 91° [1297, 1298].

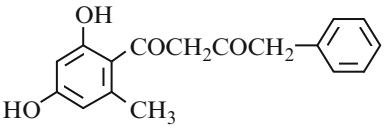
Diethyl ether $C_{20}H_{22}O_4$ mol. wt. 326.39

-Obtained by reaction of 2,4-diethoxyacetophenone with ethyl phenylacetate in the presence of sodium [3083].

m.p. 75° [1234], 74–75° [3083]; UV [3083].

1-(2,4-Dihydroxy-6-methylphenyl)-4-phenyl-1,3-butanedione

$C_{17}H_{16}O_4$ mol. wt. 284.31



Synthesis

-Refer to: [3101].

Dimethyl ether [102172-04-3]

$C_{19}H_{20}O_4$ mol. wt. 312.37

-Refer to: [3101].

b.p.$_{0.5}$ 225–230° [3101]; m.p. 69–70° [3101].

Na salt

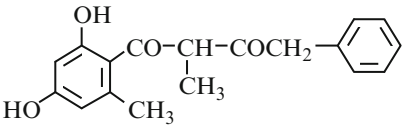
-Obtained by Claisen-condensation of orcacetophenone dimethyl ether with ethyl phenylacetate in xylene in the presence of pulverized sodium. Then, the reaction mixture was heated at 120° for 2 h [3101].

Cu (II) salt of the dimethyl ether $(C_{19}H_{19}O_4)_2Cu$ mol. wt. 686.26

m.p. 145–146° [3101].

1-(2,4-Dihydroxy-6-methylphenyl)-2-methyl-4-phenyl-1,3-butanedione

$C_{18}H_{18}O_4$ mol. wt. 298.34



Synthesis

-Refer to: [3101].

Dimethyl ether

$C_{20}H_{22}O_4$ mol. wt. 326.39

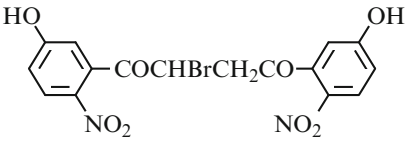
-Obtained by reaction of methyl iodide with the sodium salt of 1-(2,4-dimethoxy-6-methylphenyl)-4-phenyl-1,3-butanedione in refluxing acetone for 5 h [3101].

oil [3101].

10 Aromatic Hydroxyketones Derived from 1,4-Butanedioic Acid

1,4-Bis(5-hydroxy-2-nitrophenyl)-2-bromo-1,4-butanedione

$C_{16}H_{11}BrN_2O_8$ mol. wt. 439.18



Synthesis

-Refer to: [3369].

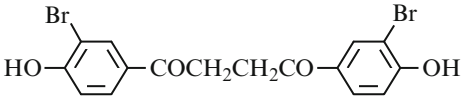
Dimethyl ether [101737-37-5]

$C_{18}H_{15}BrN_2O_8$ mol. wt. 467.23

IR [3369].

1,4-Bis(3-bromo-4-hydroxyphenyl)-1,4-butanedione

$C_{16}H_{12}Br_2O_4$ mol. wt. 428.08

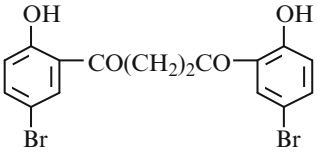


Synthesis
-Obtained by bromination of 1,4-bis (4-hydroxyphenyl)-1,4-butanedione in acetic acid [3319].

m.p. 134–136° [3319].

1,4-Bis(5-bromo-2-hydroxyphenyl)-1,4-butanedione

[16197-58-3] $C_{16}H_{12}Br_2O_4$ mol. wt. 428.08



Syntheses
-Obtained by Fries rearrangement of di-(4-bromophenyl) succinate with aluminium chloride at 130–140° for 3–4 h [594].
-Also refer to: [592].

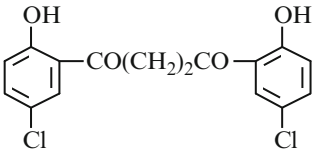
m.p. 180° [594].

Di-2,4-dinitrophenylhydrazone [16286-63-8] $C_{28}H_{20}Br_2N_8O_{10}$ mol. wt. 788.32

m.p. 250° [594].

1,4-Bis(5-chloro-2-hydroxyphenyl)-1,4-butanedione

[16197-54-9] $C_{16}H_{12}Cl_2O_4$ mol. wt. 339.17



Syntheses
-Obtained by Fries rearrangement of di-p-chlorophenyl succinate with aluminium chloride at 130–140° for 3–4 h (good yield) [594].
-Also refer to: [592].

m.p. 182° [594].

Di-2,4-dinitrophenylhydrazone [16197-55-0] $C_{28}H_{20}Cl_2N_8O_{10}$ mol. wt. 699.42

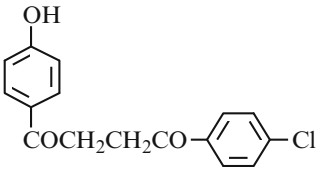
m.p. 210° [592, 594].

Dioxime [16197-64-1] $C_{16}H_{14}Cl_2N_2O_4$ mol. wt. 369.20

m.p. 175° [594].

1-(4-Chlorophenyl)-4-(4-hydroxyphenyl)-1,4-butanedione

$C_{16}H_{13}ClO_3$ mol. wt. 288.73



Synthesis
-Refer to: [2953].
Methyl ether [67756-16-5]
$C_{17}H_{15}ClO_3$ mol. wt. 302.76

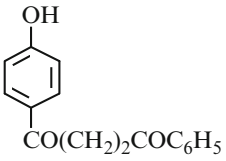
-Obtained from 4-chlorobenzaldehyde and 1-(4-methoxyphenyl)-2-propen-1-one (77 %) [2953].

-Also refer to: [1055, 2452, 2951, 3458].

m.p. 145° [2953], 136° [2951];
^{1}H NMR [1055, 2951, 2953, 3458],
^{13}C NMR [2452], IR [1055, 2951, 2953], MS [2452].

1-(4-Hydroxyphenyl)-4-phenyl-1,4-butanedione

$C_{16}H_{14}O_3$ mol. wt. 254.29



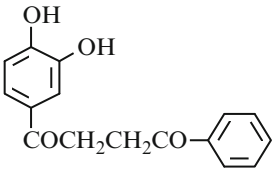
Synthesis
-Refer to: [2953].
Methyl ether [60755-22-8]
$C_{17}H_{16}O_3$ mol. wt. 268.31

-Obtained from benzaldehyde and 1-(4-methoxyphenyl)-2-propen-1-one (63 %) [2953].
-Also refer to: [1055, 1268, 1295, 1658, 2275, 2951, 3358, 3393, 3458].

m.p. 107° [2953], 106–107° [2275], 100–101° [1268, 1295], 98–100° [3393, 3436], 58–60° [3358];
^{1}H NMR [1055, 1658, 2275, 2951, 2953, 3358, 3393, 3458],
^{13}C NMR [3358, 3393, 3436],
IR [1055, 1268, 2275, 2951, 2953, 3358, 3393, 3436], UV [2275], MS [3393, 3436].

1-(3,4-Dihydroxyphenyl)-4-phenyl-1,4-butanedione

$C_{16}H_{14}O_4$ mol. wt. 270.28



Synthesis
-Refer to: [2953].
Dimethyl ether [67756-25-6]
$C_{18}H_{18}O_4$ mol. wt. 298.34

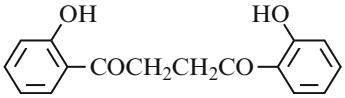
-Obtained from benzaldehyde and 1-(3,4-dimethoxyphenyl)-2-propen-1-one (60 %) [2953].
-Also refer to: [321].

m.p. 109° [2953]; ^{1}H NMR [321, 2953], IR [321, 2953].

BIOLOGICAL ACTIVITY: Antiprotozoal [321].

1,4-Bis(2-hydroxyphenyl)-1,4-butanedione

$C_{16}H_{14}O_4$ mol. wt. 270.28



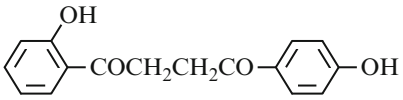
Synthesis
-Refer to: [579].
Dimethyl ether [134179-55-8]
$C_{18}H_{18}O_4$ mol. wt. 298.34

-Obtained by adding zinc dust and a small amount of iodine to a solution of 2-bromo-2′-methoxy-acetophenone. Then, the reaction mixture was heated at 65° for 16 h (26 %) [579].
-Also obtained by reduction of 1,2-bis(2-methoxybenzoyl)ethene with zinc dust in acetic acid (2 %) [1392].

colourless crystals [579];
m.p. 102–104° [1392], 98–100° [579];
^{1}H NMR [579, 1392], ^{13}C NMR [579], IR [579].

1-(2-Hydroxyphenyl)-4-(4-hydroxyphenyl)-1,4-butanedione

$C_{16}H_{14}O_4$ mol. wt. 270.28



Synthesis
-Refer to: [1392].
Dimethyl ether [134179-54-7]
$C_{18}H_{18}O_4$ mol. wt. 298.34

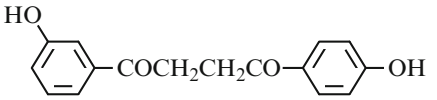
-Refer to: [1392 (8 %)].

m.p. 89–90° [1392], ^{1}H NMR [1392].

N.B.: Its name was 1-(3-methoxybenzoyl)-2-(4-methoxybenzoyl)ethane (in the paper, formula **6e** page 4813) in contradiction with formula represented page 4812.

1-(3-Hydroxyphenyl)-4-(4-hydroxyphenyl)-1,4-butanedione

$C_{16}H_{14}O_4$ mol. wt. 270.28



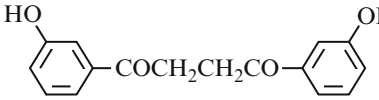
Synthesis
-Refer to: [121].
Dimethyl ether [133559-45-2]
$C_{18}H_{18}O_4$ mol. wt. 298.34

-Refer to: [699, 1156].

^{1}H NMR [121], IR [121].

1,4-Bis(3-hydroxyphenyl)-1,4-butanedione

$C_{16}H_{14}O_4$ mol. wt. 270.28



Synthesis
-Refer to: [579].
Dimethyl ether
$C_{18}H_{18}O_4$ mol. wt. 298.34

-Obtained by adding zinc dust and a small amount of iodine to a solution of 2-bromo-3′-methoxy-acetophenone. Then, the reaction mixture was heated at 65° for 16 h (60 %) [579].

-Also refer to: [2401].

colourless crystals [579]; m.p. 128° [579];
^{1}H NMR [579], ^{13}C NMR [579], IR [579], MS [579].

1,4-Bis(4-hydroxyphenyl)-1,4-butanedione

[108791-64-6] $C_{16}H_{14}O_4$ mol. wt. 270.28

Syntheses
-Obtained (by-product) by reaction of succinic anhydride with anisole in the presence of aluminium chloride in nitrobenzene or in tetrachloroethane [858].
-Preparation by treatment of dimethyl ether with aluminium chloride in nitrobenzene [3319].
-Also refer to: [2567].

m.p. 147° [2567, 3319].

Dimethyl ether [15982-64-6] $C_{18}H_{18}O_4$ mol. wt. 298.34

-Obtained by Friedel-Crafts reaction of succinyl chloride with anisole in the presence of aluminium chloride [2142],
*in carbon disulfide for 45 min at 60° (18–21 %) [478] or for 36 h (8 %) [432];
*in petroleum ether at 0°, then 2 h at r.t. [3319].
-Also obtained from 4-methoxybenzaldehyde and 1-(4-methoxyphenyl)-2-propen-1-one (47 %) [2953].
-Also prepared by reaction of trimethylsilyl enol ether obtained from p-methoxyacetophenone with lead tetraacetate in methylene chloride and tetrahydrofuran at −78° (50 %) [2148].
-Also obtained by reaction between 2′-bromo-4-methoxyacetophenone and methylmagnesium iodide (10 %) [761].
-Preparation: Ethyl p-anisoylacetate in THF was added to a suspension of NaH in THF. After hydrogen evolution had stopped, there was added in succession potassium iodide, acetone and p-methoxyphenacyl bromide. The mixture was stirred for 1 h at r.t. (75 %) [1839].
-Also obtained by reaction of α-bromo-p-phenacyl bromide with TDAE in THF in the presence of iodine at 67° for 30 min (69 %) [2291].
-Also obtained by indium (I) bromide-mediated reductive coupling of α,α-dichloro-p-methoxy-acetophenone in THF at 20° for 24 h (60 %) [2452].
-Also obtained by reduction of 1,2-bis(4-dimethoxybenzoyl)ethene with zinc dust in acetic acid [1392].
-Also obtained by hydrolysis of 2,5-bis(dimethylamino)-2,5-bis(4-methoxyphenyl) adiponitrile in refluxing THF and 30 % aqueous oxalic acid mixture (1:1) for 90 min (76 %) [3026].
-Also refer to: [93, 252 (74 %), 446, 536, 579 (32 %), 699, 1058, 1059, 1342, 1343, 1423, 1431 (84 %), 1533, 1582–1584, 1784, 1815, 1821, 2546, 2304].

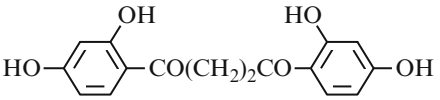
colourless crystals [252, 579];
m.p. 156–157° [1583], 155–159° [579], 154–156° [1815], 154–155° [446, 2304], 154° [478, 1342, 1343, 3319], 153–155° [3026], 153–154.5° [1839], 152° [1821], 151° [252, 2953], 150–152° [2452], 150–151° [536, 1784, 2148], 149–150° [761];
^{1}H NMR [93, 579, 761, 1533, 1583, 1815, 2452, 2546, 2953],
^{13}C NMR [579, 1583, 2452],
IR [252, 579, 761, 1533, 1583, 1815, 2452, 2546, 2953],
MS [252, 761, 1815, 2452], UV [2142];
luminescence spectroscopy [2142].

Di-2,4-dinitrophenylhydrazone of the dimethyl ether $C_{30}H_{26}N_8O_{10}$ mol. wt. 658.58

m.p. 197–198° [432].

1,4-Bis(2,4-dihydroxyphenyl)-1,4-butanedione

[16290-14-5] $C_{16}H_{14}O_6$ mol. wt. 302.28



Syntheses

-Obtained by reaction of succinic anhydride with resorcinol in the presence of zinc chloride at 170° for 2 h (25 %) [651].

-Also obtained by reaction of succinic acid with resorcinol in the presence of zinc chloride [2256].

-Also obtained by reaction of 4-(2,4-dihydroxyphenyl)-4-oxo-1-butanoic acid with resorcinol in the presence of zinc chloride [651].

-Also obtained by condensation of β-(2-hydroxy-4-methoxybenzoyl)propionic acid methyl ester with resorcinol in the presence of a mixture of aluminium chloride and sodium chloride at 190–200° for 50 min (71 %) [1669, 1670].

-Also refer to: [2567].

m.p. 319° [651], 310–312° [2567], 295–296° [1669, 1670], 142–143° [2515];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [1670, 2515], IR [651, 2515],
UV [651, 1669, 1670], MS [1670, 2515].

Isolation from natural sources

-From *Gnetum ula* (Gnetaceae) [2515].

Mono-phenylhydrazone $C_{22}H_{20}N_2O_5$ mol. wt. 392.41

m.p. 194° (d) [651].

Di-phenylhydrazone [16290-17-8] $C_{28}H_{26}N_4O_4$ mol. wt. 482.54

m.p. 208° (d) [651, 2567].

Di-2,4-dinitrophenylhydrazone $C_{28}H_{22}N_8O_{12}$ mol. wt. 662.53

m.p. 185–187° [2567].

Tetraacetate [16290-15-6] $C_{24}H_{22}O_{10}$ mol. wt. 470.43

-Obtained by reaction of acetic anhydride with the title diketone in the presence of pyridine [651].

-Also refer to: [2567].

m.p. 166° [651], 140–141° [2567].
N.B.: One of the reported melting point is obviously wrong.

Dioxime $C_{20}H_{24}N_2O_6$ mol. wt. 388.42

m.p. 218–220° [2567].

Tetramethyl ether [16290-20-3] $C_{20}H_{22}O_6$ mol. wt. 358.39

-Obtained by reaction of dimethyl sulfate with the title diketone in the presence of potassium carbonate in refluxing acetone for 10 h (63 %) [651].
-Obtained by heating a mixture of 1-(2,4-dimethoxyphenyl)-2-propen-1-one (0.026 mol), 2,4-dimethoxybenzaldehyde (0.030 mol), 3-benzyl-5-(2-hydroxyethyl)-4-methylthiazolium chloride (0.0021 mol) and triethylamine (0.014 mol) in DMF at 65° for 4.5 h (78 %) [241].
-Also obtained by Friedel-Crafts reaction of succinyl chloride with resorcinol dimethyl ether in the presence of aluminium chloride (7 %) [2142].
-Obtained: 2,4-dimethoxyacetophenone silyl enol ether was oxidatively coupled at 97° (74 %) [911].
-Also refer to: [2567].

colourless fine needles [2142];
m.p. 148–150° [2567], 148° [651], 146° [241], 145° [911], 128–129° [2142];
^{1}H NMR [241, 911, 2142], ^{13}C NMR [241, 911, 2142],
IR [241, 651, 911, 2142], UV [651, 2142],
MS [241, 911, 2142]; luminescence spectroscopy [2142].

(E,E)-Di-O-methyl oxime of the tetramethyl ether

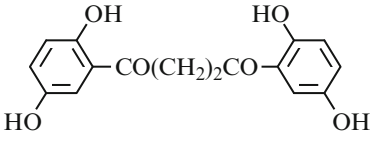
[125304-88-3] $C_{22}H_{28}N_2O_6$ mol. wt. 416.47

-Refer to: [911 (25 %)].

m.p. 122° [911];
^{1}H NMR [911], ^{13}C NMR [911], IR [911], MS [911].

1,4-Bis(2,5-dihydroxyphenyl)-1,4-butanedione

$C_{16}H_{14}O_6$ mol. wt. 302.28



Synthesis
-Refer to: [1575].

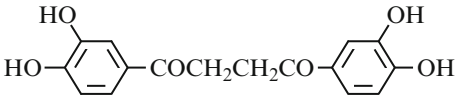
Tetramethyl ether [10365-21-6]
$C_{20}H_{22}O_6$ mol. wt. 358.39

-Obtained by reaction of succinic acid dichloride (1 mol) with hydroquinone dimethyl ether (2.5 mol) in the presence of aluminium chloride (1 mol) [1575].

m.p. 150° [1575].

1,4-Bis(3,4-dihydroxyphenyl)-1,4-butanedione

[114914-89-5] $C_{16}H_{14}O_6$ mol. wt. 302.28



Syntheses

-Obtained by treatment of its tetramethyl ether with boron tribromide in methylene chloride at −78° (74 %) [1392].

-Also refer to: [349].

m.p. 280–283° [1392]; ^{1}H NMR [1392], IR [1392].

Tetramethyl ether [4650-71-9] $C_{20}H_{22}O_6$ mol. wt. 358.39

-Obtained by adding 3,4-dimethoxyacetophenone to lithium diisopropylamide (LDA) in tetrahydrofuran at −40° under nitrogen. After 1 h, cupric chloride in DMF was added and stirring was continued overnight (25 %) [349].

-Also obtained by reduction of 1,2-bis(3,4-dimethoxybenzoyl)ethene with zinc dust in acetic acid (0.6 %) [1392]. The mixture was heated at 80° for 1 h (39 %) [1392].

-Also refer to: [321, 1279, 1533, 2379, 3088, 3133, 3363, 3364].

m.p. 181–182° [349], 180–181° [1279, 3133], 176–178° [3088], 154–156° [1392], 115.2–116.2° [3363].

N.B.: One of the reported melting point is obviously wrong.

^{1}H NMR [321, 349, 1392, 1533, 2379, 3088],

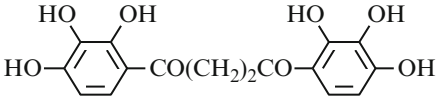
^{13}C NMR [321, 3088], IR [1392, 1533, 3364],

MS [3088].

BIOLOGICAL ACTIVITY: Antiprotozoal [321].

1,4-Bis(2,3,4-trihydroxyphenyl)-1,4-butanedione

$C_{16}H_{14}O_8$ mol. wt. 334.28



Synthesis

-Obtained by reaction of succinic anhydride with pyrogallol in the presence of zinc chloride [1574].

Hexamethyl ether [10388-38-2] $C_{22}H_{26}O_8$ mol. wt. 418.44

-Obtained by reaction of dimethyl sulfate with 1,4-bis(2,3,4-trihydroxyphenyl)-1,4-butanedione in the presence of 20 % sodium hydroxide (43 %) [1574].

m.p. 150° [1574].

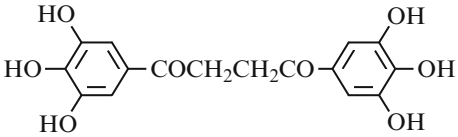
2,4-Dinitrophenylhydrazone of the hexamethyl ether

[10388-39-3] $C_{34}H_{34}N_8O_{14}$ mol. wt. 778.69

m.p. 160° [1574].

1,4-Bis(3,4,5-trihydroxyphenyl)-1,4-butanedione

$C_{16}H_{14}O_8$ mol. wt. 334.28



Synthesis

-Refer to: [349].

Hexamethyl ether [101394-53-0]

$C_{22}H_{26}O_8$ mol. wt. 418.44

-Obtained by adding 3,4,5-trimethoxyacetophenone to lithium diisopropylamide (LDA) in tetrahydrofuran at −70° under nitrogen. After 2 h, cupric chloride in DMF was added and stirring was continued for 2 more hours (49 %) [349].

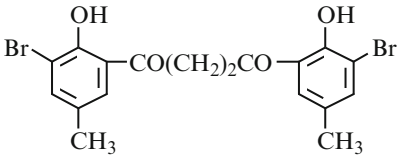
-Also refer to: [321].

white solid [349]; m.p. 189–190° [349];
^{1}H NMR [321], ^{13}C NMR [321].

BIOLOGICAL ACTIVITY: Antiprotozoal [321].

1,4-Bis(3-bromo-2-hydroxy-5-methylphenyl)-1,4-butanedione

[128733-94-8] $C_{18}H_{16}Br_2O_4$ mol. wt. 456.13



Syntheses

-Obtained by reaction of bromine with 1,1′-bis (2-hydroxy-5-methylphenyl)-1,4-butanedione in acetic acid [1035].

-Also obtained by treatment of 1,4-bis (2-hydroxy-5-methylphenyl)-1,4-butanedione with 2,4,4,6-tetrabromocyclohexa-2,5-dienone first at 0°, then at 25° for 13 h (88 %) [473].

slightly yellow solid [473];
m.p. 238–240° [473], 232° [1035]; ^{1}H NMR [473], MS [473].

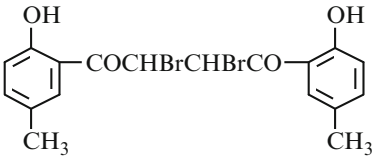
Diacetate $C_{22}H_{20}Br_2O_6$ mol. wt. 540.21

-Obtained by reaction of acetic anhydride with the title ketone in the presence of sodium acetate [1035].

m.p. 140° [1035].

1,4-Bis(2-hydroxy-5-methylphenyl)-2,3-dibromo-1,4-butanedione

$C_{18}H_{16}Br_2O_4$ mol. wt. 456.13



Synthesis
-Refer to: [1035].
m.p. 183° [1035].

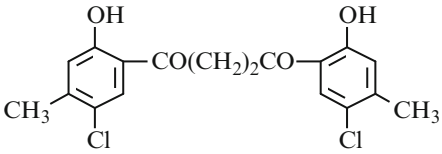
Diacetate $C_{22}H_{20}Br_2O_6$ mol. wt. 540.21

-Obtained by reaction of acetic anhydride with the title diketone in the presence of sulfuric acid [1035].

m.p. 187° [1035].

1,4-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,4-butanedione

[16197-59-4] $C_{18}H_{16}Cl_2O_4$ mol. wt. 367.23



Synthesis
-Obtained by Fries rearrangement of di-(4-chloro-3-methylphenyl) succinate with aluminium chloride at 130–140° for 3–4 h [594].
m.p. 194° [594].

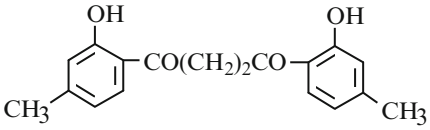
Di-2,4-dinitrophenylhydrazone [16197-60-7] $C_{30}H_{24}Cl_2N_8O_{10}$ mol. wt. 727.47

-Refer to: [592, 594].

m.p. 250° [594].

1,4-Bis(2-hydroxy-4-methylphenyl)-1,4-butanedione
(Hofmeisterin II)

[122427-50-3] $C_{18}H_{18}O_4$ mol. wt. 298.34



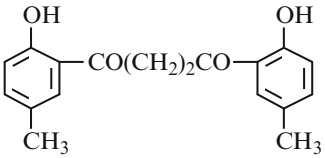
Isolation from natural sources
-From the aerial parts of *Hofmeisteria schaffneri* (Asteraceae) [2455].

colourless crystalline needles [2455]; m.p. 193° [2455];
^{1}H NMR [2455], ^{13}C NMR [2455], IR [2455], UV [2455], MS [2455]; X-ray data [2455].

BIOLOGICAL ACTIVITY: Phytotoxicity [2455].

1,4-Bis(2-hydroxy-5-methylphenyl)-1,4-butanedione

[13282-23-0] $C_{18}H_{18}O_4$ mol. wt. 298.34



Syntheses
-Obtained by Fries rearrangement of di (4-methylphenyl) succinate with aluminium chloride,
*without solvent,
-at 130° for 4 h [1035], (44 %) [3107, 3465];
-at 130–140° for 3–4 h [594], (25 %) [2013];
-at 180–185° for 2.5 h (49 %) [473].
*in refluxing chlorobenzene for 6 h (43 %) [3107].

light brown solid [2013]; light, off-white solid [473];
m.p. 189° [594, 3107], 187–188° [3465], 187° [1035], 185° [1966], 184–186° [2013], 180–189° [473];
^{1}H NMR [473, 3465], IR [2013, 3107, 3465],
UV [2013], MS [1966].

Isolation from natural sources

-From *Berberis coriaria* (Berberidaceae) [1966].
-From *Berberis acanthifolium* (Berberidaceae) [2013].

Di-2,4-dinitrophenylhydrazone [16197-56-1] $C_{30}H_{26}N_8O_{10}$ mol. wt. 658.58

m.p. 239° [594].

Dioxime [16197-57-2] $C_{18}H_{20}N_2O_4$ mol. wt. 328.37

-Refer to: [592, 594].

m.p. 269° [594].

Diacetate [69618-10-6] $C_{22}H_{22}O_6$ mol. wt. 382.40

-Obtained by reaction of acetic anhydride with the title diketone in the presence of sulfuric acid [1035].
-Also refer to: [1966].

m.p. 163° [1035], 141° [1966];
^{13}C NMR [1966], ^{1}H NMR [1966], IR [1966], UV [1966],
MS [1966].

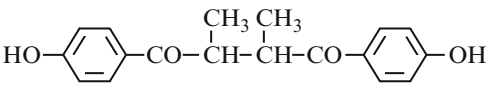
Dimethyl ether [69618-11-7] $C_{20}H_{22}O_4$ mol. wt. 326.39

-Obtained by reaction of methyl iodide with the title diketone in the presence of potassium carbonate [1966], (85 %) [2013].

m.p. 68° [1966];
^{1}H NMR [1966, 2013], ^{13}C NMR [1966], IR [1966, 2013],
UV [1966, 2013], MS [1966, 2013].

1,4-Bis(4-hydroxyphenyl)-2,3-dimethyl-1,4-butanedione

$C_{18}H_{18}O_4$ mol. wt. 298.34



Synthesis
-Refer to: [2461].

Dimethyl ether (racemic) $C_{20}H_{22}O_4$ mol. wt. 326.39

-Obtained by condensation of α-bromo-p-methoxypropiophenone (m.p. 66–69°) with p-methoxy-propiophenone (67 %) [2461].

m.p. 124–127° [2461]; ^{1}H NMR [2461], IR [2461], MS [2461].

Dimethyl ether [81096-36-8] $C_{20}H_{22}O_4$ mol. wt. 326.39

-Refer to: [2671].

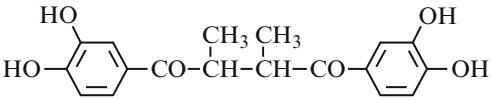
m.p. 166–168° [2671]; ^{1}H NMR [2671], IR [2671].

Dimethyl ether (meso) [222158-42-1] $C_{20}H_{22}O_4$ mol. wt. 326.39

-Refer to: [2671].

1,4-Bis(3,4-dihydroxyphenyl)-2,3-dimethyl-1,4-butanedione

$C_{18}H_{18}O_6$ mol. wt. 330.34



Synthesis
-Refer to: [1474].
Tetramethyl ether [4440-92-0]
$C_{22}H_{26}O_6$ mol. wt. 386.45

-Obtained by reaction* of a THF solution of lithium enolate of 3,4-dimethoxypropiophenone with $CuCl_2$ in DMF at −78° (31 %) [1474].
*(Oxidative dimerization of 3,4-dimethoxypropiophenone).
-Also obtained by treatment of bis-methyl ethyl veratroylacetate with sodium hydroxide in ethanol at r.t. for 24 h (48 %) [232].
-Also obtained by treatment of β-bromopropioveratrone with copper powder in refluxing xylene for 24 h [171].
-Also refer to: [85 (90 %), 678, 2535].

colourless rhombic prisms [171];
m.p. 189–190° [171, 232], 177–178° [1474], 165° [85];
^{1}H NMR [1474], IR [1474]; TLC [1474].

(meso-isomer) [36287-37-3] $C_{22}H_{26}O_6$ mol. wt. 386.45

-Refer to: [349, 2461 (3.8 %)].

white crystals [2461];
m.p. 189–190° [171], 184.5–187.5° [2461];
^{1}H NMR [2461], MS [2461].

(racemic) [27686-81-3] $C_{22}H_{26}O_6$ mol. wt. 386.45

-Refer to: [349, 350, 2461 (90.3 %)].

m.p. 145–146° [2461]; ^{1}H NMR [2461], IR [2461], MS [2461].

Monophenylhydrazone of the tetramethyl ether (racemic)

[116588-92-2] $C_{28}H_{32}N_2O_5$ mol. wt. 476.57

-Obtained by reaction of phenylhydrazine with the tetramethyl ether in refluxing ethanol for 1 h [85].

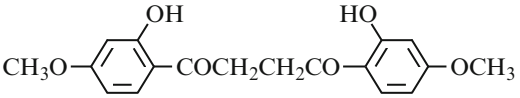
yellow needles [85]; m.p. 140° [85];
^{1}H NMR [85], IR [85].

Di-2,4-dinitrophenylhydrazone of the tetramethyl ether $C_{34}H_{34}N_8O_{12}$ mol. wt. 746.69

-Refer to: [232].

1,4-Bis(2-hydroxy-4-methoxyphenyl)-1,4-butanedione

[16290-18-9] $C_{18}H_{18}O_6$ mol. wt. 330.34



Syntheses
-Obtained by methylation of 1,4-bis (2,4-dihydroxyphenyl)-1,4-butanedione with excess diazomethane in ethyl ether at r.t. overnight (31 %) [1669, 1670].

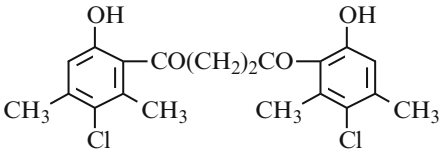
-Also refer to: [651].

Isolation from natural sources
-From *Gnetum ula* [1670, 2515].

yellow needles [1670]; yellow crystals [1669];
m.p. 200–202° [1669, 1670], 192° [651];
^{1}H NMR [1669, 1670], IR [651], UV [651],
MS [1669, 1670].

1,4-Bis(3-chloro-6-hydroxy-2,4-dimethylphenyl)-1,4-butanedione

[16197-61-8] $C_{20}H_{20}Cl_2O_4$ mol. wt. 395.29



Syntheses
-Obtained by Fries rearrangement of di-(4-chloro-3,5-dimethylphenyl) succinate with aluminium chloride at 130–140° for 3–4 h [594].

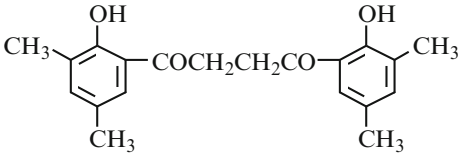
m.p. 250° [594].

Di-2,4-dinitrophenylhydrazone [16197-62-9] $C_{32}H_{28}Cl_2N_8O_{10}$ mol. wt. 755.53

m.p. 220° [594].

1,4-Bis(2-hydroxy-3,5-dimethylphenyl)-1,4-butanedione

$C_{20}H_{22}O_4$ mol. wt. 326.39



Synthesis
-Obtained by Fries rearrangement of di-(2,4-diphenyl) succinate with aluminium chloride in 1,2-dichloroethane at 125–135° for 2 h 30 min (41 %) [1443].

m.p. 206–208° [1443].

Dioxime $C_{20}H_{24}N_2O_4$ mol. wt. 356.42

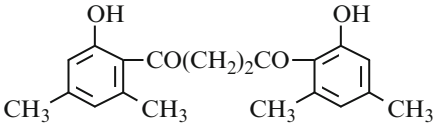
m.p. 225–230° [1443].

Diacetate $C_{24}H_{26}O_6$ mol. wt. 410.47

m.p. 161° [1443].

1,4-Bis(2-hydroxy-4,6-dimethylphenyl)-1,4-butanedione

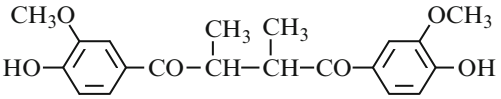
$C_{20}H_{22}O_4$ mol. wt. 326.39



Synthesis
-Obtained by Fries rearrangement of bis (3,5-dimethylphenyl) succinate with aluminium chloride [1035].
m.p. 141° [1035].

1,4-Bis(4-hydroxy-3-methoxyphenyl)-2,3-dimethyl-1,4-butanedione

[1173986-38-3] (+) $C_{20}H_{22}O_6$ mol. wt. 358.39
[1173986-37-2] (−)
[1204225-56-8] meso



Synthesis
-Refer to: [1687, 1964, 1965].

(+)-7,7′-Dioxodihydroguaiaretic [1173986-38-3] $C_{20}H_{22}O_6$ mol. wt. 358.39

-Refer to: [3380].

^{1}H NMR [3380], ^{13}C NMR [3380], MS [3380]; $(\alpha)_D^{20} = +102°$ [3380].

BIOLOGICAL ACTIVITY: Antibacterial [1642]; Antifungal [1642]; Inhibition of enzyme activity [3380].

(−)-7,7′-Dioxodihydroguaiaretic [1173986-37-2] $C_{20}H_{22}O_6$ mol. wt. 358.39

-Refer to: [1642].

$(\alpha)_D^{20} = -102°$ [3380].

BIOLOGICAL ACTIVITY: Antibacterial [1642]; Antifungal [1642]; Inhibition of enzyme activity [3380].

Meso -7,7′-Dioxodihydroguaiaretic [1204225-56-8] $C_{20}H_{22}O_6$ mol. wt. 358.39

-Refer to: [1642].

colourless cristal [1642]; m.p. 175–177° [1642];
^{1}H NMR [1642], ^{13}C NMR [1642], MS [1642]

BIOLOGICAL ACTIVITY: Antibacterial [1642]; Antifungal [1642].

Dimethyl ether [4440-92-0] $C_{22}H_{26}O_6$ mol. wt. 386.45

-Refer to: [85, 171, 232, 678, 1474, 2535].

m.p. 189–190° [171, 232]; 177–178° [1474]; 165° [85];
^{1}H NMR [1474], ^{13}C NMR [1474], IR [1474], MS [1474].

Meso isomer [36287-37-3] $C_{22}H_{26}O_6$ mol. wt. 386.45

-Refer to: [349, 2461].

m.p. 186–190° [2461]; ^{1}H NMR [2461], MS [2461].

Racemic [27686-81-3] $C_{22}H_{26}O_6$ mol. wt. 386.45

-Refer to: [349, 350, 2461].

m.p. 145–146° [2461]; ^{1}H NMR [2461], IR [2461], MS [2461].

Diethyl ether [986-89-0] $C_{24}H_{30}O_6$ mol. wt. 414.50

-Obtained by heating α-bromo-4-ethoxy-3-methoxypropiophenone with freshly precipitated copper in xylene for 24 h (7 %) [1687].
-Also refer to: [1964, 1965].

needles [1687]; m.p. 185–186° [1687], 185° [1964, 1965];
^{1}H NMR [1964, 1965], IR [1964, 1965],
UV [1687, 1964], MS [1964, 1965].

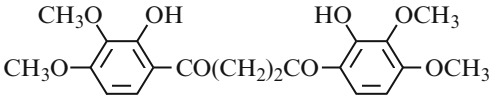
Methyl and ethyl ether [749-41-7] $C_{23}H_{28}O_6$ mol. wt. 400.47

-Following the conditions used for the benzylation of propiophenone, sodium O-ethylpropio-vanillone and α-bromopropioveratrone afforded two products separated after alumina chromatography by crystallisation from methanol. Only the minor more-soluble product consisted of the titled diketone [1687].

m.p. 161° [1687].

1,4-Bis(2-hydroxy-3,4-dimethoxylphenyl)-1,4-butanedione

[10351-89-0] $C_{20}H_{22}O_8$ mol. wt. 390.39

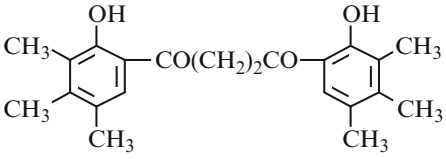


Synthesis
-Obtained by reaction of succinic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride in tetrachloroethane [1574].

m.p. 208° [1574].

1,4-Bis(2-hydroxy-3,4,5-trimethylphenyl)-1,4-butanedione

$C_{22}H_{26}O_4$ mol. wt. 354.45



Synthesis
-Obtained (by-product) by Fries rearrangement of 2,3,5-trimethylphenyl succinate with aluminium chloride (2 mol) in tetrachloroethane at 140° for several hours (20 %) [2908].

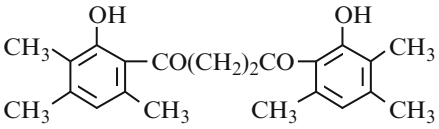
m.p. 246–248° [2908].

Diacetate $C_{26}H_{30}O_6$ mol. wt. 438.52

m.p. 213–214° [2908].

1,4-Bis(2-hydroxy-3,4,6-trimethylphenyl)-1,4-butanedione

[860705-13-1] $C_{22}H_{26}O_4$ mol. wt. 354.45



Syntheses

-Obtained by Fries rearrangement of 2,3,5-trimethylphenyl succinate with aluminium chloride for 1.5 h at 140–150°,

*in tetrachloroethane (31 %) [2908];
*in stannic chloride (24 %) [2908];
*in o-dichlorobenzene (20 %) (very impure) [2908];
*without solvent (10 %) [2908].

-Also obtained by Friedel-Crafts reaction of succinic acid with 2,3,5-trimethylphenol in the presence of boron trifluoride etherate (9 %) [2908].

-Also obtained by hydrolysis of the acetate by action for 48 h of boiling aqueous methanol containing hydrochloric acid (79 %) [2908].

m.p. 207–209° [2908].

Diacetate $C_{26}H_{30}O_6$ mol. wt. 438.52

-Obtained by reaction of acetic anhydride with the title diketone in boiling pyridine for 2 h (60 %) [2908].

m.p. 154–156° [2908].

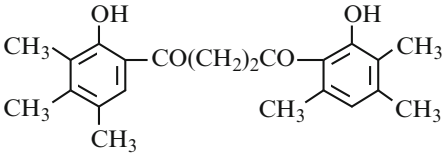
Dimethyl ether $C_{24}H_{30}O_4$ mol. wt. 382.50

-Obtained by reaction of methyl iodide with the disodium salt of the title diketone in xylene (50 %) [2908].

m.p. 124–125° [2908].

1-(2-Hydroxy-3,4,5-trimethylphenyl)-4-(2-hydroxy-3,4,6-trimethylphenyl)-1,4-butanedione

$C_{22}H_{26}O_4$ mol. wt. 354.45



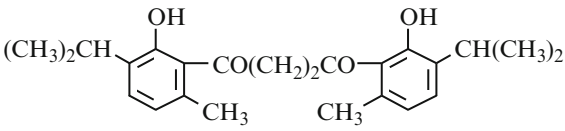
Synthesis

-Obtained (by-product) by Fries rearrangement of 2,3,5-trimethylphenyl succinate with aluminium chloride (2 mol) in tetrachloroethane at 140° for several hours [2908].

m.p. 246–248° [2908].

1,4-Bis[2-hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1,4-butanedione
(Succinothymon)

[124135-37-1] $C_{24}H_{30}O_4$ mol. wt. 382.50

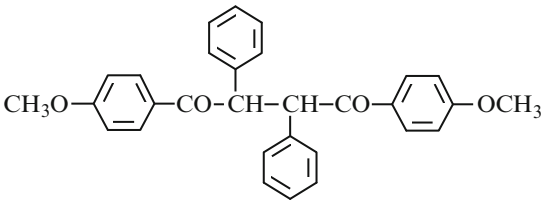


Synthesis
-Obtained by reaction of succinic acid with thymol in the presence of aluminium chloride on heating at reflux for 12 h (40 %) [2960].

m.p. 44° [2960].

1,4-Bis(4-methoxyphenyl)-2,3-bis(phenyl)-1,4-butanedione

[30839-20-4] $C_{30}H_{26}O_4$ mol. wt. 450.53



Syntheses
-Refer to: [2142, 2604, 2875].
m.p. 264° [2604];
IR [2604].

racemic [135680-27-2] $C_{30}H_{26}O_4$ mol. wt. 450.53

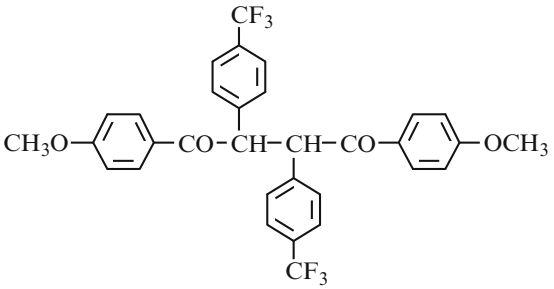
colourless microcrystalline powder [2142]; m.p. 136–137° [2142];
^{1}H NMR [2142, 2143], ^{13}C NMR [2142], IR [2142],
UV [2142], MS [2142]; luminescence spectroscopy [2142].

meso $C_{30}H_{26}O_4$ mol. wt. 450.53

colourless powder [2142]; m.p. 258–260° [2142];
^{1}H NMR [2142], ^{13}C NMR [2142], IR [2142],
UV [2142], MS [2142], luminescence spectroscopy [2142].

1,4-Bis(4-methoxyphenyl)-2,3-bis[(4-trifluoromethyl)phenyl]-1,4-butanedione

$C_{32}H_{24}F_6O_4$ mol. wt. 586.53



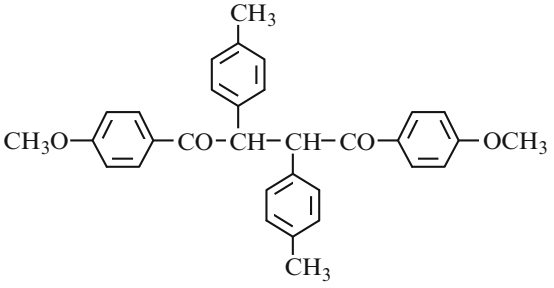
Synthesis
-Refer to: [2142].
racemic
$C_{32}H_{24}F_6O_4$ mol. wt. 586.53
colourless powder [2142];
^{1}H NMR [2142],
^{13}C NMR [2142],
IR [2142], UV [2142], MS [2142];
luminescence spectroscopy [2142].

meso $C_{32}H_{24}F_6O_4$ mol. wt. 586.53

colourless powder [2142];
^{1}H NMR [2142], ^{13}C NMR [2142], UV [2142], IR [2142], MS [2142];
luminescence spectroscopy [2142].

1,4-Bis(4-methoxyphenyl)-2,3-bis(4-methylphenyl)-1,4-butanedione

$C_{32}H_{30}O_4$ mol. wt. 478.59



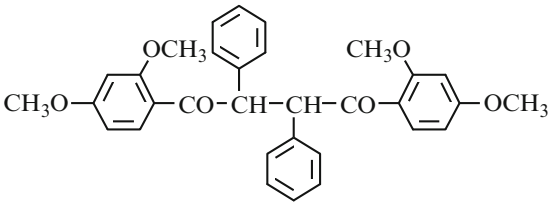
Synthesis
-Refer to: [2142].
racemic
$C_{32}H_{30}O_4$ mol. wt. 478.59
colourless plates [2142];
m.p. 196–198° [2142];
^{1}H NMR [2142],
^{13}C NMR [2142],
IR [2142], UV [2142], MS [2142];
luminescence spectroscopy [2142].

meso $C_{32}H_{30}O_4$ mol. wt. 478.59

colourless crystals [2142]; m.p. 229–230° [2142];
^{1}H NMR [2142], ^{13}C NMR [2142], IR [2142], UV [2142],
MS [2142]; luminescence spectroscopy [2142].

1,4-Bis(2,4-dimethoxyphenyl)-2,3-bis(phenyl)-1,4-butanedione

$C_{32}H_{30}O_6$ mol. wt. 510.58



Synthesis
-Refer to: [2142].
racemic
$C_{32}H_{30}O_6$ mol. wt. 510.58
colourless powder [2142];

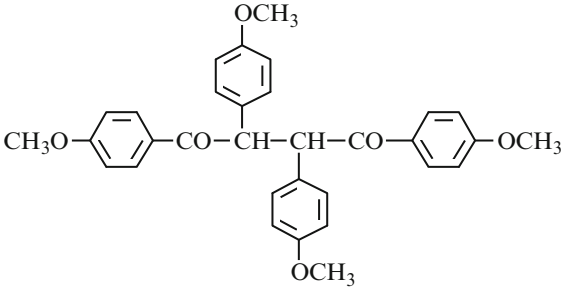
m.p. 164–165° [2142];
^{1}H NMR [2142], ^{13}C NMR [2142], IR [2142], UV [2142],
MS [2142]; luminescence spectroscopy [2142].

meso $C_{32}H_{30}O_6$ mol. wt. 510.58

colourless powder [2142]; m.p. 214–216° [2142];
^{1}H NMR [2142], ^{13}C NMR [2142], IR [2142], UV [2142],
MS [2142]; luminescence spectroscopy [2142].

1,4-Bis(4-methoxyphenyl)-2,3-(4-methoxyphenyl)-1,4-butanedione

[103326-23-4] $C_{32}H_{30}O_6$ mol. wt. 510.58



Syntheses
-Refer to: [781, 2142, 2157].
m.p. 208° [781];
^{1}H NMR [2157],
^{13}C NMR [2157],
UV [781].

racemic $C_{32}H_{30}O_6$ mol. wt. 510.58

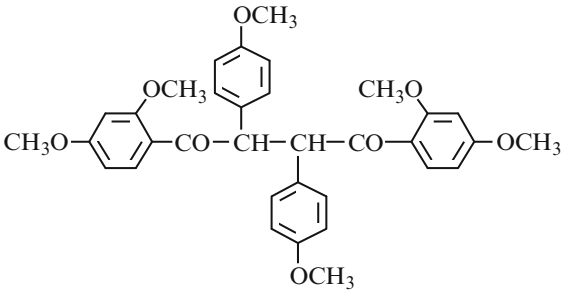
colourless needles [2142]; m.p. 151–152° [2142];
^{1}H NMR [2142], ^{13}C NMR [2142], IR [2142], UV [2142],
MS [2142]; luminescence spectroscopy [2142].

meso $C_{32}H_{30}O_6$ mol. wt. 510.58

colourless microcrystalline powder [2142]; m.p. 203–204° [2142];
^{1}H NMR [2142], ^{13}C NMR [2142], IR [2142], UV [2142],
MS [2142]; luminescence spectroscopy [2142].

1,4-Bis(2,4-dimethoxyphenyl)-2,3-(4-methoxyphenyl)-1,4-butanedione

$C_{34}H_{34}O_8$ mol. wt. 570.64



Synthesis
-Refer to: [2142].
racemic
$C_{34}H_{34}O_8$ mol. wt. 570.64
colourless needles [2142];
m.p. 133–134° [2142];
^{1}H NMR [2142],

^{13}C NMR [2142], IR [2142], UV [2142],
MS [2142]; luminescence spectroscopy [2142].

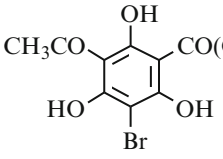
meso $C_{34}H_{34}O_8$ mol. wt. 570.64

colourless crystals [2142]; m.p. 172–173° [2142];
^{1}H NMR [2142], ^{13}C NMR [2142], IR [2142], UV [2142],
MS [2142]; luminescence spectroscopy [2142].

11 Diketones Derived from Acetic and 1-Butanoic Acids

1-(3-Bromo-5-acetyl-2,4,6-trihydroxyphenyl)-1-butanone

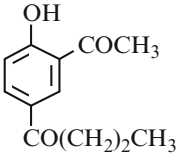
$C_{12}H_{13}BrO_5$ mol. wt. 317.14



Synthesis
-Obtained by acylating the phloroglucinol with appropriate acyl chloride or acid anhydride in the presence of boron trifluoride [3391].
m.p. 109–110° [3391].

1-[3-Acetyl-4-hydroxyphenyl]-1-butanone

[173469-74-4] $C_{12}H_{14}O_3$ mol. wt. 206.24

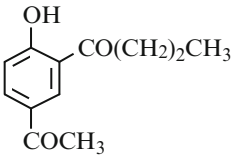


Synthesis
-Obtained by reaction of butyryl chloride with 2-hydroxyacetophenone in the presence of aluminium chloride in carbon disulfide (90 %) [345].

m.p. 57–58° [345]; ^{1}H NMR [345], IR [345].

1-(5-Acetyl-2-hydroxyphenyl)-1-butanone

[92757-66-9] $C_{12}H_{14}O_3$ mol. wt. 206.24



Syntheses

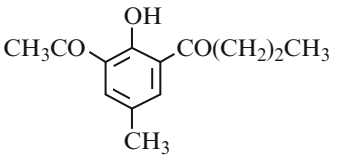
-Preparation by Fries rearrangement of 4-(butyryl-oxy) acetophenone with aluminium chloride (4 mol) without solvent at 150° for 3 h (58 %) [1305].

-Also obtained by Friedel-Crafts acylation of 4-hydroxy-acetophenone with butyryl chloride in the presence of aluminium chloride (4 mol) in tetrachloroethane at 130° for 4 h (47 %) [1305].

m.p. 54–55° [1305]; ^{1}H NMR [1305], IR [1305].

1-(3-Acetyl-2-hydroxy-5-methylphenyl)-1-butanone

[213622-17-4] $C_{13}H_{16}O_3$ mol. wt. 220.27



Synthesis

-Obtained by reaction of butyryl chloride with 2-hydroxy-5-methylacetophenone in the presence of aluminium chloride in carbon disulfide at r.t. for 1 h (90 %) [344].

m.p. 53–55° [344]; ^{1}H NMR [344], IR [344].

Benzoate [213622-22-1] $C_{20}H_{20}O_4$ mol. wt. 324.38

-Obtained by reaction of benzoyl chloride with 1-(3-acetyl-2-hydroxy-5-methylphenyl)-1-butanone in the presence of pyridine (95 %) [344].

m.p. 90–91° [344].

p-Chlorobenzoate [213622-23-2] $C_{20}H_{19}ClO_4$ mol. wt. 358.82

-Obtained by reaction of p-chlorobenzoic acid and phosphorous oxychloride with 1-(3-acetyl-2-hydroxy-5-methylphenyl)-1-butanone in the presence of pyridine (90 %) [344].

m.p. 101–102° [344].

p-Methylbenzoate [213622-24-3] $C_{21}H_{22}O_4$ mol. wt. 338.40

-Obtained by reaction of p-toluic acid and phosphorous oxychloride with 1-(3-acetyl-2-hydroxy-5-methylphenyl)-1-butanone in the presence of pyridine (95 %) [344].

m.p. 65–66° [344].

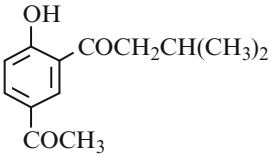
p-Methoxybenzoate [213622-25-4] $C_{21}H_{22}O_5$ mol. wt. 354.40

-Obtained by reaction of p-toluic acid and phosphorous oxychloride with 1-(3-acetyl-2-hydroxy-5-methylphenyl)-1-butanone in the presence of pyridine (95 %) [344].

m.p. 73–75° [344].

1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone
(Desmethylespeleton)

[62458-64-4] $C_{13}H_{16}O_3$ mol. wt. 220.27



Syntheses

-Preparation by Fries rearrangement of 4-acetylphenyl isovalerate in the presence of aluminium chloride without solvent at 140–160° for 2.5 h (51 %) [402] or at 150° for 3 h (32 %) [1305].

-Also obtained by Friedel-Crafts acylation of 4-hydroxyacetophenone with isovaleryl chloride (4 mol) in tetrachlroethane at 130° for 4 h (37 %) [1305].

-Also obtained by treatment of its methyl ether with 48 % hydrobromic acid in refluxing acetic acid for 6 h (65 %) [2220].

-Also obtained by treatment of 2-isovaleroyl-4-(1-hydroxyethyl)phenol with manganese dioxide in ethyl ether for 2 h [3444].

Isolation from natural sources

-From the genus *Flourensia cernua* DC in Sub-tribe *Helianthinae* (Tribe Heliantheae) (Compositae) [396].

-From the aerial parts of *Ophryosporus floribundus* (Compositae, tribe Eupatorieae) [3443].

-From sliced yacon tubers after inoculation with the bacterium *Pseudomonas cichorii* and incubation at 20° for 3 days, then extraction with acetone. Yacon (*Polymnia sonchifolia*) (Compositae) is cultivated in South America and has recently been introduced in Japan [3035].

-From the aerial parts of *Ophryosporus axilliflorus* (Griseb.) Hieron (Asteraceae) [979, 2353].

-From *Helichrysum argyrophyllum* DC (86/18, Hogsback) [1488].

-From *Brachyclados megalanthus* [3444].

colourless oil [396]; white crystals [2353];
b.p.$_{.4}$ 156–158° [2220];
m.p. 94.5–96° [3035], 64–66° [1305, 2353], 61.5° [402].
N.B.: One of the reported melting points is obviously wrong.
^{1}H NMR [396, 1305, 2353, 3035, 3444],
^{13}C NMR [2353, 3035], IR [396, 1305, 3035], UV [3035],
MS [396, 3035]; TLC [3444].

BIOLOGICAL ACTIVITY: Antiinflammatory [979, 2353].

Methyl ether [51995-98-3] $C_{14}H_{18}O_3$ mol. wt. 234.30
(Espeleton)

Syntheses

-Obtained by oxidation of 1-[5-(1-hydroxyethyl)-2-methoxyphenyl]-3-methyl-1-butanone with chromium trioxide in pyridine at 25° for 15 h [399, 409].
-Also obtained by treatment of 5-ethyl-2-methoxyisovalerophenone,
*with DDQ in refluxing dioxane for 70 h (60 %) [2220];
*with BTAP (benzyltriethylammonium permanganate) in acetic acid at 30° for 2 days (26 %) [2701].

Isolation from natural sources

-From *Espeletia Schultzii* Wedd. (Tribe Heliantheae; Compositae) [399].
-From *Heteroplexis microcephala* (Compositae) [971].
-From *Otanthus maritimus* (Asteraceae) [662].
-From the aerial parts of *Eupatorium aschenborniana* Schauer (Asteraceae) [2626].
-From *Ageratina glabrata* (HBK) King et Rob (Eupatorium Groupe) [409].
-From aerial parts of *Ageratina pichinchensis* var. bustamenta (DC) R.M. King and H. Rob., Axihuitl [46].
-From *Bahianthus viscidus* [408].
-From aerial parts of *Verbesina luetzelburgl* [407].

colourless oil [399];
b.p.$_1$ 140–142° [2701], b.p.$_5$ 151–153° [2220];
^{1}H NMR [399, 2701], IR [399, 2701], UV [399], MS [399].

USE: Antifungal [2626]; Insecticidal [662]; Cytotoxic activity [971]; Active against dermatophytes [2626]; Antimicrobial [2626].

Glucoside 1-[5-Acetyl-2-(β-D-glucopyranosyloxy)phenyl]-3-methyl-1-butanone

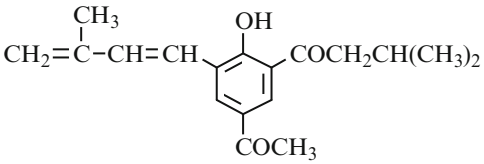
[934302-22-4] $C_{19}H_{26}O_8$ mol. wt. 382.41

-From the aerial parts of *Ophryosporus axilliflorus* (Griseb.) Hieron (Asteraceae) [2353].
-Also obtained by treatment of 1-(5-acetyl-2-hydroxyphenyl)-3-methyl-1-butanone with Brassica napus hairy roots.

pale yellow crystals [2353];
^{1}H NMR [2353], ^{13}C NMR [2353]; $(\alpha)_D^{25} = -40.8°$ (methanol) [2353].

1-[5-Acetyl-2-hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]-3-methyl-1-butanone *(E)*

[148707-32-8] $C_{18}H_{22}O_3$ mol. wt. 286.37



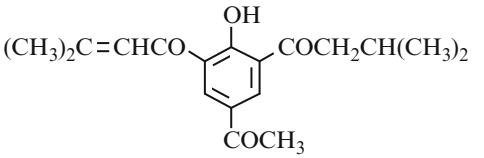
Synthesis

N.B.: After several days in a $CDCl_3$ solution used for the ^1H NMR measurements, 3-(3-hydroxy-3-methyl-1-butenyl)-5-isovaleryl-4-hydroxyacetophenone (*E*) (**3a**) was converted into the titled substance (**3b**) [2880].

^1H NMR [2880].

1-[5-Acetyl-2-hydroxy-3-(3-methyl-1-oxo-2-butenyl)phenyl]-3-methyl-1-butanone

$C_{18}H_{22}O_4$ mol. wt. 302.37



Synthesis

-Obtained by oxidation of 4-hydroxy-3-(1-hydroxy-3,3-dimethylallyl)-5-isovalerylacetophenone with manganese dioxide in ethyl ether for 30 min (60 %) [395].

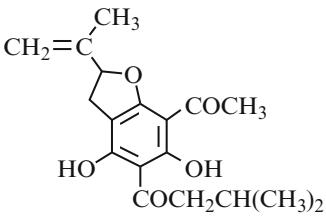
Isolation from natural source

-From the roots of *Gerbera piloselloides* Cass. (Family of Compositae, Tribe Arctotideae) [395].

colourless oil [395]; ^1H NMR [395], IR [395], MS [395].

1-[7-Acetyl-2,3-dihydro-4,6-dihydroxy-2-(1-methylethenyl)-5-benzofuranyl]-3-methyl-1-butanone

[119998-65-1] $C_{18}H_{22}O_5$ mol. wt. 318.37



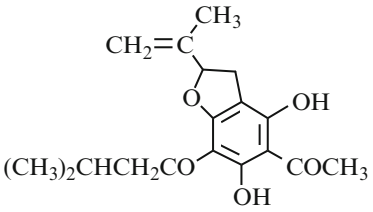
Synthesis

-Obtained by acid-catalyzed of Sessiliflorene with p-toluenesulfonic acid in toluene at 110° [601].

^1H NMR [601], ^{13}C NMR [601],
IR [601], UV [601], MS [601].

1-[5-Acetyl-2,3-dihydro-4,6-dihydroxy-2-(1-methylethenyl)-7-benzofuranyl]-3-methyl-1-butanone

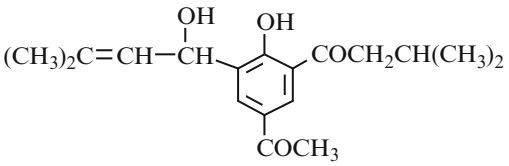
[119998-66-2] $C_{18}H_{22}O_5$ mol. wt. 318.37



Synthesis
-Obtained by acid-catalyzed of Sessiliflorene with p-toluenesulfonic acid in toluene at 110° [601].
^{1}H NMR [601], ^{13}C NMR [601], IR [601], UV [601], MS [601].

1-[5-Acetyl-2-hydroxy-3-(1-hydroxy-3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone
(Hydroxypiloselloidon)

[94413-27-1] $C_{18}H_{24}O_4$ mol. wt. 304.39
[54963-61-0]

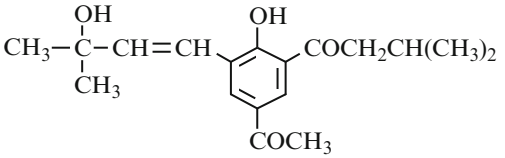


Isolation from natural sources
-From the aerial parts of *Ophryosporus peruvianus* Gmel. K. et R. (Compositae) [410].
-From the roots of *Gerbera piloselloides* Cass. (Compositae) [395].

colourless oil [395];
^{1}H NMR [395], IR [395], MS [395]; $(\alpha)_D^{24} = -50.4°$ (chloroform) [395].

1-[5-Acetyl-2-hydroxy-3-(3-hydroxy-3-methyl-1-butenyl)phenyl]-3-methyl-1-butanone *(E)*
(Hydroxyisopiloselloidon)

[54963-60-9] $C_{18}H_{24}O_4$ mol. wt. 304.39



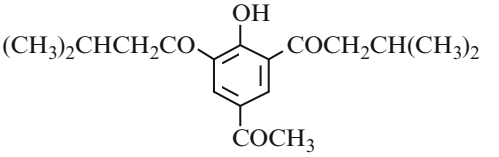
Isolation from natural sources
-From the aerial parts of *Ophryosporus charua* Griseb. Hieron (Compositae) [831].
-From the aerial parts of *Ophryosporus macrodon* Griseb. (Compositae, tribe Eupatorieae) [2880].
-From the leaves of *Ophryosporus axilliflorus* (Griseb.) Hieron (Asteraceae-Asteroideae/Eupatorieae) [979].
-From the roots of *Gerbera piloselloides* Cass. (Family of Compositae, Tribe Arctotideae) [395].

colourless crystals [395]; m.p. 103–105° [2880], 97° [395]; ^{1}H NMR [395, 979, 2880], ^{13}C NMR [979], IR [395]; UV [395], MS [395, 2880].

BIOLOGICAL ACTIVITY: Antiinflammatory [979].

1,1′-[5-Acetyl-2-hydroxy-1,3-phenylene]bis-3-methyl-1-butanone

[94413-28-2] $C_{18}H_{24}O_4$ mol. wt. 304.39

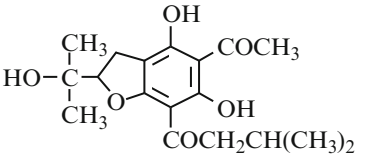


Isolation from the natural sources
-From the aerial parts of Ophryosporus peruvianus Gmel. K. et R. (Compositae) [410].

^{1}H NMR [410], IR [410], MS [410]; TLC [410].

1-[5-Acetyl-2,3-dihydro-4,6-dihydroxy-2-(1-hydroxy-1-methylethyl)-7-benzofuranyl]-3-methyl-1-butanone
(Sessiliflorol A)

[119998-60-6] $C_{18}H_{24}O_6$ mol. wt. 336.38

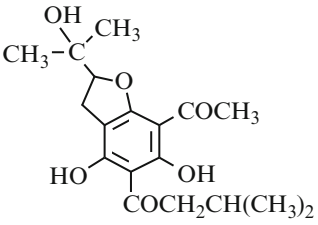


Isolation from natural sources
-From the Plant *melicope sessiliflora* (Rutaceae) [601].
m.p. 105–107° [601];
^{1}H NMR [601],
^{13}C NMR [601], IR [601],
UV [601], MS [601]; X-ray data [601].

BIOLOGICAL ACTIVITY: *In vitro* antiherpes activity [601].

1-[7-Acetyl-2,3-dihydro-4,6-dihydroxy-2-(1-hydroxy-1-methylethyl)-5-benzofuranyl]-3-methyl-1-butanone
(Sessiliflorol B)

[119998-61-7] $C_{18}H_{24}O_6$ mol. wt. 336.38

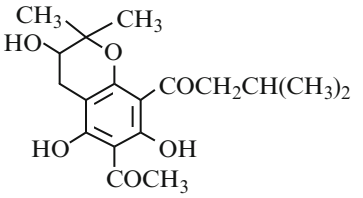


Isolation from natural sources
-From the Plant *melicope sessiliflora* (Rutaceae) [601].
^{1}H NMR [601],
^{13}C NMR [601], IR [601],
UV [601], MS [601].

BIOLOGICAL ACTIVITY: *In vitro* antiherpes activity [601].

1-(6-Acetyl-3,4-dihydro-3,5,7-trihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-3-methyl-1-butanone

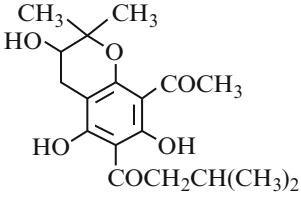
[119998-64-0] $C_{18}H_{24}O_6$ mol. wt. 336.38



Synthesis
-Obtained by acid-catalyzed of Sessiliflorene with p-toluenesulfonic acid in toluene at 110° [601].
^{1}H NMR [601], ^{13}C NMR [601], IR [601], UV [601], MS [601].

1-(8-Acetyl-3,4-dihydro-3,5,7-trihydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-3-methyl-1-butanone

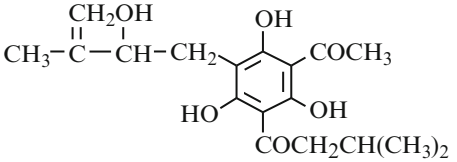
[119998-63-9] $C_{18}H_{24}O_6$ mol. wt. 336.38



Synthesis
-Obtained by acid-catalyzed of Sessiliflorene with p-toluenesulfonic acid in toluene at 110° [601].
^{1}H NMR [601], ^{13}C NMR [601], IR [601], UV [601], MS [601].

1-[3-Acetyl-2,4,6-trihydroxy-5-(2-hydroxy-3-methyl-3-butenyl)phenyl]-3-methyl-1-butanone
(Sessiliflorene)

[119998-59-3] $C_{18}H_{24}O_6$ mol. wt. 336.38

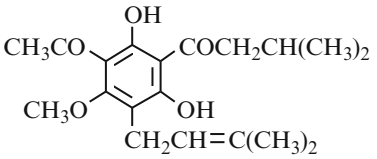


Isolation from natural sources
-From the Plant *melicope sessiliflora* (Rutaceae) [337, 601].
m.p. 117–120° [601];
^{1}H NMR [601],
^{13}C NMR [601], IR [601],
UV [601], MS [601].

BIOLOGICAL ACTIVITY: *In vitro* antiherpes [601]; Antiprotozoal and antimicrobial [337].

1-[3-Acetyl-2,6-dihydroxy-4-methoxy-5-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone
(Acronyculatin C)

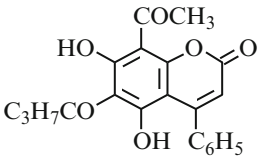
[578716-69-5] $C_{19}H_{26}O_5$ mol. wt. 334.41



Isolation from natural sources
-From *Acronychia pedunculata* (L.) Miq. (Rutaceae) [2969].
^{1}H NMR [2969], ^{13}C NMR [2969], IR [2969], UV [2969], MS [2969].

5,7-Dihydroxy-6-(1-butanoyl)-8-acetyl-4-phenyl-2*H*-1-benzopyran-2-one
(Racemosone)

$C_{21}H_{18}O_6$ mol. wt. 366.37



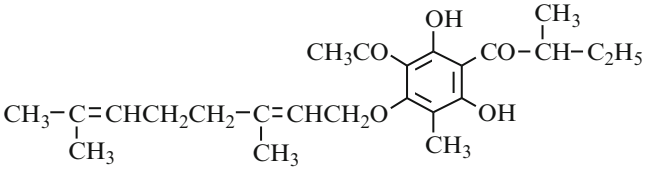
Synthesis
-Obtained by reaction of acetyl chloride with 5,7-dihydroxy-6-(1-butanoyl)-4-phenyl-2*H*-1-benzopyran-2-one in the presence of aluminium chloride in carbon disulfide, then in refluxing nitromethane (11 %) [2146].

Isolation from natural sources
-From the leaves of *Mesua racemosa* (Clusiaceae) [2146].

m.p. 149–150° [2146];
^{1}H NMR [2146], ^{13}C NMR [2146], IR [2146], UV [2146], MS [2146].

1-[3-Acetyl-4-[[(2*E*)-3,7-dimethyl-2,6-octadienyl]oxy]-2,6-dihydroxy-5-methylphenyl]-2-methyl-1-butanone

[267009-82-5] $C_{24}H_{34}O_5$ mol. wt. 402.53



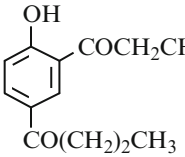
Isolation from natural sources
-From *Hypericum japonicum* (Guttiferae) [1386].

colourless oil [1386];
^{1}H NMR [1386], ^{13}C NMR [1386], IR [1386], UV [1386], MS [1386]; $(\alpha)_D^{31.2} = -7.02$ (methanol) [1386].

12 Diketones Derived from Propionic and 1-Butanoic Acids

1-[4-Hydroxy-3-(1-oxopropyl)phenyl]-1-butanone

[173469-67-5] $C_{13}H_{16}O_3$ mol. wt. 220.27



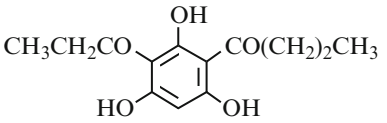
Synthesis

-Obtained by reaction of butyryl chloride with 2-hydroxypropiophenone in the presence of aluminium chloride in carbon disulfide (90 %) [345].

m.p. 81–82° [345]; ^{1}H NMR [345], IR [345].

1-[2,4,6-Trihydroxy-3-(1-oxopropyl)phenyl]-1-butanone

[96573-40-9] $C_{13}H_{16}O_5$ mol. wt. 252.27



Syntheses

-Obtained by reaction of butyryl chloride with phloropropiophenone in the presence of aluminium chloride in nitrobenzene for 3 days at r.t. (5–10 %) [421].

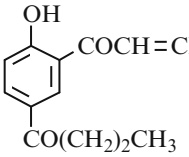
-Also refer to: [3033].

m.p. 135° [421]; ^{1}H NMR [421], IR [421], MS [421].

BIOLOGICAL ACTIVITY: Inhibitory effects of treatment with this acylphenol on TPA induced EBV-EA activation [3033].

1-[4-Hydroxy-3-(1-oxo-3-phenyl-2-propenyl)phenyl]-1-butanone

[173469-75-5] $C_{19}H_{18}O_3$ mol. wt. 294.35



Synthesis

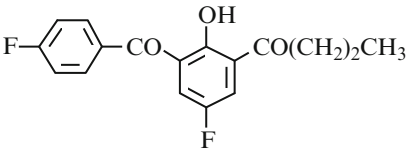
-Obtained by reaction of benzaldehyde with 1-(3-acetyl-4-hydroxyphenyl)-1-butanone in the presence of potassium hydroxide in methanol at r.t. (95 %) [345].

m.p. 99–100° [345]; ^{1}H NMR [345], IR [345].

13 Diketones Derived from Benzoic and 1-Butanoic Acids

1-[5-Fluoro-3-(4-fluorobenzoyl)-2-hydroxyphenyl]-1-butanone

[2250-71-7] $C_{17}H_{14}F_2O_3$ mol. wt. 304.29



Synthesis

-Obtained by Fries rearrangement of 2-butyryl-4-fluorophenyl 4-fluorobenzoate (1 mol) with aluminium chloride (4–5 mol) at 160° for 6 h [1550].

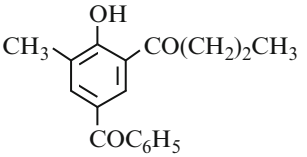
m.p. 150° [1550].

2,4-Dinitrophenylhydrazone $C_{23}H_{18}F_2N_4O_6$ mol. wt. 428.39

m.p. 147° [1550].

1-(5-Benzoyl-2-hydroxy-3-methylphenyl)-1-butanone

[101789-78-0] $C_{18}H_{18}O_3$ mol. wt. 282.34



Syntheses

-Obtained by Fries rearrangement of 4-benzoyl-2-methyl-phenyl butyrate with aluminium chloride (50 %) [106].

-Also obtained by reaction of benzoyl chloride with 2-butyryl-6-methylphenol in the presence of aluminium chloride [106].

m.p. 75° [106].

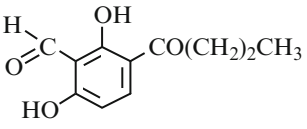
Acetate [102159-08-0] $C_{20}H_{20}O_4$ mol. wt. 324.38

m.p. 82° [106].

14 Diketones Derived from Formic and 1-Butanoic Acids

2,6-Dihydroxy-3-(1-oxobutyl)benzaldehyde

[855875-24-0] $C_{11}H_{12}O_4$ mol. wt. 208.21



Synthesis

-Obtained from resbutyrophenone; zinc cyanide, potassium chloride; aluminium chloride and hydrogen chloride (26 %) [2821].

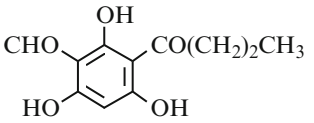
yellow needles [2821]; m.p. 42–43° [2821].

Semicarbazone $C_{12}H_{15}N_3O_4$ mol. wt. 265.27

m.p. 242–245° (d) [2821].

2,4,6-Trihydroxy-3-(1-oxobutyl)benzaldehyde

[96573-30-7] $C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis

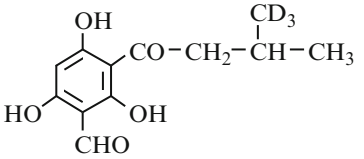
-Obtained by reaction of ethyl orthoformate with 2,4,6-trihydroxybutyrophenone in the presence of aluminium chloride in methylene chloride with cooling in an ice bath for 30 min (70 %) [421].

m.p. 163–165° (d) [421]; ^{1}H NMR [421], IR [421], MS [421].

BIOLOGICAL ACTIVITY: As photosynthetic electron transport (PET) [3405].

2,4,6-Trihydroxy-3-(3-methyl-(d_3)-1-oxobutyl)benzaldehyde

$C_{12}H_{11}D_3O_5$ mol. wt. 238.24



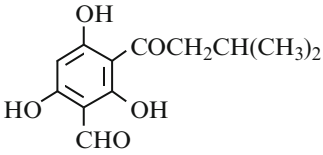
Syntheses

-Obtained by reaction of ethyl orthoformate with phloroisovalerophenone in the presence of aluminium chloride in methylene chloride at 0° for 30 min (70 %) [421, 3415].

m.p. 74° [3415]; ^{1}H NMR [3415], IR [3415], MS [3415].

2,4,6-Trihydroxy-3-(3-methyl-1-oxobutyl)benzaldehyde

[78423-49-1] $C_{12}H_{14}O_5$ mol. wt. 238.24



Syntheses

-Obtained by reaction of ethyl orthoformate with 2,4,6-trihydroxyisobutyrophenone in the presence of aluminium chloride in methylene chloride with cooling in an ice bath for 30 min (70 %) [421].

-Also obtained by adding DMF and phosphoryl chloride (Vilsmeier-Haack reagent) to a solution of phloroglucinol in ethyl acetate. The reaction mixture was further stirred for 30 min at r.t. [334], (70 %) [335, 337, 621].

-Also obtained by reaction of zinc cyanide with 2,4,6-trihydroxyisovalerophenone (Houben-Hoesch reaction) [2534].

-Also refer to: [336, 3033, 3405, 3408].

m.p. 137–139° [2534], 74° [421];

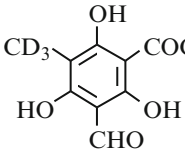
N.B.: One of the reported melting point is obviously wrong.

^{1}H NMR [421, 2534], IR [421], MS [421, 2534].

BIOLOGICAL ACTIVITY: Effects on transpiration and stomatal closure [3408]; Germination inhibition [421]; Inhibitory effects of treatment with this acylphenol on TPA induced EBV-EA activation [3033]; As photosynthetic electron transport (PET) [3405].

2,4,6-Trihydroxy-3-methyl-(d_3)-5-(3-methyl-1-oxobutyl)benzaldehyde
(Deuterated grandinol)

$C_{13}H_{13}D_3O_5$ mol. wt. 255.24

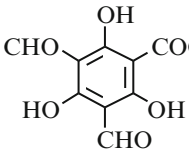


Synthesis
-Obtained by heating a mixture of 3-formylphloro-isovalerophenone, potassium hydroxide, d_3-iodomethane, d_4-methanol and deuterium oxide at 70° for 4 h (28 %) [3415].
m.p. 125–130° [3415];

^{1}H NMR [3415], UV [3415], IR [3415], MS [3415].

2,4,6-Trihydroxy-5-(3-methyl-1-oxobutyl)-1,3-benzenedicarboxaldehyde
(Jensenone)

[96573-43-2] $C_{13}H_{14}O_6$ mol. wt. 266.25



Syntheses
-Obtained by reaction of hexamethylenetetramine with 2,4,6-trihydroxyisovalerophenone in the presence of trifluoroacetic acid at 70° (40 %) [335].
-Also obtained by reaction of 3-methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-butanone with dichloromethyl methyl ether in the presence of titanium tetrachloride in methylene chloride at −20° under argon. Then the mixture was allowed to stand at −20° for 2 h (41.6 %) [642].
Isolation from natural sources
-From fresh leaves of *Eucalyptus grandis* (Myrtaceae) [337, 1754].
-From *Eucalyptus jensenii* Maiden (Myrtaceae) [337, (approximatively 70 % of the oil) 419, 1106, 1453, 2037].
-From the leaf essential oil of *Eucalyptus apodophylla* (Myrtaceae) [2046].
-Also refer to: [1107, 3033].

BIOLOGICAL ACTIVITY: Antiprotozoal and antimicrobial [337]; Antifeedant [337]; A marsupial antifeedant [2037]; Inhibitory effects of treatment with this acylphenol on TPA induced EBV-EA activation [3033].

white solid [419]; pink crystals [642];
m.p. 198–200° [421], 113–114° [642], 102° [419];
N.B.: One of the reported melting point is obviously wrong.

^{1}H NMR [419, 421, 642], ^{13}C NMR [419], IR [419, 421, 642], UV [642], MS [419, 421, 642, 2046];
GC-FID [2037]; GC-MS [419, 2037, 2046]; LC-UV [2037];
LC-MS [2037].

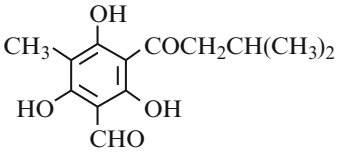
Triacetate [143183-56-6] $C_{19}H_{20}O_9$ mol. wt. 392.36

-Obtained by reaction of acetic anhydride with Jensenone in the presence of pyridine at r.t. for 48 h [419].

^{1}H NMR [419], ^{13}C NMR [419], IR [419], MS [419].

2,4,6-Trihydroxy-3-methyl-5-(3-methyl-1-oxobutyl)benzaldehyde
(Grandinol)

[63861-11-0] $C_{13}H_{16}O_5$ mol. wt. 252.27



Syntheses

-Obtained by reaction of methyl iodide with 3-formyl-phloroisovalerophenone in the presence of potassium hydroxide in methanol [334, 335, 421, 3415].
-Also obtained by reaction of triethyl orthoformate with 3-isovaleroyl-2,4,6-trihydroxytoluene [3176] according to [641].
-Also obtained by formylation of 3-methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-butanone using dichloromethyl methyl ether reagent and titanium tetrachloride as catalyst in methylene chloride at 0° for 1 h (25 %) [3437].
-Also obtained by reaction of 3-methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-butanone with dichloromethyl methyl ether in the presence of titanium tetrachloride in methylene chloride at −20° under argon. Then the mixture was allowed at −20° for 2 h (41.6 %) [642].

Isolation from natural sources

-From fresh leaves of *Eucalyptus grandis* (Myrtaceae) [337, 419, 421, 769, 1346, 1754, 3405, 3406, 3413–3415, 3437].
-From *Eucalyptus grandis* W. Hill ex Maiden [1106, 1107].
-From fresh leaves and stems of *Eucalyptus pulverulenta* [419–421] Sims [1106].
-From the leaves of *Eucalyptus perriniana* [2235] F. Muell. ex Rodway [1106].
-From *Eucalyptus jensenii* Maiden (Myrtaceae) [419].
-From *Eucalyptus* [642].
-Also refer to: [1753, 3033].

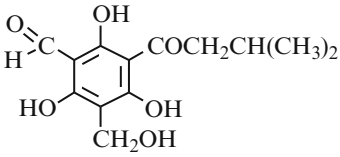
colourless crystals; yellowish powder [2235]; pink crystals [642];
m.p. 131–133° [420], 130–132° [421, 769, 3413, 3437], 130° [2235], 113–114° [642];
^{1}H NMR [420, 421, 642, 769, 2235, 3413], IR [421, 642, 769, 2235, 3413],

UV [642, 769, 2235, 3413], MS [420, 421, 642, 769, 2235, 3413];
X-ray analysis [421]; GC-MS [420]; TLC [2235]; HPLC [3413].

BIOLOGICAL ACTIVITY: Antiprotozoal and antimicrobial [337]; G-inhibitor (plant growth regulator) [419, 1107, 3413]; A rooting inhibitor in adult tissues of *Eucalyptus grandis* [769, 3415]; A potent germination inhibitor was found in *Eucalyptus pulverulenta* [420]; Antibacterial [2235]; Effects on transpiration and stomatal closure [3408]; Germination inhibition [421, 3414]; Inhibitory effects of treatment with this acylphenol on TPA induced EBV-EA activation [3033]; Strongly inhibit photosynthesis as well as germination of cress seeds [1346]; As photosynthetic electron transport (PET) [3405]; PET inhibitory activity [3414].

2,4,6-Trihydroxy-3-(hydroxymethyl)-5-(3-methyl-1-oxobutyl)benzaldehyde

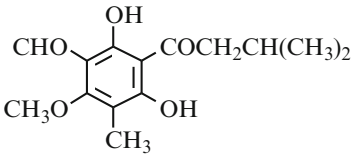
$C_{13}H_{16}O_6$ mol. wt. 268.27



Synthesis
-Refer to: [1106].
N.B.: A precursor of Jensenone [1106].

2,4-Dihydroxy-6-methoxy-5-methyl-3-(3-methyl-1-oxobutyl)benzaldehyde

[63861-20-1] $C_{14}H_{18}O_5$ mol. wt. 266.29

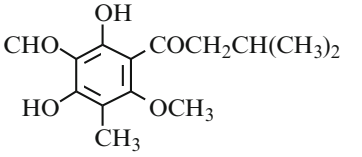


Synthesis
-Obtained by treatment of Grandinol with diazomethane [769].
m.p. 89–89.5° [769];
^{1}H NMR [769], ^{13}C NMR [769],
UV [769], MS [769]; X-ray data [769].

BIOLOGICAL ACTIVITY: Germination inhibition [421].

2,6-Dihydroxy-4-methoxy-5-methyl-3-(3-methyl-1-oxobutyl)benzaldehyde

[63861-21-2] $C_{14}H_{18}O_5$ mol. wt. 266.29

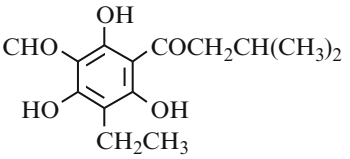


Synthesis
-Obtained by treatment of Grandinol with diazomethane [769].
m.p. 78–78.5° [769];
^{1}H NMR [769], UV [769], MS [769].

BIOLOGICAL ACTIVITY: Germination inhibition [421].

3-Ethyl-2,4,6-trihydroxy-5-(3-methyl-1-oxobutyl)benzaldehyde

[96573-34-1] $C_{14}H_{18}O_5$ mol. wt. 266.29



Syntheses

-Obtained by reaction of ethyl iodide with 2,4,6-tri-hydroxy-3-(3-methyl-1-oxobutyl)benzaldehyde in the presence of potassium hydroxide in aqueous methanol at 65° for 24 h (30 %) [421].

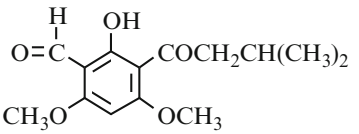
-Also refer to: [3033].

m.p. 126–126.5° [421]; ^{1}H NMR [421], IR [421], MS [421].

BIOLOGICAL ACTIVITY: Germination inhibition [421]; Inhibitory effects of treatment with this acylphenol on TPA induced EBV-EA activation [3033].

2-Hydroxy-4,6-dimethoxy-3-(3-methyl-1-oxobutyl)benzaldehyde

[179630-54-7] $C_{14}H_{18}O_5$ mol. wt. 266.29



Syntheses

-Obtained by reaction of dichloromethyl methyl ether with 2-hydroxy-4,6-dimethoxyisovalerophenone in the presence of titanium tetrachloride in methylene chloride at −10°. Then, the reaction mixture was stored at r.t. for 1 h (98 %) [643].

-Obtained by reaction of isovaleryl chloride with 2,4-dimethoxy-6-hydroxybenzaldehyde in the presence of aluminium chloride in methylene chloride for 20 h at r.t. (80 %) [2576].

-Also refer to: [270].

colourless solid [2576]; m. p. 91° [2576], 62° [643];

N.B.: One of the reported melting point is obviously wrong.

^{1}H NMR [643, 2576], ^{13}C NMR [643, 2576], IR [643, 2576], UV [643], MS [643];

X-ray data [270]; TLC [2576].

Tert-Butyldimethylsilyl derivative [233751-78-5] $C_{20}H_{32}O_5Si$ mol. wt. 380.56

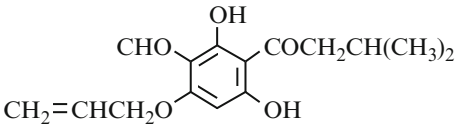
-Obtained by reaction of TBSCl (tert-butyldimethylsilyl chloride) with the title ketone in the presence of ethyldimethylamine and DMAP (4-dimethylaminopyridine) in methylene chloride for 20 h at r.t. (76 %) [2576].

colourless solid [2576]; m. p.105.8° [2576];

^{1}H NMR [2576], ^{13}C NMR [2576], IR [2576]; TLC [2576].

2,4-Dihydroxy-3-(3-methyl-1-oxobutyl)-6-(2-propen-1-yloxy)benzaldehyde

[918814-59-2] $C_{15}H_{18}O_5$ mol. wt. 278.30



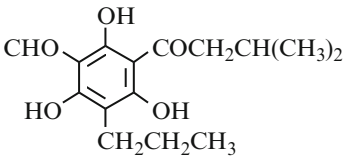
Synthesis
-Obtained from 1-(2,6-dihydroxy-4-allyloxy)-isovalerophenone further upon Vilsmeier-Haack formylation (40 %) [337].

light violet solid [337]; m.p. 96–98° [337];
^{1}H NMR [337], ^{13}C NMR [337], IR [337], UV [337], MS [337].

BIOLOGICAL ACTIVITY: *In vitro* antileishmanial [337]; Cytotoxicity [337].

2,4,6-Trihydroxy-3-(3-methyl-1-oxobutyl)-5-propylbenzaldehyde

[96573-35-2] $C_{15}H_{20}O_5$ mol. wt. 280.32



Syntheses
-Obtained by reaction of propyl iodide with 2,4,6-trihydroxy-3-(3-methyl-1-oxobutyl) benzaldehyde in the presence of potassium hydroxide in aqueous methanol at 65° for 24 h (30 %) [421].

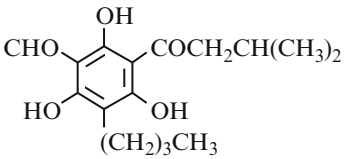
-Also refer to: [3033].

m.p. 124–125° [421]; ^{1}H NMR [421], IR [421], MS [421].

BIOLOGICAL ACTIVITY: Inhibitory effects of treatment with this acylphenol on TPA induced EBV-EA activation [3033].

3-Butyl-2,4,6-trihydroxy-5-(3-methyl-1-oxobutyl)benzaldehyde

[96573-36-3] $C_{16}H_{22}O_5$ mol. wt. 294.35

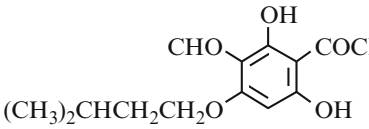


Synthesis
-Obtained by reaction of butyl iodide with 2,4,6-tri-hydroxy-3-(3-methyl-1-oxobutyl) benzaldehyde in the presence of potassium hydroxide in aqueous methanol at 65° for 24 h (30 %) [421].

m.p. 101–102° [421]; ^{1}H NMR [421], IR [421], MS [421].

2,4-Dihydroxy-6-(3-methylbutoxy)-3-(3-methyl-1-oxobutyl)-1-butanone

[918814-63-8] $C_{17}H_{24}O_5$ mol. wt. 308.38



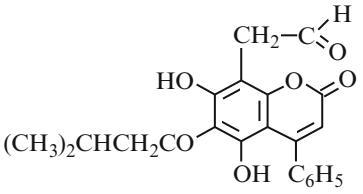
Synthesis
-Obtained from 1-(2,6-dihydroxy-4-isopentyloxy)-isovalerophenone further upon Vilsmeier-Haack formylation (40 %) [337].

off white solid [337]; m.p. 85–87° [337];
^{1}H NMR [337], ^{13}C NMR [337], IR [337], UV [337], MS [337].

BIOLOGICAL ACTIVITY: *In vitro* antileishmanial [337]; Cytotoxicity [337].

[5,7-Dihydroxy-6-(3-methylbutyryl)-2-oxo-4-phenyl-2*H*-chromen-8-yl] acetaldehyde

[37972-56-8] $C_{22}H_{20}O_6$ mol. wt. 380.40

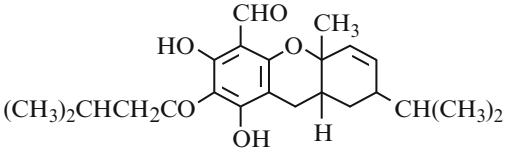


Synthesis
-Formation by simple fission of the double bond of 5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one obtained by ozonization in acetic acid at 15° (64 %) [1007].

pale yellow needles [1007]; m.p. 175–183° [1007];
IR [1007], UV [1007].

Euglobal-IIc

[77794-62-8] $C_{23}H_{30}O_5$ mol. wt. 386.49



Isolation from natural sources
-From the flower buds of *Eucalyptus globulus* LABILL [1753, 3033].

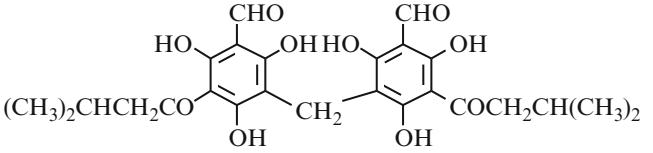
colourless oil [1754];
$(\alpha)_D^{20} = -137°$ (chloroform) [1754]; $(\alpha)_D^{20} = -144°$ (chloroform) [1753];
^{1}H NMR [1753, 1754], ^{13}C NMR [1753], IR [1753, 1754],
UV [1753, 1754], MS [1754]; circular dichroism [1753].

Refer to: [1754 (**5**), 3033 (**7**)].

BIOLOGICAL ACTIVITY: Inhibitory effects of treatment with this acylphenol on TPA induced EBV-EA activation [3033]; Active in the fertile egg test [1753].

1,1′-Methylenebis[2,4,6-trihydroxy-3-(1-oxomethyl)-5,1-phenylene]bis-3-methyl-1-butanone
Methylenebis(3-formyl-5-isopentanoyl)-2,4,6-trihydroxybenzene
(Robustaol A)

$C_{25}H_{28}O_{10}$ mol. wt. 488.49



Syntheses
-Refer to: [621 (30 %), [2534].

Isolation from natural sources
-From the leaves of *Eucalyptus robusta,* a plant used in Chinese herbal medicine [1819].

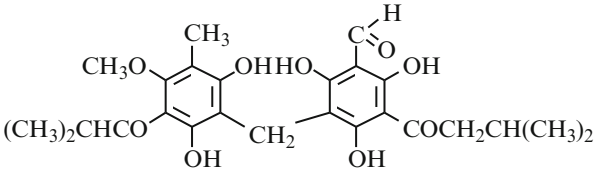
cream coloured solid [621]; m.p. 228–230° [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621], MS [621].

BIOLOGICAL ACTIVITY: Antimalarial [1819, 2534].

-Also refer to: [621].

5-[2,6-Dihydroxy-4-methoxy-3-methyl-5-(2-methyl-1-oxopropyl)phenyl] methyl-3-(3-methyl-1-oxobutyl)-2,4,6-trihydroxybenzaldehyde
(Robustaol A)

$C_{25}H_{30}O_9$ mol. wt. 474.50

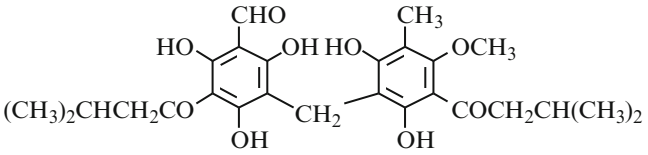


Isolation from natural sources
-From the leaves of *Eucalyptus robusta* Sm. (Myrtaceae) [2534].

m.p. 163–164° [2534];
^{1}H NMR [2534], IR [2534], UV [2534], MS [2534].
N.B.: Identification from its alkaline degradation products [2534].

2,4,6-Trihydroxy-5-(3-methyl-1-oxobutyl)-3-[2,6-dihydroxy-4-methoxy-3-(3-methyl-1-oxobutyl)-5-methylphenyl]methylbenzaldehyde
(Robustaol A)

$C_{26}H_{32}O_9$ mol. wt. 488.53

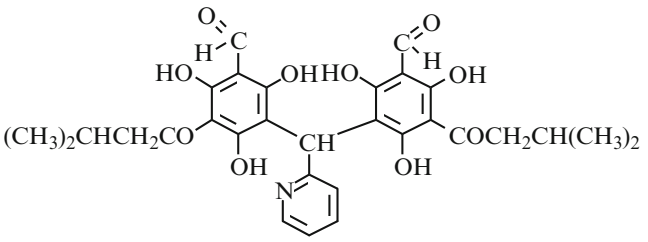


Isolation from natural sources
-From the leaves of *Eucalyptus robusta* Smith (Myrtaceae) [1106].

BIOLOGICAL ACTIVITY: Antimalarial [1106].

1-[3-Formyl-5-[(5-formyl-3-isopentanoyl-2,4,6-trihydroxyphenyl)pyridin-2-yl-methyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{30}H_{31}NO_{10}$ mol. wt. 565.58



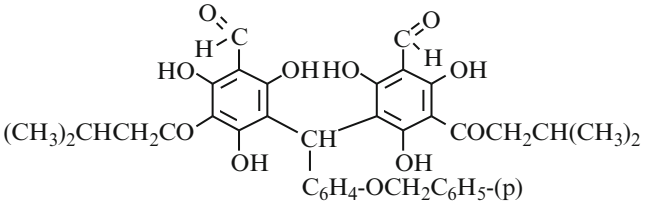
Synthesis
-Obtained by irradiation of a 3-formyl phloroiso-valerophenone in chloroform, p-TsCl and 2-formylpyridine mixture with microwave radiations (750 W) in domestic microwave oven for 10–15 min (44 %) [621].

yellow solid [621]; m.p. 148–149° [621];
^{1}H NMR [621], ^{13}C NMR [621], IR [621], UV [621], MS [621].

BIOLOGICAL ACTIVITY: Cytotoxicity [621].

1-[3-Formyl-5-[(5-formyl-3-isopentanoyl-2,4,6-trihydroxyphenyl)-4-benzyloxyphenyl-methyl]-2,4,6-trihydroxyphenyl]-3-methyl-1-butanone

$C_{38}H_{38}O_{11}$ mol. wt. 670.71



Syntheses

-Obtained by irradiation of a 3-formyl phloroiso-valerophenone in chloroform, p-TsCl and 4-benzyloxybenzaldehyde mixture with microwave radiations (750 W), in domestic microwave oven for 10–15 min (40 %) [621].

-Also refer to: [620 (33 %)].

cream colour solid [620, 621]; m.p. 195–197° [620], 180° [621]; ^{1}H NMR [620, 621], ^{13}C NMR [620, 621], IR [621], UV [621], MS [620, 621].

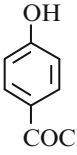
BIOLOGICAL ACTIVITY: Cytotoxicity [621].

15 Aromatic Hydroxy-4-Oxo-1-Butanoic Acids

15.1 Unsubstituted Hydroxyketones

4-(4-Hydroxyphenyl)-2,3-dibromo-4-oxo-1-butanoic acid

$C_{10}H_8Br_2O_4$ mol. wt. 351.98



Synthesis

-Refer to: [2593].

Ethyl ether

$C_{12}H_{12}Br_2O_4$ mol. wt. 380.03

-Obtained by treatment of p-ethoxybenzoylacrylic acid (m.p. 141–142°) with bromine in acetic acid [2593].

m.p. 151° (d) [2593].

Methyl ether [103862-60-8] $C_{11}H_{10}Br_2O_4$ mol. wt. 366.01

-Refer to: [1095, 2592, 2753, 2794].

m.p. 164° (higher-melting form) [2592, 2794],
140–141° [2794], 140° (lower-melting form) [2592].

BIOLOGICAL ACTIVITY: Antifungal [1095].

-Also refer to: [2753].

Methyl ester of the methyl ether

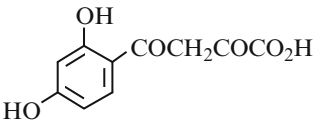
[92017-91-9] $C_{12}H_{12}BrO_4$ mol. wt. 380.03
[27117-71-1] (threo)
[27117-72-2] (erythro)

-Refer to: [2592, 2795].

m.p. 115–116° (erythro) [255, 2795], 115° [2592],
68–69° (threo) [255], 57–58.5° [2795].

4-(2,4-Dihydroxyphenyl)-2,4-dioxo-1-butanoic acid

$C_{10}H_8O_6$ mol. wt. 224.17



Synthesis
-Refer to: [2456].

Ethyl ester of the dimethyl ether [80081-75-0] $C_{14}H_{16}O_6$ mol. wt. 280.28

-Obtained by reaction of resacetophenone dimethyl ether with ethyl oxalate in the presence of sodium [2456].

yellow crystals [2456]; m.p. 86–87° [2456].

Methyl ester of the dimethyl ether [39757-32-9] $C_{13}H_{14}O_6$ mol. wt. 266.25

m.p. 100–101° [117].

Methyl ester of the dibenzyl ether $C_{25}H_{22}O_6$ mol. wt. 418.45

m.p. 160–164° [167].

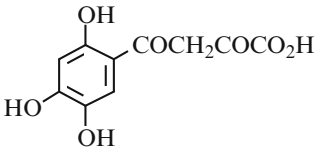
Ethyl ester of the diethyl ether $C_{16}H_{20}O_6$ mol. wt. 308.33

m.p. 152° [1742].

Ethyl ester of the dibenzyl ether [170283-09-7] $C_{26}H_{24}O_6$ mol. wt. 432.47

4-(2,4,5-Trihydroxyphenyl)-2,4-dioxo-1-butanoic acid

$C_{10}H_8O_7$ mol. wt. 240.17



Synthesis
-Refer to: [2196].
Triethyl ether [63213-34-3]
$C_{16}H_{20}O_7$ mol. wt. 324.33
2,4,5-Triethoxy-α,γ-dioxobenzenebutanoic acid

-Preparation: An oil dispersion of sodium hydride was added to a mixture of 2,4,5-triethoxy-acetophenone, diethyl oxalate and benzene. The mixture was stirred at 65–70° for 1 h. The ethyl ester obtained (90 %, m.p. 153–155°) was dissolved in sulfuric acid at r.t. for 2 h (65 %) [2196].

m.p. 178–181° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

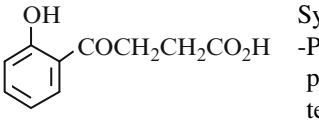
Ethyl ester of the triethyl ether [63213-44-5] $C_{18}H_{24}O_7$ mol. wt. 352.38

-Refer to: [2196].

m.p. 153–155° [2196].

4-(2-Hydroxyphenyl)-4-oxo-1-butanoic acid
γ-o-hydroxyphenyl-γ-ketobutyric acid

[39560-34-4] $C_{10}H_{10}O_4$ mol. wt. 194.19



Syntheses
-Preparation by reaction of succinic anhydride with phenol in the presence of aluminium chloride in tetrachloroethane at 130–140° for 2 h (62 %) [2100], (55 %) [197], (30–35 %) [2571], (26–28 %) [222], (20 %) [990].
-Also obtained by Fries rearrangement of phenyl hydrogen succinate with aluminium chloride at 117° for 2.5 h in tetrachloroethane (58 %) or in chlorobenzene (41 %) [1987].
-Also obtained from 4-(2-hydroxyphenyl)-4-oxobutyronitrile [2649].
-Also refer to: [222 (54 %), 676, 997 (2 %), 3291 (0.4 %)].

colourless crystals [2100]; long colourless needles [990];
m.p. 146° [197, 2097, 2571], 145–146° [222],
145° [2100, 2649], 139–140° [222, 990, 3291],
127–130° [997];
^{1}H NMR [676, 997, 3291], IR [676, 997, 3291].

Methyl ether [103987-16-2] $C_{11}H_{12}O_4$ mol. wt. 208.21

-Obtained by reaction of methyl iodide with o-benzoylpropionic acid in the presence of potassium carbonate in refluxing acetone for 8 h. Then, hydrolysis of the methyl β-o-anisoylpropionate obtained [222].
-Also obtained by methylation of the title ketone [2571].
-Also obtained by Robinson's method [2571].
-Also refer to: [391, 805 (86 %), 1032, 1131, 3139].

m.p. 100–101° [222], 98° [3139], 97–98° [2571], 95.6–96.6° [805], 86–88° [1032]; ^{1}H NMR [1032], IR [391].

BIOLOGICAL ACTIVITY: Human zinc insulin; Delivery of [1131].

Methyl ester of the methyl ether [99046-13-6] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained from o-bromoanisole and β-carbomethoxypropionyl chloride (Grignard reaction) (43 %) [805].

b.p.$_{1.5}$ 161–162° [805], 160° [3139].

Methyl ester [56871-93-3] $C_{11}H_{12}O_4$ mol. wt. 208.21

-Refer to: [915, 997, 3122].

b.p.$_{0.4}$ 135° [3122]; m.p. 33–34° [997];
^{1}H NMR [915, 997], ^{13}C NMR [915], IR [997],
MS [915].

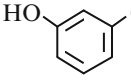
Ethyl ester [39496-84-9] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Refer to: [216, 2571].

colourless liquid [2571];
b.p.$_{0.1}$ 112–113° [216], b.p.$_{184}$ 255° [2571].

4-(3-Hydroxyphenyl)-4-oxo-1-butanoic acid

[56872-07-2] $C_{10}H_{10}O_4$ mol. wt. 194.19

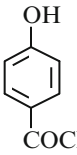


Syntheses
-Refer to: [665, 1706, 1993].

m.p. 146.5° [1706], 146–147° [665], 144–145° [1993].

4-(4-Hydroxyphenyl)-4-oxo-1-butanoic acid
γ-p-hydroxyphenyl-γ-ketobutyric acid

[56872-39-0] $C_{10}H_{10}O_4$ mol. wt. 194.19



Syntheses
-Preparation by reaction of succinic anhydride with phenol in the presence of aluminium chloride in tetrachloroethane at 130–140° for 2 h [222], (6 %) [197], (2–3 %) [2571].
-Also obtained by treatment of its methyl ether with hydrogen bromide in refluxing acetic acid (86 %) [2652].
-Also refer to: [43, 496, 990 (3 %), 1208, 1341, 1482, 1561, 1706, 1779, 1939, 2100, 2438, 3007].

lustrous needles [222]; slightly yellow [990];
m.p. 160–161° [222], 159–160° [3007], 159° [2652], 157° [1706], 156–159° [1561], 156° [2571], 155–156° [1341], 154–156° [990];
^{1}H NMR [1208, 1341], ^{13}C NMR [1341].

BIOLOGICAL ACTIVITY: Feeble choleretic [496].

Methyl ether [3153-44-4] $C_{11}H_{12}O_4$ mol. wt. 208.21

-Preparation by reaction of succinic anhydride with anisole in the presence of aluminium chloride [257, 258, (90 %) 2392, 3401],
*in tetrachloroethane [858] first at 0°, then at r.t. overnight (83 %) [2649], (80 %) [2100];
*in tetrachloroethane and nitrobenzene mixture (85 %) [987], at r.t. for 2.5–3 h (75 %) [2579];
*in nitrobenzene: [858, 1281], first at 0°, then at r.t. overnight (72 %) [606] or at 60° for 3 h (77 %) [1745];
*in benzene at 60° for 30 min (77 %) [1302];
*in carbon disulfide [257, 891, 1209];
*in methylene chloride with ice-ethanol bath cooling and stirring for 3 h (55 %) [878].
-Also obtained by basic hydrolysis of its methyl ester [1093].

-Also refer to: [71, 72, 99, 262, 437, 806, 837, 945, 977, 980, 991, 1061, 1131, 1169, 1410, 1503, 1520, 1529, 1635, 1664, 1667, 1668, 1779, 1854, 1953, 1955, 2015, 2128, 2129, 2358, 2359, 2383, 2427, 2529, 2546, 2733 (80 %), 2817, 2831]

large hexagonal prisms [1209]; white flaky solid [2546];
b.p. 154° [2579];
m.p. 148–151° [1302], 148–150° [2579], 147.5–148.5° [606], 147–149° [2733], 147–148° [1281, 1766, 2392], 147° [1209], 146–148° [878], 146–147° [987, 2358, 2359, 2546], 146° [2099, 2100, 2649], 145–146° [3401], 144.5–146.5° [1529], 144–146° [1093], 144–145° [257, 258], 142–143° [1745];

^{1}H NMR [606, 891, 1061, 1131, 1410, 1520, 1635, 1668, 1745, 1953, 2427, 2546, 2831],
^{13}C NMR [1520, 1635, 1745],
IR [837, 1520, 1635, 1745, 1953, 2427, 2546, 2817], UV [806, 1169],
MS [606, 1520, 1635, 1745, 2546].

BIOLOGICAL ACTIVITY: Feeble choleretic [496]; Human zinc insulin, delivery of [1131]; Inhibition of aggregation of thrombocytes [1779]; Antinociceptive [891].

Methyl ester of the methyl ether [5447-74-5] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by bubbling hydrogen chloride in 1-(4-methoxyphenyl)-4-oxo-1-butanoic acid in methanol for 1.5 h [257, 258].
-Also obtained by reaction between anisole and 3-carbomethoxypropanoic acid in the presence of PPA for 2.5 h at 45° (75 %) [1093].
-Also obtained by treatment of the methyl ether with diazomethane in ethyl ether [339, 806, 1169, 1189, 1512, 1635, 1745 (99 %), 2668].

$b.p._{\cdot 0.6}$ 147–152° [1274], $b.p._{1}$ 160–161° [1189];
m.p. 48–49° [1093], 47–48.5° [1189], 46–47° [257, 258, 1169, 1512], 46° [1745];
^{1}H NMR [339, 1512, 1635, 1745, 2668], ^{13}C NMR [1635, 1745, 2668],
IR [339, 1189, 1512, 1635, 1745, 2668], UV [806, 1169],
MS [1512, 1635, 1745, 2668].

Ethyl ester of the methyl ether [15118-67-9] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by reaction of ethyl succinyl chloride with anisole in the presence of aluminium chloride in methylene chloride first at 0°, then at r.t. for 15 h (67 %) [1436].
-Also refer to: [312, 1055, 1209, 1485, 1840, 1954, 1955, 2592, 2644, 2689 (26 %), 2733 (87 %), 3139].

$b.p._{\cdot 0.04}$ 160° [312];
m.p. 57° [3139], 55–57° [2733], 52° [1209], 51–53° [2689], 49–50° [1436], 33–35° [1955];
^{1}H NMR [1055, 1436, 1485, 1840, 1954, 1955], ^{13}C NMR [1485, 1840],
IR [1055, 1436, 1485, 1840, 1954].

Ethyl ether [53623-37-3] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by Friedel-Crafts reaction of succinic anhydride and phenetole (82 %) [2579], (59 %) [2593].
-Also refer to: [1075, 2392 (88 %), 3140].

b.p. 172° [2579];
m.p. 140–142° [1667], 138–139° [1075, 2392, 2593], 137–139° [2579], 137–138° [3140], 136–137° [2794];
MS [1567, 3038].

Methyl ester of the ethyl ether [319494-44-5] $C_{13}H_{16}O_4$ mol. wt. 236.27

m.p. 53° [2593]; ^{1}H NMR [3038], MS [1567, 3038].

Ethyl ester of the ethyl ether $C_{14}H_{18}O_4$ mol. wt. 250.29

m.p. 52° [3140], 51° [2593].

Ethyl ester [66123-43-1] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by treatment of ethyl 4-(4-methoxyphenyl)-4-oxobutanoate,
*with boron tribromide in methylene chloride, first at 0°, then at r.t. for 15 h (62 %) [1436];
*with 48 % HBr in refluxing acetic acid for 20 h (33 %) [878].
-Refer to: [1399, 1482, 2571].

m.p. 111–112° [1436], 111° [2571], 108–110° [878];
^{1}H NMR [1436], IR [1436], MS [1399].

Butyl ether [63471-88-5] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by Friedel-Crafts reaction of succinic anhydride and n-butyl phenyl ether (72 %) [2579].

b.p. 210° [2579]; m.p. 112° [3140], 110–112° [2579].

Phenyl ether [36330-86-6] $C_{16}H_{14}O_4$ mol. wt. 270.28

-Obtained by Friedel-Crafts reaction of succinic anhydride and phenyl ether in the presence of aluminium chloride (94 %) [2579], in carbon disulfide (93 %) [1692].

b.p. 252° [2579];
m.p. 185° [1667], 172° [286, 1115], 119–120° [1396, 1646, 2579], 119° [2818], 118–119° [2308, 2491, 2594], 117–119° [648, 649], 117° [1692];
^{1}H NMR [286, 1115, 1352], ^{13}C NMR [1352].

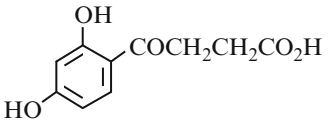
BIOLOGICAL ACTIVITY: Antiinflammatory [649]; Hypolipidemic [1646].

Semicarbazone of the phenyl ether [94960-09-5] $C_{17}H_{17}N_3O_4$ mol. wt. 327.34

m.p. 203° [2308].

4-(2,4-Dihydroxyphenyl)-4-oxo-1-butanoic acid

[13335-54-1] $C_{10}H_{10}O_5$ mol. wt. 210.19



Syntheses

-Obtained by reaction of succinic anhydride with resorcinol in the presence of aluminium chloride [651, 1669].

-Also obtained by treatment of its dimethyl ether with hydrogen bromide in refluxing acetic acid (47 %) [2652].

-Also obtained by reaction of succinonitrile with resorcinol (Hoesch reaction) [1669].

-Also obtained by condensation of resorcinol with succinonitrile (Hoesch reaction) [2187].

-Also refer to: [351, 445, 796, 815, 856, 999, 1790, 2186, 3245, 3485].

m.p. 206–207° [3245], 205° [351, 796], 203° [794, 2652], 201.5–203° [3485], 199–200° [856, 1790, 2186, 2187], 197° [445], 196–200° [999].
^{1}H NMR [999, 3344], IR [999], UV [999].

Na salt $C_{10}H_9O_5Na$, 3 H_2O mol. wt. 263.22

m.p. 199–200° [2187].

Ba, **Ca**, **Pb** and **Ag** salts insoluble in water [794].

4-Nitrophenylhydrazone $C_{16}H_{15}N_3O_6$ mol. wt. 345.31

m.p. 194° [856].

Dibenzoate $C_{24}H_{18}O_7$ mol. wt. 418.40

m.p. 146–147° [2187].

Dimethyl ether [14617-06-2] $C_{12}H_{14}O_5$ mol. wt. 238.24

-Preparation by a Friedel-Crafts reaction with succinic anhydride and resorcinol dimethyl ether [257, 258, 815, (49 %) 2579].

-Preparation by a Friedel-Crafts reaction with succinic anhydride and resorcinol dimethyl ether in the presence of aluminium chloride in nitrobenzene (60 %) [2652].

-Obtained by reaction of succinic anhydride with resorcinol dimethyl ether in the presence of aluminium chloride,

*in tetrachloroethane at 50–60° for 3 h, then at r.t. overnight (79 %) [2100];

*in refluxing carbon disulfide for 3 h [2456].

-Also obtained by treatment of 4-(2,4-dihydroxyphenyl)-4-oxo-1-butanoic acid with dimethyl sulfate [2187].

-Also obtained by refluxing 2,4-dimethoxyphenyl-γ-ketobutyric acid ethyl ester ($C_{14}H_{18}O_5$ mol. wt. 266.29; b.p.$_5$ 198–200°, m.p. 66°) with 10 % caustic potash for 3 h (92 %) [2100].
-Also refer to: [223, 258, 262, 794, 795, 1149, 1246, 1293, 1790, 2100, 2186, 2187, 2409, 2427, 2458, 2579, 2652, 3485].

b.p. 214° [2579];
m.p. 150–151.5° [2579], 150° [2652], 149.5° [3485], 148° [794, 795, 2186, 2187], 147° [1790, 2100], 146–148° [2456, 2458], 146° [257, 258], 124–125° [2187], 106–107° [223].
^{1}H NMR [2427], IR [2427].

Oxime of the dimethyl ether $C_{12}H_{15}NO_5$ mol. wt. 253.25

m.p. 155–156° [2187].

Methyl ester of the dimethyl ether [14563-41-8] $C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained from dimethyl ether in refluxing methanol for 2 h in the presence of 20 % sulfuric acid [2456].

m.p. 58° [2456], 57.5–58.5° [3485], 49° [2595].

Ethyl ester of the dimethyl ether [858445-94-0] $C_{14}H_{18}O_5$ mol. wt. 266.29

-Preparation by reaction of $ClCH_2CH_2CO_2C_2H_5$ with resorcinol dimethyl ether in the presence of aluminium chloride [2456].
-Also refer to: [2499].

b.p.$_5$ 198–200° [2100]; 70° [795], 68.5° [2595], 66° [2100], 44° [2595].

Diethyl ether [39560-29-7] $C_{14}H_{18}O_5$ mol. wt. 266.29

2,4-Diethoxy-γ-oxo-benzenebutanoic acid

-Obtained by condensation of resorcinol diethyl ether with succinic anhydride (65 %) [2579], (40 %) [1451].
-Also refer to: [2196].

b.p. 235° [2579];
m.p. 148.5–150.5° [2579], 146–147° [1451].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

Dipropyl ether $C_{16}H_{22}O_5$ mol. wt. 294.35

-Obtained by condensation of resorcinol dipropyl ether with succinic anhydride [1451].

m.p. 111° [1451].

Dibutyl ether $C_{18}H_{26}O_5$ mol. wt. 322.40

-Obtained by condensation of resorcinol dibutyl ether with succinic anhydride (69 %) [2579], (50 %) [1451].

b.p. 290° [2579];
m.p. 118–119° [2579], 117° [1451].

Di-*iso*-amyl ether $C_{20}H_{30}O_5$ mol. wt. 350.46

-Obtained by condensation of resorcinol di-*iso*-amyl ether with succinic anhydride (85 %) [1451].

m.p. 111° [1451].

Methyl ester [13335-55-2] $C_{11}H_{12}O_5$ mol. wt. 224.21

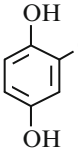
m.p. 138° [794], 130–131° [3485], 130° [3245], 129° [445]; ^{1}H NMR [3344].

Ethyl ester [133535-21-4] $C_{12}H_{14}O_5$ mol. wt. 238.24

b.p.$_3$ 193–195° [3370]; m.p. 100° [794]; IR [3370].

4-(2,5-Dihydroxyphenyl)-4-oxo-1-butanoic acid

[59701-65-4] $C_{10}H_{10}O_5$ mol. wt. 210.19



Syntheses
-Obtained by treatment of its dimethyl ether,
*with hydrogen iodide (81 %) [2331];
*with hydrogen bromide (85 %) [2652];
*with pyridinium chloride for 40 min at 200° (63 %) [1349].

-Also obtained by photo-Fries rearrangement of 1,4-dihydroxyphenyl monosuccinate (55 %) [2004].
-Also refer to: [696 (25–30 %), 747, 997 (55 %), 1878, 1891].

yellow columns [2331]; dark orange crystals [1891];
m.p. 186.5° [747], 183.5–184.5° [997, 2004], 181–182° [1349, 2652], 180–182° [2331],
179–181.5° [1891], 177° [696, 2652], 159–162° [1878],
^{1}H NMR [997, 1878, 1891, 2004], ^{13}C NMR [1878],
IR [997, 1349, 1891, 2004], MS [1878, 1891];
X-ray crystallographic analysis [1891].

Dimethyl ether [1084-74-8] $C_{12}H_{14}O_5$ mol. wt. 238.24

-Preparation by reaction of succinic anhydride with hydroquinone dimethyl ether in the presence of aluminium chloride [257, 258, 622, (96 %) 696, (80 %) 2566, (58 %) 3387],
*in nitrobenzene first at 0°, then was allowed to warm from 5 to 29° over a 3.5 h period [(81 %) 2140, (79 %) 3320];
*in methylene chloride first at 10°, then 3 days at r.t. (67 %) [1454];
*in nitromethane first at 0°, then at 25° for 12 h (81 %) [3343];
*in dichloroethane first from 10 to 57°, then at 57° for 2.5 h (95 %) [304].
-Also obtained by treatment of its methyl ester with boiling dilute alcoholic potassium hydroxide for 2 h (90 %) [2661].
-Also refer to: [99, 157, 258, 459, 747, 768, 795, 990 (6.3 %), 1349, 1503, 1937 (59 %), 1953, 2062, 2331, 2462, 2708, 3289, 3485].

very pale yellow solid [3320];
m.p. 107° [258, 795], 103–105° [2062], 103–104° [157], 103° [747], 102.5–103.5° [1937], 102–104° [3485], 102–103° [2661], 102° [304, 1454], 101–102° [990, 2140, 2331], 101–101.5° [3387], 100–103° [2566], 99–100° [257, 258], 96–97° [768], 94–97° [3289], 86–88° [2708],
^{1}H NMR [768, 1454, 1953, 2566, 2708, 3320, 3387],
IR [1454, 1953, 2566, 2708],
MS [2708, 3387].

Methyl ester of the dimethyl ether [1086-77-7] $C_{13}H_{16}O_5$ mol. wt. 252.27

-Preparation by treatment of 4-(2,5-dihydroxyphenyl)-4-oxo-1-butanoic acid with diazomethane (72 %) [1454].
-Also obtained by treatment of 2,5-dimethoxybenzoylpropionic acid with methanol in the presence of hydrogen chloride in refluxing benzene for 5 h [696].
-Also obtained by reaction of succinic acid monomethyl ester with hydroquinone dimethyl ether in the presence of stannic chloride in benzene for 17 h at r.t. (47.5 %) [2661].
-Also refer to: [1040].

b.p.$_1$ 150° [696], b.p.$_{14}$ 235° [696], b.p.$_{20}$ 223–224° [2661];
m.p. 55° [1454], 54° [795], 52–53° [3485], 49.5–50° [2661], 49–50° [696];
^{1}H NMR [1454], IR [1454], MS [1454].

BIOLOGICAL ACTIVITY: Radioprotector [1040].

LD_{50} [1040].

Ethyl ester of the dimethyl ether $C_{14}H_{18}O_5$ mol. wt. 266.29

-Obtained by treatment of 2,5-dimethoxybenzoylpropionic acid with ethanol in the presence of hydrogen chloride in refluxing benzene for 5 h [696].
-Also refer to: [2499].

pale yellow oil; b.p.$_{13}$ 202° [696]; m.p. 46° [795].

Tert-butyl ester of the dimethyl ether [63171-82-4] $C_{16}H_{22}O_5$ mol. wt. 294.35

-Preparation by reaction of liquid isobutene with 4-(2,5-dihydroxyphenyl)-4-oxo-1-butanoic acid in the presence of sulfuric acid in methylene chloride at r.t. (62 %) [1454].

m.p. 70–72° [1454]; ^{1}H NMR [1454], IR [1454].

Diethyl ether [63213-46-7] $C_{14}H_{18}O_5$ mol. wt. 266.29

2,5-Diethoxy-γ-oxobenzenebutanoic acid

-Obtained by condensation of hydroquinone diethyl ether with succinic anhydride (62 %) [1451], (57 %) [2579].
-Also refer to: [747, 768, 989, 1451].

m.p. 151° [747], 148–150° [2579], 147.4–148.6° [989], 145° [1451];
^{1}H NMR [768].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

Dipropyl ether $C_{16}H_{22}O_5$ mol. wt. 294.35

-Obtained by condensation of hydroquinone dipropyl ether with succinic anhydride (68 %) [1451].

m.p. 95° [1451].

Dibutyl ether $C_{18}H_{26}O_5$ mol. wt. 322.40

-Obtained by condensation of hydroquinone dibutyl ether with succinic anhydride (71 %) [1451].

m.p. 89° [1451].

2-Ethoxy-5-methoxy [107327-72-0] (di-ether mix) $C_{13}H_{16}O_5$ mol. wt. 252.27

needles [747]; m.p. 137.5° [747].

5-Ethoxy-2-methoxy [107327-65-1] (di-ether mix) $C_{13}H_{16}O_5$ mol. wt. 252.27

needles [747]; m.p. 105.5° [747].

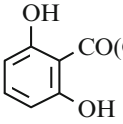
Methyl ester [127275-13-2] $C_{11}H_{12}O_5$ mol. wt. 224.21

-Refer to: [997].

m.p. 129–130° [997]; ^{1}H NMR [997], IR [997].

4-(2,6-Dihydroxyphenyl)-4-oxo-1-butanoic acid

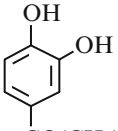
$C_{10}H_{10}O_5$ mol. wt. 210.19



Synthesis
-Refer to: [3141].
m.p. 198–199° [3141].

4-(3,4-Dihydroxyphenyl)-4-oxo-1-butanoic acid
3-protocatechuoylpropanoic acid

[57596-02-8] $C_{10}H_{10}O_5$ mol. wt. 210.19



Syntheses
-Obtained by treatment of 6-(3,4-dimethoxy)-4,5-dihydro-3(2*H*)-pyridazinone with boiling aqueous 48 % HBr (16 %) [1269].
-Also refer to: [1451, 2196, 3057, 3067, 3363, 3364].

m.p. 190–191° [1269], 171–172° [3363], 170–173° [3057], 150–154° [3067], 142° [1451];
^{1}H NMR [1269, 3067], IR [1269, 3067, 3364].

Dimethyl ether [5333-34-6] $C_{12}H_{14}O_5$ mol. wt. 238.24

3,4-Dimethoxy-γ-oxobenzenebutanoic acid

-Preparation by reaction of succinic anhydride with veratrole in the presence of aluminium chloride, [257, 258, (60 %) 2579],
*in nitrobenzene,
-first at 0–10° for 24 h, then at 45° for 1 h (93 %) [1246];
-for 24 h at r.t. (85 %) [1280];
-at 60° for 3 h (81.4 %) [1745].
*in methylene chloride first at 0°, then at reflux for 4–8 h (53 %) [3190].
*in tetrachloroethane and nitrobenzene mixture at 0° for 3 days (67 %) [987].
-Also refer to: [537, 1269, 1451, 2071 (78.6 %), 2196].

colourless solid [2071];
b.p. 206° [2579];
m.p. 165° [1246], 163–164° [2579], 162–163° [1745], 161.6–162° [2071], 160–161° [257, 258, 1246, 1280], 159–161° [3190], 157–159° [987].
^{1}H NMR [1745, 2071, 3190], ^{13}C NMR [1745, 2071], IR [1745, 2071], MS [2071].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

Methyl ester of the dimethyl ether [14563-40-7] $C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained by treatment of the methyl ether with diazomethane in ethyl ether (99 %) [1745].
-Preparation by reaction of 3-carbomethoxypropanoic acid with veratrole in the presence of PPA at 45–50° for 1 h, then at r.t. overnight (65.5 %) [2915].
-Preparation by reaction of 3-carbomethoxypropanoyl chloride with veratrole in the presence of PPA at 40° for 2.5 h (79.6 %) [2915].
-Also refer to: [432, 722, 795, 984, 1246, 1247, 1635, 1667, 3485].

m.p. 95° [795], 94–95° [2915], 92° [984], 90.5–91° [3485],
90–91° [432], 89° [1246, 1247], 87° [1635, 1745];
^{1}H NMR [984, 1635, 1745, 2915],
^{13}C NMR [1635, 1745], IR [984, 1635, 1745, 2915],
MS [1635, 1745].

Ethyl ester of the dimethyl ether [56872-60-7] $C_{14}H_{18}O_5$ mol. wt. 266.29

-Ethyl succinyl chloride was added to a suspension of aluminium chloride in methylene chloride at 0°, and the mixture was stirred at 0° for 15 min. To this was added veratrole at 0°. The reaction mixture was stirred at r.t. for 15 h (81 %) [1436].
-Also refer to: [28, 795, 1286, 2499, 2879].

colourless oil [1436];
m.p. 70° [795], 62° [28], 57–58° [1286];
^{1}H NMR [1436], IR [1436].

Diethyl ether [63213-42-3] $C_{14}H_{18}O_5$ mol. wt. 266.29

3,4-Diethoxy-γ-oxobenzenebutanoic acid

-Obtained by condensation of pyrocatechol diethyl ether with succinic anhydride (80 %) [1451].
-Also refer to: [807, 2196].

m.p. 113° [1451], 108–109° [807];
^{1}H NMR [807], IR [807], UV [807].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

Dipropyl ether [568553-00-4] $C_{16}H_{22}O_5$ mol. wt. 294.35

-Obtained by condensation of pyrocatechol dipropyl ether with succinic anhydride (62 %) [1451].

m.p. 115° [1451].

Dibutyl ether [856809-73-9] $C_{18}H_{26}O_5$ mol. wt. 322.40

-Obtained by condensation of pyrocatechol dibutyl ether with succinic anhydride (78 %) [1451].

m.p. 107° [1451].

Diamyl ether [859059-36-2] $C_{20}H_{30}O_5$ mol. wt. 350.46

-Obtained by condensation of pyrocatechol diamyl ether with succinic anhydride (53 %) [1451].

m.p. 88° [1451].

Dihexyl ether [856807-53-9] $C_{22}H_{34}O_5$ mol. wt. 378.51

-Obtained by condensation of pyrocatechol dihexyl ether with succinic anhydride (57 %) [1451].

m.p. 94–95° [1451].

Methylenedioxy ether [41764-07-2] $C_{11}H_{10}O_5$ mol. wt. 222.20

-Obtained by refluxing for 2.5 h a mixture of methyl piperonylate, acetone and sodium hydride in tetrahydrofuran (36 %) [1258].
-Also refer to: [2156].

m.p. 91–92° [2156], 89.5–91° [1258].

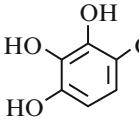
Ethyl ester [56872-61-8] $C_{12}H_{14}O_5$ mol. wt. 238.24

-Obtained by treatment of ethyl 4-(3,4-dimethoxyphenyl)-4-oxobutanoate with boron tribromide in methylene chloride, first at 0°, then at r.t. for 15 h (45 %) [1436].
-Refer to: [1399, 1482, 2571, 2913].

colourless crystals [1436];
m.p. 118–119° [1436], 116–117° [2913], 111° [2571];
^{1}H NMR [1436], IR [1436], MS [1399].

4-(2,3,4-Trihydroxyphenyl)-4-oxo-1-butanoic acid

[74882-04-5] $C_{10}H_{10}O_6$ mol. wt. 226.19



Syntheses
-Obtained *via* initial Friedel-Crafts reaction of 1,2,3-trimethoxybenzene and monomethyl succinate in the presence of 70 % PPA; followed by alkaline hydrolysis of the product ester (95 %) [1671].
-The free acid is generated *in situ* during the strongly acidic conditions of the Clemmensen reduction, but no isolated [231].

Ethyl ester $C_{12}H_{14}O_6$ mol. wt. 254.24

-Obtained by reaction of succinic anhydride with pyrogallol in the presence of boron trifluoride etherate in dioxan, first at −30°, then at r.t. for 24 h (20 %) [231].

^{1}H NMR [58, 231], ^{13}C NMR [231].

Trimethyl ether [63213-41-2] $C_{13}H_{16}O_6$ mol. wt. 268.27

2,3,4-Trimethoxy-γ-oxobenzenebutanoic acid

-Obtained by reaction of pyrogallol trimethyl ether with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h [2196].
-Also obtained by reaction of succinic anhydride with pyrogallol trimethyl ether [2196].
-Also obtained by hydrolysis of its ethyl ester ($C_{15}H_{20}O_6$; m.p. 57°) with aqueous alkali [1981] or in refluxing 8 % alcoholic alkali for 3 h (35 %) [2440].
-Also obtained by basic hydrolysis of its methyl ester [535, 1093].
-Also refer to: [1671, 2463, 2487].

long needles [1981];
m.p. 89–90° [1093], 89° [1981], 88–89° [2440];
^{1}H NMR [2440, 2487], IR [2440], MS [2440].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

Methyl ester of the trimethyl ether [51686-50-1] $C_{14}H_{18}O_6$ mol. wt. 282.29

-Obtained by Friedel-Crafts reaction of succinic acid monomethyl ester with pyrogallol trimethyl ether [535].
-Also obtained by reaction between 1,2,3-trimethoxybenzene and 3-carbomethoxypropanoic acid in the presence of PPA for 2.5 h at 45° (86 %) [2915], (78.8 %) [1093].
-Also refer to: [1302, 2487].

m.p. 48–49° [1093, 2915], 41–42° [1302];
^{1}H NMR [2487, 2915], IR [2915].

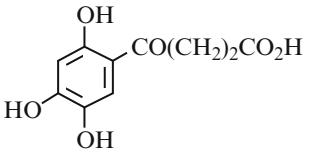
Ethyl ester of the trimethyl ether [102222-55-9] $C_{15}H_{20}O_6$ mol. wt. 296.32

-Obtained by reaction of ethyl succinoyl chloride with 1,2,3-trimethoxybenzene in the presence of stannic chloride in methylene chloride at 0° for 5 h (62 %) [2440].
-Also refer to: [1981].

m.p. 57° [1981, 2440];
^{1}H NMR [2440], IR [2440], MS [2440].

4-(2,4,5-Trihydroxyphenyl)-4-oxo-1-butanoic acid

[63213-28-5] $C_{10}H_{10}O_6$ mol. wt. 226.19



Synthesis
-Obtained by treatment of trimethyl ether with 57 % aqueous hydriodic acid at 130–140° for 3 h (36 %) [2196].
m.p. 234–235° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

Trimethyl ether [31914-19-9] $C_{13}H_{16}O_6$ mol. wt. 268.27

2,4,5-Trimethoxy-γ-oxobenzenebutanoic acid

-Obtained by reaction of 1,2,4-benzenetriol trimethyl ether with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h [2196].
-Also obtained by reaction of succinic anhydride with 1,2,4-benzenetriol trimethyl ether in the presence of aluminium chloride [257, 258, 2196].
-Also refer to: [99, 472, 1578, 2018, 2794, 3084].

m.p. 171.5–172° [472], 170–171° [2794],
168–169° [257, 258, 3084];
^{1}H NMR [3084], IR [3084].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

Methyl ester of the trimethyl ether [82961-09-9] $C_{14}H_{18}O_6$ mol. wt. 282.29

-Obtained by bubbling hydrogen chloride in 1-(2,4,5-trimethoxyphenyl)-4-oxo-1-butanoic acid in methanol for 1.5 h [258].

m.p. 110–111° [258].

Triethyl ether [41826-92-0] $C_{16}H_{22}O_6$ mol. wt. 310.35

2,4,5-Triethoxy-γ-oxobenzenebutanoic acid

-Obtained by heating a mixture of 1,2,4-benzenetriol triethyl ether and succinic acid monomethyl ester in the presence of PPA at 50–55° for 40 min. Ice-water was added to the mixture, the resulting aqueous mixture was diluted with acetic acid and heated at 80–90° for 50 min (45 %) [2196].
-Preparation from 1,2,4-triethoxybenzene by reaction with succinic anhydride or succinic acid chloride ethyl ester [2195].

m.p. 150–151° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

Ethyl ester of the triethyl ether [63213-26-3] $C_{18}H_{26}O_6$ mol. wt. 338.40

2,4,5-Triethoxy-γ-oxobenzenebutanoic acid ethyl ester

-The 3-(2,4,5-triethoxybenzoyl)propionic acid was esterified with a hot ethanol-sulfuric acid mixture (quantitative yield) [2196].
-Also refer to: [2192].

m.p. 97–98° [2192], 75° [2196].
N.B.: One of the reported melting point is obviously wrong.

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

Tripropyl ether [63213-39-8] $C_{19}H_{28}O_6$ mol. wt. 352.43

2,4,5-Tripropoxy-γ-oxo-benzenebutanoic acid

-Obtained by reaction of phloroglucinol tripropyl ether with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h [2196].

m.p. 109–111° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

Tributyl ether [41827-09-2] $C_{22}H_{34}O_6$ mol. wt. 394.51

2,4,5-Tributoxy-γ-oxobenzenebutanoic acid

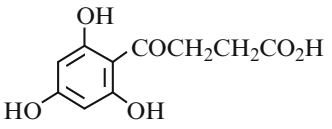
-Obtained by reaction of phloroglucinol tributyl ether with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h [2196].

m.p. 117–118° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

4-(2,4,6-Trihydroxyphenyl)-4-oxo-1-butanoic acid

[4890-45-3] $C_{10}H_{10}O_6$ mol. wt. 226.19



Syntheses
-Refer to: [1669, 2196, 2354, 2355].
m.p. 238° [2354, 2355], 219–220° [1669].

Trimethyl ether [63213-25-2] $C_{13}H_{16}O_6$ mol. wt. 268.27

2,4,6-Trimethoxy-γ-oxobenzenebutanoic acid

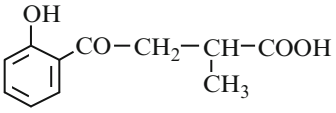
-Obtained by reaction of phloroglucinol trimethyl ether with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h (72 %) [2196].
-Also obtained from succinic anhydride and phloroglucinol trimethyl ether [2196].

m.p. 142–143° [2196].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

4-(2-Hydroxyphenyl)-2-methyl-4-oxo-1-butanoic acid

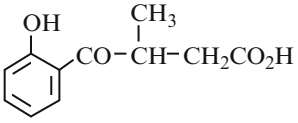
[99865-80-2] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Refer to: [223, 2098].
m.p. 161° [2098], 158.5–159.5° [223].

4-(2-Hydroxyphenyl)-3-methyl-4-oxo-1-butanoic acid

[59010-62-7] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Refer to: [687, 1032, 2913].
m.p. 95–97° [687, 2913].

Methyl ether [133101-50-5] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Preparation: A solution of KHMDS in toluene was diluted in THF and cooled to −78°. To this mixture was added dropwise a solution of 1-(2-methoxyphenyl)-1-propanone in THF and the solution was stirred at −78° for 1 h. Then a solution of methyl bromoacetate in THF was added dropwise, and the solution was stirred at −78° for 1 h. The mixture was quenched in 1 N HCl (80 %) [1032].
-Also refer to: [223].

m.p. 68–70° [1032], 55–57° [223];
^{1}H NMR [1032], IR [1032].

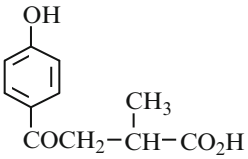
Methoxymethyl ether [133101-52-7] $C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained from 1-(2-methoxymethoxyphenyl)-1-propanone (to see above) (66 %) [1032].

oil [1032]; ^{1}H NMR [1032], IR [1032].

4-(4-Hydroxyphenyl)-2-methyl-4-oxo-1-butanoic acid

$C_{11}H_{12}O_4$ mol. wt. 208.21



Synthesis
-Refer to: [2733].
Methyl ether [5717-16-8]
$C_{12}H_{14}O_4$ mol. wt. 222.24

-Refer to: [223, 262, 1074, 1170, 2039, 2098, 2427, 2537, 2733 (77 %), 2844, 2845].

m.p. 145–146° [2537], 144° [2098], 143–144° [223, 1170, 2733], 141° [2039];
^{1}H NMR [1074, 2427, 2844, 2845],
^{13}C NMR [1074, 2844, 2845], IR [2427, 2844, 2845].

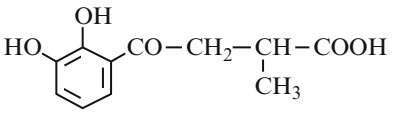
Ethyl ester of the methyl ether [15118-68-0] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Refer to: [1055, 2039, 2098, 2733 (96 %)].

b.p.$_{0.1}$ 110–112° [2733], b.p.$_5$ 185–187° [2098], b.p.$_{30}$ 190° [2039];
^{1}H NMR [1055];
$n_D^{35.7} = 1.5170$ [2039].

4-(2,3-Dihydroxyphenyl)-2-methyl-4-oxo-1-butanoic acid
(Plumbagic acid)

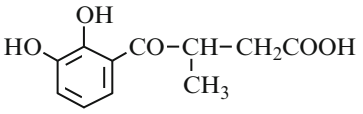
$C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis
-Refer to: [141].
m.p. 109° [141]; ^{1}H NMR [141], ^{13}C NMR [141], IR [141], MS [141], UV [141].

4-(2,3-Dihydroxyphenyl)-3-methyl-4-oxo-1-butanoic acid
(Plumbagic acid)

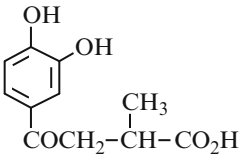
$C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis
-Refer to: [880].
m.p. 112° [880]; ^{1}H NMR [880], ^{13}C NMR [880], IR [880], MS [880], UV [880]; CD [880].

4-(3,4-Dihydroxyphenyl)-2-methyl-4-oxo-1-butanoic acid

$C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis
-Refer to: [3190].

Dimethyl ether

$C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained by reaction of 3,4-dimethoxyphenyl-magnesium bromide with 2-methylsuccinic anhydride in THF first 30 min at 0°, then at r.t. overnight (31 %) [3190].

N.B.: One obtained an inseparable mixture of the regioisomers 2-methyl and 3-methyl (ratio 4:6).
-Also obtained by reaction of methylsuccinic anhydride with veratrole in the presence of aluminium chloride in nitrobenzene at r.t. for 50 h [2632].
-Also refer to: [431, 2427].

m.p. 107–108° [431, 2632], 94–95° [3190];
^{1}H NMR [2427, 3190], IR [2427].

Methyl ester of the dimethyl ether $C_{14}H_{18}O_6$ mol. wt. 282.29

-Refer to: [431, 2632].

m.p. 74–75° [431, 2632].

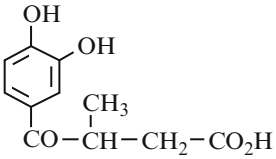
2,4-Dinitrophenylhydrazone of the dimethyl ether and methyl ester $C_{20}H_{22}N_4O_8$ mol. wt. 446.41

-Refer to: [431, 2632].

m.p. 155–156° [431, 2632].

4-(3,4-Dihydroxyphenyl)-3-methyl-4-oxo-1-butanoic acid

$C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis
-Refer to: [3190].

Dimethyl ether [358369-06-9]

$C_{13}H_{16}O_5$ mol. wt. 252.27

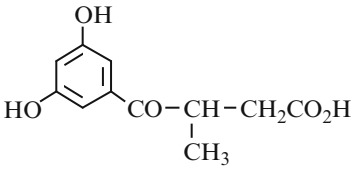
-Obtained by adding TFA to a solution of malonic acid di(tert-butyl) ester in methylene chloride. The reaction mixture was stirred at r.t. for 1.5 h and then refluxed for 3 h. After removal of the solvent in vacuo, acetic acid was added to the residue and the mixture was refluxed for 3 h (69 %) [3190].
-Also refer to: [265, 266, 431, 1282, 2632].

m.p. 129° [1282], 118–123° [3190];
^{1}H NMR [3190].

Methyl ester of the dimethyl ether $C_{14}H_{18}O_5$ mol. wt. 266.29

m.p. 74–75° [431, 2632].

4-(3,5-Dihydroxyphenyl)-3-methyl-4-oxo-1-butanoic acid $C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis
-Refer to: [1030].
Dimethyl ether [17103-73-0]
$C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained from α-bromo-3,5-dimethoxypropiophenone (40–45 %) [1030].

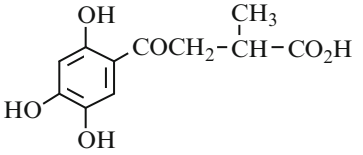
m.p. 105.5–106.5° [1030].

Semicarbazone of the dimethyl ether [101117-26-4] $C_{14}H_{19}N_3O_5$ mol. wt. 309.32

m.p. 160–161° [1030].

4-(2,4,5-Trihydroxyphenyl)-2-methyl-4-oxo-1-butanoic acid

$C_{11}H_{12}O_6$ mol. wt. 240.21



Synthesis
-Refer to: [2196].
Trimethyl ether [1702-68-7]
$C_{14}H_{18}O_6$ mol. wt. 282.29

-Obtained by reaction of methylsuccinic anhydride with 1,2,4-trimethoxybenzene in the presence of aluminium chloride,
*in sym-tetrachloroethane at 10° for 2 days (30 %) [975];
*in carbon disulfide for 15 h at r.t. (27 %) [3303].
-Also refer to: [145].

m.p. 164–165° [145], 161° [975], 160–161° [3303];
UV [145].

Methyl ester of the trimethyl ether [1702-69-8] $C_{15}H_{20}O_6$ mol. wt. 296.32

-Obtained by treatment of above trimethyl ether with diazomethane in ethyl ether [3303].

m.p. 92–93° [3303].

Triethyl ether [63213-32-1] $C_{17}H_{24}O_6$ mol. wt. 324.37

2,4,5-Triethoxy-α-methyl-γ-oxo-benzene-butanoic acid

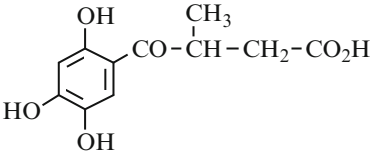
-Preparation by reaction of 1,2,4-triethoxybenzene with 2-methylsuccinic anhydride in the presence of aluminium chloride in carbon tetrachloride at 70° for 2 h (40 %) [779, 2196].

m.p. 138–139° [2196]; ^{1}H NMR [2196].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

4-(2,4,5-Trihydroxyphenyl)-3-methyl-4-oxo-1-butanoic acid

$C_{11}H_{12}O_6$ mol. wt. 240.21



Synthesis
-Refer to: [3303].

Trimethyl ether [1702-70-1]
$C_{14}H_{18}O_6$ mol. wt. 282.29

-Obtained by reaction of methylsuccinic anhydride with 1,2,4-trimethoxybenzene in the presence of aluminium chloride in sym-tetrachloroethane,
*at 40° for 8 h (20 %) [3303];
*at 10° for 2 days (10 %) [975].

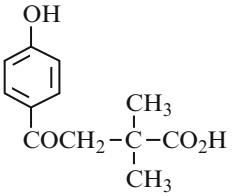
m.p. 130–131.5° [145], 128–129° [1250], 125–126° [975], 123–125° [3303]; UV [145].

Methyl ester of the trimethyl ether [2010-80-2] $C_{15}H_{20}O_6$ mol. wt. 296.32

m.p. 90–92° [1250].

4-(4-Hydroxyphenyl)-2,2-dimethyl-4-oxo-1-butanoic acid

$C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Refer to: [2358].

Methyl ether [15118-48-6]
$C_{13}H_{16}O_4$ mol. wt. 236.27
-Obtained by reaction of dimethylsuccinic anhydride with anisole in the presence of aluminium chloride [2359].

-Also refer to: [2358, 2733 (51 %)].

m.p. 162–164° [2358, 2359, 2733]; pK [2358];
^{1}H NMR [2733], IR [2733].

BIOLOGICAL ACTIVITY: Anorexigen [2358].

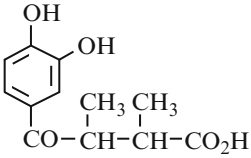
Methyl ester of the methyl ether [15118-69-1] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Refer to: [2733 (70 %)].

m.p. 60–61° [2733].

4-(3,4-Dihydroxyphenyl)-2,3-dimethyl-4-oxo-1-butanoic acid

$C_{12}H_{14}O_5$ mol. wt. 238.24



Synthesis

-Refer to: [1280].

Dimethyl ether [358369-08-1]

$C_{14}H_{18}O_5$ mol. wt. 266.29

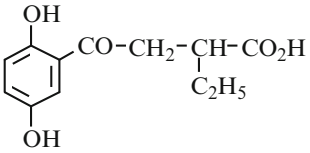
-Obtained by reaction of *cis* or *trans* α,β-dimethylsuccinic anhydride with veratrole in the presence of aluminium chloride in nitrobenzene at r.t. for 24 h (38 %) [1280].

-Also obtained by reaction of 3,4-dimethoxyphenylmagnesium bromide with 2,3-dimethylsuccinic anhydride (D,L and meso) in THF first 30 min at 0°, then at r.t. overnight (45 %) [3190].

m.p. 165–166° [1280], 163–166° [3190]; ^{1}H NMR [3190].

2-Ethyl-4-(2,5-dihydroxyphenyl)-4-oxo-1-butanoic acid

$C_{12}H_{14}O_5$ mol. wt. 238.24



Synthesis

-Refer to: [472].

Dimethyl ether [132330-85-9]

$C_{14}H_{18}O_5$ mol. wt. 266.29

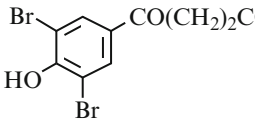
-Obtained by reaction of ethylsuccinic anhydride with hydroquinone dimethyl ether in the presence of aluminium chloride in nitropropane first at 0–5°, then 18 h at 3–8° (85 %) [472].

m.p. 121° [472].

15.2 Substituted Hydroxyketones

4-(3,5-Dibromo-4-hydroxyphenyl)-4-oxo-1-butanoic acid

[392304-69-7] $C_{10}H_8Br_2O_4$ mol. wt. 351.98



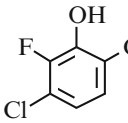
Synthesis

-Refer to: [1446].

^{1}H NMR [1446].

4-(4-Chloro-3-fluoro-2-hydroxyphenyl)-4-oxo-1-butanoic acid

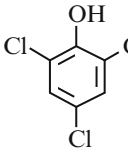
[1208265-79-5] $C_{10}H_8ClFO_4$ mol. wt. 246.62



Synthesis
-Refer to: [1008].
^{1}H NMR [1008].

4-(3,5-Dichloro-2-hydroxyphenyl)-4-oxo-1-butanoic acid

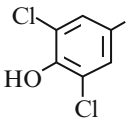
[62903-22-4] $C_{10}H_8Cl_2O_4$ mol. wt. 263.08



Syntheses
-Refer to: [2703, 2705].
m.p. 166–167° [2703, 2705].

4-(3,5-Dichloro-4-hydroxyphenyl)-4-oxo-1-butanoic acid

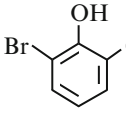
[62903-25-7] $C_{10}H_8Cl_2O_4$ mol. wt. 263.08



Syntheses
-Refer to: [1532, 2703, 2705].
m.p. 180–183° [1532, 2703, 2705].

4-(3-Bromo-2-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{10}H_9BrO_4$ mol. wt. 273.08



Synthesis
-Refer to: [2579].

Methyl ether

$C_{11}H_{11}BrO_4$ mol. wt. 287.14

-Obtained by Friedel-Crafts reaction of succinic anhydride with o-bromoanisole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4), first at 0–5° for 1–2 h, then at r.t. for 3 days (59 %) [2579].

b.p. 218° [2579]; m.p. 189.5–191.5° [2579].

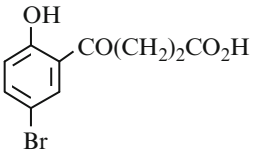
Ethyl ether $C_{12}H_{13}BrO_4$ mol. wt. 301.14

-Obtained by Friedel-Crafts reaction of succinic anhydride with o-bromophenetole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4), first at 0–5° for 1–2 h, then at r.t. for 3 days (86 %) [2579].

b.p. 224° [2579]; m.p. 201–202° [2579].

4-(5-Bromo-2-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{10}H_9BrO_4$ mol. wt. 273.08



Synthesis
-Refer to: [2579].

Phenyl ether

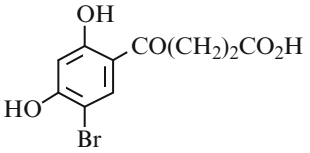
$C_{16}H_{13}BrO_4$ mol. wt. 349.18

-Obtained by Friedel-Crafts reaction of succinic anhydride with p-bromophenyl phenyl ether in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4), first at 0–5° for 1–2 h, then at r.t. for 3 days (82 %) [2579].
-Also refer to: [1958].

b.p. 305° [2579]; m.p. 161.5–162.5° [2579].

4-(5-Bromo-2,4-dihydroxyphenyl)-4-oxo-1-butanoic acid

[854676-84-9] $C_{10}H_9BrO_5$ mol. wt. 289.08



Syntheses
-Refer to: [853, 2196].
m.p. 190° [853].

Dimethyl ether [63213-40-1]

$C_{12}H_{13}BrO_5$ mol. wt. 317.14

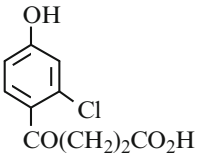
-Obtained by reaction of 4-bromoresorcinol dimethyl ether with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h [2196].

m.p. 188–189° [2196], 179° [853], 178° [795].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

4-(2-Chloro-4-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{10}H_9ClO_4$ mol. wt. 228.63



Synthesis
-Obtained by Fries rearrangement of 3-chlorophenyl hydrogen succinate with aluminium chloride in tetrachloroethane or in toluene at 117° for 2.5 h [224].

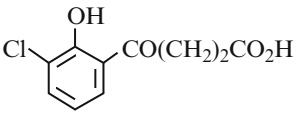
Methyl ether [15572-03-9] $C_{11}H_{11}ClO_4$ mol. wt. 242.66

-Obtained by Friedel-Crafts reaction of succinic anhydride with m-chloroanisole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4), first at 0–5° for 1–2 h, then at r.t. for 3 days [224].
-Also refer to: [861].

m.p. 145° [861], 100–102° [224]; IR [224].

4-(3-Chloro-2-hydroxyphenyl)-4-oxo-1-butanoic acid

[15572-06-2] $C_{10}H_9ClO_4$ mol. wt. 228.63



Syntheses
-Obtained by Fries rearrangement of 2-chlorophenyl hydrogen succinate with aluminium chloride in tetrachloroethane or in toluene at 117° for 2.5 h [224].

-Also obtained by Friedel-Crafts reaction of succinic anhydride with o-chlorophenol in the presence of aluminium chloride in tetrachloroethane, first at r.t. overnight, then the mixture was heated on a water bath for 4–5 h (20 %) [224].

m.p. 147–149° [224]; IR [224].

Methyl ether $C_{11}H_{11}ClO_4$ mol. wt. 242.66

-Obtained by treatment of the title ketone with diazomethane in ethyl ether [224].

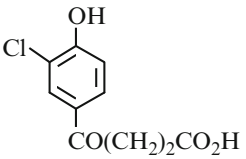
Ethyl ether $C_{12}H_{13}ClO_4$ mol. wt. 256.69

-Obtained by Friedel-Crafts reaction of succinic anhydride with o-chlorophenetole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4), first at 0–5° for 1–2 h, then at r.t. for 3 days [224], (79 %) [2579].

b.p. 208° [2579]; m.p. 190–191.5° [2579], 184° [1333].

4-(3-Chloro-4-hydroxyphenyl)-4-oxo-1-butanoic acid

[56872-21-0] $C_{10}H_9ClO_4$ mol. wt. 228.63



Syntheses
-Obtained by Fries rearrangement of 2-chlorophenyl hydrogen succinate with aluminium chloride in tetrachloroethane or in toluene at 117° for 2.5 h [224].
-Also refer to: [688, 1667, 1779, 2912, 2913, 3099].

m.p. 170° [1667], 160–162° [688, 2912, 2913], 159° [3099].

Methyl ether [39496-87-2] $C_{11}H_{11}ClO_4$ mol. wt. 242.66

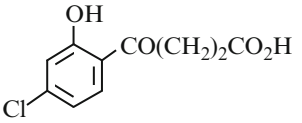
-Obtained by Friedel-Crafts reaction of succinic anhydride with o-chloroanisole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4), first at 0–5° for 1–2 h, then at r.t. for 3 days [224].
-Also refer to: [216, 1779, 2703, 2705].

m.p. 192–198° [2703, 2705], 189° [1333], 188–189° [224], 187–189° [208, 216], 186–188° [1779];
IR [224].

BIOLOGICAL ACTIVITY: Inhibition of aggregation of thrombocytes [1779]; Antiinflammatory efficacy [1779].

4-(4-Chloro-2-hydroxyphenyl)-4-oxo-1-butanoic acid

[15572-01-7] $C_{10}H_9ClO_4$ mol. wt. 228.63



Syntheses
-Obtained by Fries rearrangement of 3-chlorophenyl hydrogen succinate with aluminium chloride in tetrachloroethane or in toluene at 117° for 2.5 h [224].

-Also refer to: [2705].

m.p. 180–181° [2705], 176–178° [224]; IR [224].

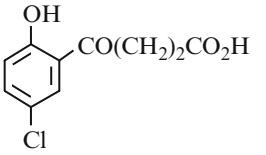
Methyl ether [15572-02-8] $C_{11}H_{11}ClO_4$ mol. wt. 242.66

-Obtained by Friedel-Crafts reaction of succinic anhydride with m-chloroanisole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4), first at 0–5° for 1–2 h, then at r.t. for 3 days [224].

m.p. 163–164° [224]; IR [224].

4-(5-Chloro-2-hydroxyphenyl)-4-oxo-1-butanoic acid

[62903-23-5] $C_{10}H_9ClO_4$ mol. wt. 228.63



Syntheses
-Obtained by Fries rearrangement of 4-chlorophenyl hydrogen succinate with aluminium chloride in tetrachloroethane or in toluene at 117° for 2.5 h [224].
-Also refer to: [676, 797, 997 (20 %), 2703, 2705, 3289].

m.p. 181–182° [2703, 2705], 180–181° [224], 178–182° [3289], 178–180° [997], 178° [797], 173–174° [676];
^{1}H NMR [676, 997], IR [224, 676, 997].

Methyl ether [63213-94-5] $C_{11}H_{11}ClO_4$ mol. wt. 242.66

-Obtained by Friedel-Crafts reaction of succinic anhydride with p-chloroanisole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4), first at 0–5° for 1–2 h, then at r.t. for 3 days [224], (25 %) [2579].
-Also refer to: [447, 797, 1403, 3289].

b.p. 200° [2579];
m.p. 120° [797], 119–121° [224, 2579], 118–119° [1403], 113–115° [3289];
IR [224].

Methyl ester of the methyl ether [15572-05-1] $C_{12}H_{13}ClO_4$ mol. wt. 256.69

-Obtained by treatment of 4-(5-chloro-2-hydroxyphenyl)-4-oxo-1-butanoic acid with dimethyl sulfate in the presence of potassium carbonate in acetone [224].

m.p. 66–67° [224]; IR [224].

Ethyl ether [105475-33-0] $C_{12}H_{13}ClO_4$ mol. wt. 256.69

-Obtained by Friedel-Crafts reaction of succinic anhydride with p-chlorophenetole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4), first at 0–5° for 1–2 h, then at r.t. for 3 days [224], (20 %) [2579].
-Also refer to: [797].

b.p. 212° [2579]; m.p. 157° [797], 156–158° [2579].

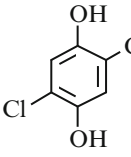
Methyl ester [99854-21-4] $C_{11}H_{11}ClO_4$ mol. wt. 242.66

-Refer to: [797, 997].

m.p. 50° [797], 44–49° [997]; ^{1}H NMR [997], IR [997].

4-(4-Chloro-2,5-dihydroxyphenyl)-4-oxo-1-butanoic acid

$C_{10}H_9ClO_5$ mol. wt. 244.63



Synthesis
-Refer to: [2196].

Dimethyl ether [41827-05-8]
$C_{12}H_{13}ClO_5$ mol. wt. 272.68
4-Chloro-2,5-dimethoxy-γ-oxobenzenebutanoic acid

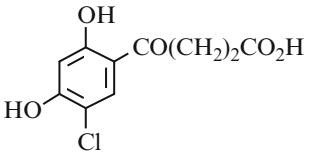
-Obtained by reaction of 2-chlorohydroquinone dimethyl ether with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h [2196].

m.p. 186–188° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

4-(5-Chloro-2,4-dihydroxyphenyl)-4-oxo-1-butanoic acid

$C_{10}H_9ClO_5$ mol. wt. 244.63



Synthesis
-Refer to: [2196].

Dimethyl ether [41826-97-5]
$C_{12}H_{13}ClO_5$ mol. wt. 272.68
5-Chloro-2,4-dimethoxy-γ-oxobenzenebutanoic acid

-Obtained by heating a mixture of 4-chlororesorcinol dimethyl ether and succinic acid monomethyl ester in the presence of PPA at 50–55° for 40 min. Ice-water was added to the mixture, the resulting aqueous mixture was diluted with acetic acid and heated at 80–90° for 50 min [2196].

m.p. 185–187° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

Diethyl ether [41827-02-5] $C_{14}H_{17}ClO_5$ mol. wt. 300.74

5-Chloro-2,4-diethoxy-γ-oxobenzenebutanoic acid.

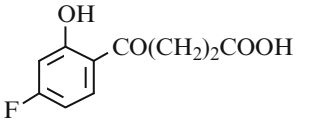
-Obtained by reaction of 4-chlororesorcinol diethyl ether with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h [2196].

m.p. 172–173° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

4-(4-Fluoro-2-hydroxyphenyl)-4-oxo-1-butanoic acid

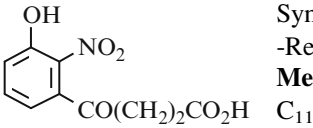
[202715-97-7] $C_{10}H_9FO_4$ mol. wt. 212.18



Synthesis
-Refer to: [1901].
m.p. 134° [1901]; ^{1}H NMR [1008], IR [1901].

4-(3-Hydroxy-2-nitrophenyl)-4-oxo-1-butanoic acid

$C_{10}H_9NO_6$ mol. wt. 239.18



Synthesis
-Refer to: [3369].

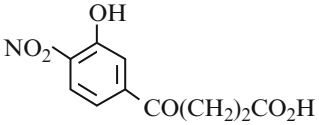
Methyl ether [103646-41-9]
$C_{11}H_{11}NO_6$ mol. wt. 253.21

-Refer to: [631, 1744, 2687, 3369].

m.p. 148.5–149° [1744, 2687],
139–139.5° (Unstable modification) [1744, 2687], 139° [631];
^{1}H NMR [631], ^{13}C NMR [631], IR [631, 3369].

4-(3-Hydroxy-4-nitrophenyl)-4-oxo-1-butanoic acid

[62893-18-9] $C_{10}H_9NO_6$ mol. wt. 239.18



Syntheses
-Refer to: [1554, 2913].
m.p. 158–160.5° [1554, 2913].

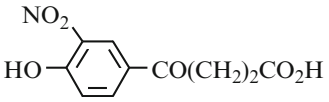
Methyl ether [93534-71-5] $C_{11}H_{11}NO_6$ mol. wt. 253.21

-Refer to: [1554 (33 %)].

m.p. 137–138.5° [1554].

4-(4-Hydroxy-3-nitrophenyl)-4-oxo-1-butanoic acid

[56872-41-4] $C_{10}H_9NO_6$ mol. wt. 239.18



Syntheses
-Refer to: [2494, 2912, 2913].
m.p. 172–174° [2912, 2913].

Methyl ether [26976-83-0] $C_{11}H_{11}NO_6$ mol. wt. 253.21

-Preparation by nitration of β-anisoylpropionic acid [2494].
-Also refer to: [953, 954, 2491].

pale yellow prisms [2494];
m.p. 158–159° [953, 954, 2491], 148° [652];
IR [652].

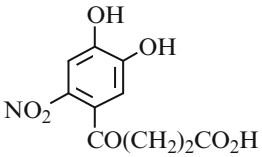
Ethyl ether [74362-69-9] $C_{12}H_{13}NO_6$ mol. wt. 267.24

-Refer to: [2494].

colourless needles; m.p. 153° [2494].

4-(4,5-Dihydroxy-2-nitrophenyl)-4-oxo-1-butanoic acid

$C_{10}H_9NO_7$ mol. wt. 255.18



Synthesis
-Refer to: [1246].

Dimethyl ether [87364-84-9]
$C_{12}H_{13}NO_7$ mol. wt. 283.24

-Obtained by adding nitric acid (d = 1.42) and sulfuric acid (d = 1.84) to a cold solution of β-3,4-dimethoxybenzoylpropionic acid in acetic acid [1246].
-Also obtained by treatment of β-veratroylpropionic acid with a mixture of nitric acid (d = 1.42) and acetic acid at 0° for 2 h (82 %) [2073].
-Also refer to: [596, 984, 2760].

m.p. 212° [1246, 2073], 210–212° [2760], 115° [596];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [984], IR [984], MS [984].

Methyl ester of the dimethyl ether $C_{13}H_{15}NO_7$ mol. wt. 297.26

-Refer to: [1246].

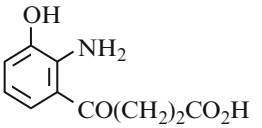
greenish-yellow needles [1246];
m.p. 118° [1246].

Ethyl ester of the dimethyl ether [87374-67-2] $C_{14}H_{17}NO_7$ mol. wt. 311.29

m.p. 84–85° [984];
^{1}H NMR [984], IR [984], MS [984].

4-(2-Amino-3-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{10}H_{11}NO_4$ mol. wt. 209.20

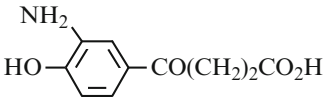


Synthesis
-Obtained by hydrogenation of 4-(3-hydroxy-2-nitrophenyl)-4-oxo-2-butenoic acid in solution in ethyl acetate/acetic acid with hydrogen gas at r.t. in the dark for 3 h (47 %) [2109].

m.p. 134–135° [2109];
^{1}H NMR [2109], ^{13}C NMR [2109], IR [2109], UV [2109], MS [2109]; Fluorescence spectroscopy [2109].

4-(3-Amino-4-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{10}H_{11}NO_4$ mol. wt. 209.20



Synthesis
-Refer to: [2494].
Methyl ether [39496-86-1]
$C_{11}H_{13}NO_4$ mol. wt. 223.23

-Obtained by reduction of its nitro derivative [2494].
-Also refer to: [216].

colourless needles [2494];
m.p. 138° [2494], 136–137° [216].

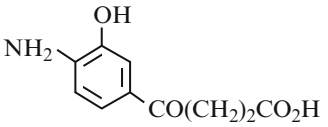
Ethyl ether $C_{12}H_{15}NO_4$ mol. wt. 237.26

-Obtained by reduction of its nitro derivative [2494].

colourless plates [2494]; m.p. 144–146° [2494].

1-(4-Amino-3-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{10}H_{11}NO_4$ mol. wt. 209.20



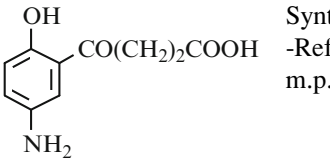
Synthesis
-Refer to: [1554].
Methyl ether [92422-41-8]
$C_{11}H_{13}NO_4$ mol. wt. 223.23

-Obtained by adding at r.t. a solution of 3-methoxy-4-nitrobenzoylpropionic acid in 2 N ammonia to an aqueous solution of ferrous sulfate. Then, boiling the mixture for few min (80 %) [1554].

m.p. 152–153° [1554].

1-(5-Amino-2-hydroxyphenyl)-4-oxo-1-butanoic acid

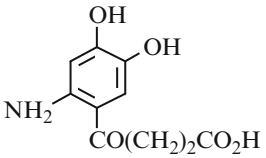
[56872-54-9] $C_{10}H_{11}NO_4$ mol. wt. 209.20



Syntheses
-Refer to: [687, 688, 2912, 2913].
m.p. 158–160° [687, 688, 2912, 2913].

4-(2-Amino-4,5-dihydroxyphenyl)-4-oxo-1-butanoic acid

$C_{10}H_{11}NO_5$ mol. wt. 225.20



Synthesis
-Refer to: [1246].

Dimethyl ether [854677-84-2]
$C_{12}H_{15}NO_5$ mol. wt. 253.25

-Obtained by treatment of 4,5-dimethoxy-2-nitrobenzoylpropionic acid in dilute ammonia with hydrated ferrous sulfate at 100° for 30 min [1246, 2073].
-Also refer to: [100, 1247, 2760].

m.p. 143–144° [2760], 141–142.5° [2073], 141° [1247], 139–141° [100], 118° [1246];
N.B.: One of the reported melting point is obviously wrong.

Acetylamino of the dimethyl ether $C_{14}H_{17}NO_6$ mol. wt. 295.29

-Refer to: [1246].

m.p. 187° [1246].

Benzoylamino of the dimethyl ether $C_{19}H_{19}NO_6$ mol. wt. 357.36

-Refer to: [1246].

m.p. 225° [1246].

Methyl ester of the dimethyl ether [4848-01-5] $C_{13}H_{17}NO_5$ mol. wt. 267.28

-Obtained by reaction of 4-(2-Amino-4,5-dimethoxyphenyl)-4-oxo-1-butanoic acid with boiling methanol in the presence of concentrated sulfuric acid for 4 h (59 %) [100].
-Also refer to: [1246, 1247].

yellow needles [100];
m.p. 127–128° [100], 127° [1246, 1247].

Ethyl ester of the dimethyl ether [87364-85-0] $C_{14}H_{19}NO_5$ mol. wt. 281.31

-Refer to: [984, 2760].

m.p. 110–111° [984], 103–104.5° [2760];
^{1}H NMR [984], IR [984], MS [984].

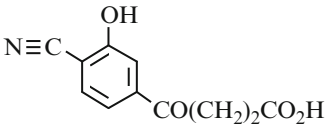
Monohydrate of the dimethyl ether $C_{12}H_{15}NO_5, H_2O$ mol. wt. 271.26

-Refer to: [1246, 1247].

m.p. 118° [1246, 1247].

1-(4-Cyano-3-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{11}H_9NO_4$ mol. wt. 219.20



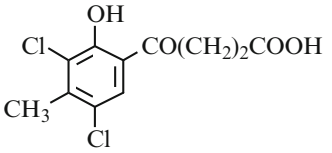
Synthesis
-Refer to: [1554].
Methyl ether [93041-47-5]
$C_{12}H_{11}NO_4$ mol. wt. 233.22

-Obtained by reaction of cuprous cyanide to a solution of diazonium salt of 4-amino-3-methoxy-benzoylpropionic acid, first at <4°, then at 70° for 1 h (60 %) [1554].

m.p. 153–154° [1554].

4-(3,5-Dichloro-2-hydroxy-4-methylphenyl)-4-oxo-1-butanoic acid

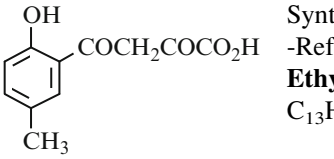
[62903-11-1] $C_{11}H_{10}Cl_2O_4$ mol. wt. 277.10



Syntheses
-Refer to: [2703, 2705].
m.p. 185–187° [2703, 2705].

4-(2-Hydroxy-5-methylphenyl)-2,4-dioxo-1-butanoic acid

$C_{11}H_{10}O_5$ mol. wt. 222.20



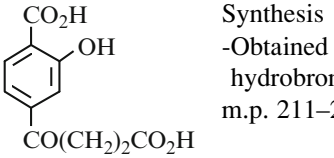
Synthesis
-Refer to: [193].
Ethyl ester
$C_{13}H_{14}O_5$ mol. wt. 250.25

-Refer to: [193].

needles [193]; m.p. 78–79° [193].

1-(4-Carboxy-3-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{11}H_{10}O_6$ mol. wt. 238.20



Synthesis
-Obtained by refluxing its methyl ether below with 48 % hydrobromic acid in acetic acid overnight (7 %) [1554].
m.p. 211–214° [1554].

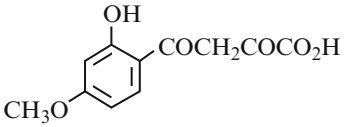
Methyl ether [91964-06-6] $C_{12}H_{12}O_6$ mol. wt. 252.22

-Obtained by refluxing a solution of 4-cyano-3-methoxybenzoylpropionic acid in 10 % aqueous sodium hydroxide and ethanol for 2.5 h under nitrogen (70 %) [1554].

m.p. 158–159.5° [1554].

4-(2-Hydroxy-4-methoxyphenyl)-2,4-dioxo-1-butanoic acid

$C_{11}H_{10}O_6$ mol. wt. 238.20



Synthesis
-Refer to: [1739].

Ethyl ester

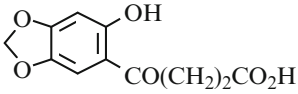
$C_{13}H_{14}O_6$ mol. wt. 266.25

-Refer to: [1739];

m.p. 107–108° [1739].

4-(6-Hydroxybenzodioxol-5-yl)-4-oxo-1-butanoic acid

$C_{11}H_{10}O_6$ mol. wt. 238.20



Synthesis
-Refer to: [2196].

Methyl ether [41827-06-9] $C_{12}H_{12}O_6$ mol. wt. 252.22

6-Methoxy-γ-oxo-1,3-benzodioxole-5-butanoic acid

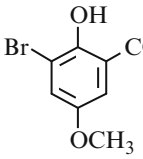
-Obtained by reaction of 5-methoxybenzodioxol with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h [2196].
-Also obtained by condensation of 5-hydroxybenzodioxol with succinic anhydride (70 %) [1451].

m.p. 140–141° [878], 140° [1451].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

4-(3-Bromo-2-hydroxy-5-methoxyphenyl)-4-oxo-1-butanoic acid

[87338-25-8] $C_{11}H_{11}BrO_5$ mol. wt. 303.11



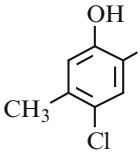
Synthesis

-Obtained by reaction of bromine with 4-(2-hydroxy-5-methoxyphenyl)-4-oxo-1-butanoic acid in acetic acid in the presence of sodium acetate at r.t. (81 %) [3045].

m.p. 191° [3045].

4-(5-Chloro-2-hydroxy-4-methylphenyl)-4-oxo-1-butanoic acid

[62903-21-3] $C_{11}H_{11}ClO_4$ mol. wt. 242.66



Syntheses

-Obtained by treatment of its methyl ether with hydrogen bromide in refluxing acetic acid (89 %) [2652].

-Also refer to: [997 (7 %), 2703, 2705].

m.p. 181–182° [2703, 2705], 180–181° [2652], 178–182° [997];
^{1}H NMR [997], IR [997].

Methyl ether [857229-77-7] $C_{12}H_{13}ClO_4$ mol. wt. 256.69

-Obtained by reaction of succinic anhydride (Bernstein anhydride) with 4-chloro-3-methylanisole in the presence of aluminium chloride in nitrobenzene for 24 h at r.t. (42.5 %) [2652].

m.p. 160–161° [2652].

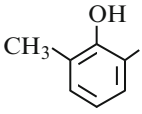
Methyl ester [127275-14-3] $C_{12}H_{13}ClO_4$ mol. wt. 256.69

-Refer to: [997].

m.p. 95–97° [997];
^{1}H NMR [997], IR [997].

4-(2-Hydroxy-3-methylphenyl)-4-oxo-1-butanoic acid

[854677-51-3] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses

-Obtained by reaction of succinic anhydride with o-cresol in the presence of aluminium chloride in tetrachloroethane at 120–130° for 2 h (21 %) [197], (35–40 %) [2571].

m.p. 136–137° [2571].

Methyl ester $C_{12}H_{14}O_4$ mol. wt. 222.24

m.p. 78° [2571].

Ethyl ester $C_{13}H_{16}O_4$ mol. wt. 236.27

m.p. 78° [2571].

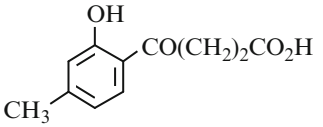
Ethyl ether $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by Friedel-Crafts reaction of succinic anhydride and o-cresyl ethyl ether (79 %) [2579].

b.p. 192° [2579]; m.p. 172–173° [341, 2579].

4-(2-Hydroxy-4-methylphenyl)-4-oxo-1-butanoic acid

[59010-46-7] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses

-Obtained by Fries rearrangement of m-tolyl hydrogen succinate with aluminium chloride at 117° for 2.5 h,

*in tetrachloroethane (41 %) [197], (60–65 %) [2571];

*in nitrobenzene (42 %) [197];

*in chlorobenzene (44 %) [197];

*m-xylene (44 %) [197].

-Also obtained by reaction of succinic anhydride with m-cresol in the presence of aluminium chloride [685, 804].

-Also obtained by treatment of its methyl ether with hydrogen bromide in refluxing acetic acid (90 %) [2652].

-Also refer to: [397, 997 (4 %), 1524].

m.p. 155–156° [716], 154–157° [997],
154° [804, 2571], 153–154° [2652];
^{1}H NMR [997], IR [997].

Methyl ether [91497-61-9] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by reaction of m-cresol methyl ether with succinic anhydride in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture (75 %) [2579], (23 %) [1530], (4 %) [930].

-Also refer to: [814, 1524, 1767, 2652 (95 %), 2804, 2832, 3139].

b.p. 177° [2579];
m.p. 138° [2649], 137–137.5° [2579], 127–128° [1524], 126–128° [814], 126–127° [1767], 126° [3139], 124–126° [930], 121–123.5° [1530];
^{1}H NMR [2804].

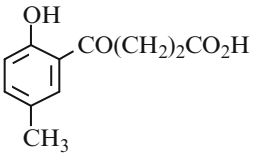
Methyl ester [59010-47-8] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Refer to: [687, 997].

m.p. 61–63° [687], 59–61° [997]; ^{1}H NMR [997], IR [997].

4-(2-Hydroxy-5-methylphenyl)-4-oxo-1-butanoic acid

[103987-17-3] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses

-Obtained by Fries rearrangement of p-tolyl hydrogen succinate with aluminium chloride at 117° for 2.5 h in tetrachloroethane (66 %), in nitrobenzene (56 %) or in chlorobenzene (38 %) [1987], (21 %) [197].

-Also obtained directly by Friedel-crafts reaction of succinic anhydride with p-cresol in the presence of aluminium chloride in tetrachloroethane first at 55°, then, at 135° for 2.5 h (52 %) [2263].

-Also obtained by treatment of its methyl ether with hydrogen bromide in refluxing acetic acid (94 %) [2652].

-Also refer to: [997 (18 %), 1667, 2263, 2571 (40–45 %), 2649].

m.p. 136–137° [2263, 2649], 136° [2652], 135–136° [3337], 132–134° [910], 131–134° [997], 122–124° [1667];
^{1}H NMR [997], IR [997], UV [1827].

BIOLOGICAL ACTIVITY: Refer to: [1827, 2167].

Methyl ether [55007-22-2] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by succinoylation of p-cresol methyl ether in a 4:1 mixture of tetrachloroethane and nitrobenzene at 0° for 24 h (84 %) [910], (65 %) [2579].

-Also refer to: [690, 858, 2649, 3065, 3273, 3289].

b.p. 176° [2579];
m.p. 115–117° [2649, 3337], 114–115.5° [690], 114–115° [3065], 107–109° [910], 107–108° [2579], 95.5–96.5° [690], 95° [588], 92° [3273], 89–94° [3289];
N.B.: The discrepancy between the found and the reported melting point is not explained at present [910].

Semicarbazone of the methyl ether $C_{13}H_{17}N_3O_4$ mol. wt. 279.29

m.p. 179° [3065].

Methyl ester of the methyl ether [20483-30-1] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by reaction of methanol with β-(2-methoxy-5-methylbenzoyl)propionic acid in the presence of concentrated sulfuric acid at reflux for 24 h (65 %) [910].

-Also refer to: [818].

m.p. 53–54.5° [910], 43.5–47.5° [818];
UV [910].

Ethyl ether [873396-80-6] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by Friedel-Crafts reaction of succinic anhydride and p-cresyl ethyl ether (52 %) [2579].
-Also refer to: [341].

b.p. 192° [2579]; m.p. 140° [341], 139–141° [2579].

Semicarbazone of the ethyl ether $C_{14}H_{19}N_3O_4$ mol. wt. 293.32

m.p. 130° [341].

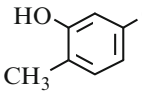
Methyl ester [123471-86-3] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Refer to: [997].

m.p. 52–53° [997]; ^{1}H NMR [997], IR [997].

4-(3-Hydroxy-4-methylphenyl)-4-oxo-1-butanoic acid

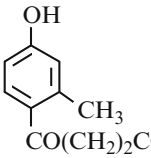
[56872-34-5] $C_{11}H_{12}O_4$ mol. wt. 208.21



Synthesis
-Refer to: [1993].
m.p. 172–173° [1993].

4-(4-Hydroxy-2-methylphenyl)-4-oxo-1-butanoic acid

[319494-43-4] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Obtained by Fries rearrangement of m-tolyl hydrogen succinate with aluminium chloride at 117° for 2.5 h in tetrachloroethane (1–2 %) [2571].
-Also obtained by heating its methyl ether with aluminium chloride at 150° [2649].
-Also obtained by treatment of its methyl ether with hydrogen bromide in refluxing acetic acid (22 %) [2652].
-Also refer to: [716, 1667, 2392, 2857].

m.p. 179.5–180.5° [2392], 172° [2571, 2857], 170° [716], 155° [2652], 108–110° [1667].
N.B.: One of the reported melting point is obviously wrong.

Methyl ether [67405-48-5] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by reaction of m-cresol methyl ether with succinic anhydride [2649] in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture (47 %) [1530].
-Obtained by reaction of β-carbethoxypropionyl chloride with 3-methylanisole in the presence of aluminium chloride in tetrachloroethane at 0° for 3–4 h (90 %) [2392].

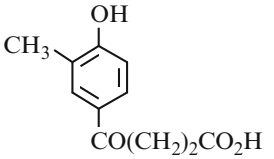
-Also refer to: [303, 340, 534, 858, 930, 1767, 2804, 2832, 2934, 3179].

m.p. 54° (monohydrate) [858];
m.p. 138–139° [1767], 138° [2649], 136.5–138° [2934], 136–137° [2392], 135–137.5° [2579], 135–136° [2804], 134–135° [534], 131–132° [303], 130–133° [1530];
^{1}H NMR [534, 2804, 2832], IR [534, 2804, 2832] .

BIOLOGICAL ACTIVITY: Refer to: [3179].

4-(4-Hydroxy-3-methylphenyl)-4-oxo-1-butanoic acid

[91541-03-6] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Obtained by reaction of succinic anhydride with o-cresol in the presence of aluminium chloride in tetrachloroethane at 120–130° for 2 h (27 %) [197], (15–20 %) [2571].
-Also obtained by treatment of its methyl ether with hydrogen bromide in refluxing acetic acid (97 %) [2652].

-Also refer to: [1619, 1667].

m.p. 198° [1667], 186° [2652], 184° [2571]; IR [1619].

Methyl ether [33446-14-9] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by reaction of succinic anhydride with o-cresol methyl ether in the presence of aluminium chloride (80 %) [982],
*in nitrobenzene first at 0°, then at r.t. for 24 h (85 %) [3476] or at 40–45° (74 %) [2649];
*in nitrobenzene as usual (73 %) [2728], for 40 h (88 %) [288], for 60 h [858];
*in nitrobenzene at r.t. overnight (83.6 %) [1566].
-Also refer to: [261, 692, 857, 1033, 1972, 2645, 3233].

m.p. 166.4–169.2° [1972], 152° [3233], 151° [2645], 150.5–152° [288], 150° [692, 857, 858], 147° [3476], 146° [2649], 143° [261, 2728], 142–143° [1566];
^{1}H NMR [288, 1033, 1972, 3476], ^{13}C NMR [288],
IR [692, 3476], UV [692], MS [1972, 3476].

Ethyl ester of the methyl ether [2954-68-9] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of β-(4-methoxy-3-methylbenzoyl)propionic acid with ethanol in the presence of sulfuric acid for 6 h at reflux (80 %) [692].

silvery plates [692]; m.p. 55° [692]; IR [692].

Semicarbazone of the methyl ether and ethyl ester

[4605-98-5] $C_{15}H_{21}N_3O_4$ mol. wt. 307.35

m.p. 134° [692]; UV [692].

Methyl ester [115763-03-6] $C_{12}H_{14}O_4$ mol. wt. 222.24

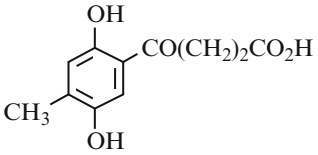
m.p. 108° [2571].

Ethyl ester $C_{13}H_{16}O_4$ mol. wt. 236.27

m.p. 106° [2571].

4-(2,5-Dihydroxy-4-methylphenyl)-4-oxo-1-butanoic acid

$C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis
-Refer to: [2196].

Dimethyl ether [856809-86-4]
$C_{13}H_{16}O_5$ mol. wt. 252.27

-Preparation from 2,5-dimethoxytoluene (90 %) [1937].
-Also refer to: [157, 2135].

m.p. 179° [2135], 177° [1937], 176–177° [157].

Methyl ester of the dimethyl ether $C_{14}H_{18}O_5$ mol. wt. 266.29

m.p. 89–90° [1755]; ^{1}H NMR [1755], IR [1755].

Ethyl ester of the dimethyl ether $C_{15}H_{20}O_5$ mol. wt. 280.32

m.p. 74° [157].

Diethyl ether [41827-11-6] $C_{15}H_{20}O_5$ mol. wt. 280.32

2,5-Diethoxy-4-methyl-γ-oxobenzenebutanoic acid

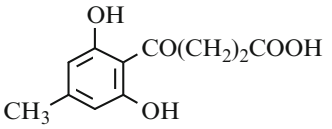
-Obtained by reaction of succinic anhydride with 2,5-diethoxytoluene in the presence of aluminium chloride in carbon tetrachloride first at r.t., then at 70° for 2 h [2196].

m.p. 128–129° [2196].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

4-(2,6-Dihydroxy-4-methylphenyl)-4-oxo-1-butanoic acid

[854679-09-7] $C_{11}H_{12}O_5$ mol. wt. 224.21



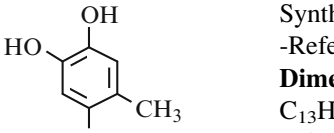
Synthesis
-Refer to: [856].
m.p. 207° [856].

4-Nitrophenylhydrazone $C_{17}H_{17}N_3O_6$ mol. wt. 359.33

m.p. 203–204° [856].

4-(4,5-Dihydroxy-2-methylphenyl)-4-oxo-1-butanoic acid

$C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis
-Refer to: [2196].
Dimethyl ether [6575-51-5]
$C_{13}H_{16}O_5$ mol. wt. 252.27
4,5-Dimethoxy-2-methyl-γ-oxobenzenebutanoic acid

-Obtained by condensation of 1-methyl-3,4-dimethoxybenzene with succinic anhydride in the presence of aluminium chloride in carbon disulfide/nitrobenzene mixture. This one was left at r.t. overnight, then heated under reflux for 30 min (52 %) [1544].
-Also obtained by Friedel-Crafts succinoylation of 3,4-dimethoxytoluene [1837] according to [2835].
-Also obtained by treatment of homoveratrole with succinic anhydride in the presence of aluminium chloride in nitrobenzene for 24 h at r.t. (78.6 %) [2835].
-Also refer to: [2196].

m.p. 128–130° [1544], 108–112° [1837], 97° [2835];
^{1}H NMR [1837], IR [1837].

BIOLOGICAL ACTIVITY: Choleretic action [2196].

Diethyl ether [41826-96-4] $C_{15}H_{20}O_5$ mol. wt. 280.32

4,5-Diethoxy-2-methyl-γ-oxobenzenebutanoic acid

-Obtained by reaction of succinic anhydride with 3,4-diethoxytoluene in the presence of aluminium chloride in carbon tetrachloride first at r.t., then at 70° for 2 h (44 %) [2196].
-Also refer to: [2191, 2192, 2194, 3037–3039].

m.p. 116–117° [2191, 2192, 2196, 3037, 3039];
^{1}H NMR [3038].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

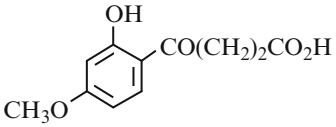
Ethyl ester of the ethyl ether [41827-10-5] $C_{17}H_{24}O_5$ mol. wt. 308.38

-Refer to: [2191, 3037].

m.p. 81–82° [2191, 3037].

4-(2-Hydroxy-4-methoxyphenyl)-4-oxo-1-butanoic acid
γ-2-hydroxy-4-methoxyphenyl-γ-ketobutyric acid

[14617-02-8] $C_{11}H_{12}O_5$ mol. wt. 224.21



Syntheses
-Obtained (by-product) by reaction of succinic anhydride with resorcinol dimethyl ether in the presence of aluminium chloride,
*in tetrachloroethane at 50–60° for 3 h, then at r.t. overnight (12 %) [2100];
*without solvent on the water bath for 3 h [2456].
-Also obtained by reaction of succinic anhydride with m-methoxyphenol in the presence of aluminium chloride in nitrobenzene at 49° for 1 h 30 min (32 %) [821];
-Also obtained by treatment of its methyl ester with boiling 2 % alcoholic potassium hydroxide for 24 h [615].
-Also obtained from anhydrobrazilic acid by its decomposition by baryta [2456].
-Also refer to: [660, 676, 795, 796, 2458, 3485].

m.p. 160–161° [615], 156° [660, 795, 796, 2456, 3485], 155–156° [676, 2458], 154° [2100], 148° [821];
^{1}H NMR [676], IR [615, 676].

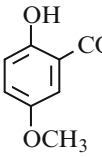
Methyl ester [42907-96-0] $C_{12}H_{14}O_5$ mol. wt. 238.24

-Obtained by methylation of β-(2,4-dihydroxybenzoyl)propionic acid,
*with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 2 h (35 %) [1669];
*with diazomethane in ethyl ether at r.t. overnight (53 %) [1669].
-Also obtained by esterification of this acid with methanol/boron trifluoride [821].
-Also obtained from title acid in refluxing methanol for 2 h in the presence of 20 % sulfuric acid [2456].
-Also refer to: [615, 999, 1153, 1670].

m.p. 90–92° [1669], 87° [2456], 85.5–86° [821], 85° [1153], 73–76° [999];
^{1}H NMR [999, 1669], IR [999], UV [999];
TLC [1669].

4-(2-Hydroxy-5-methoxyphenyl)-4-oxo-1-butanoic acid

[75501-54-1] $C_{11}H_{12}O_5$ mol. wt. 224.21



Syntheses

-Obtained by partial demethylation of β-(2,5-dimethoxybenzoyl)propionic acid with aluminium chloride,
*in chlorobenzene [2331];
*in acetonitrile at 65° (70 %) [3045].

-Also obtained by condensation of hydroquinone dimethyl ether with succinic anhydride in nitrobenzene in the presence of aluminium chloride. During this addition, which required 1 h, the reaction mixture was stirred and cooled in an ice bath. The temperature was maintained below 35°. The resulting solution was warmed slowly to 60° and stirred at this temperature for 3 h (51 %) [2262].
-Also obtained by photo-Fries rearrangement of 4-methoxyphenyl monosuccinate (60 %) [2004].
-Also refer to: [676, 747, 997 (60 %), 3320].

yellow crystals [2262];
m.p. 145–146° [2262], 145° [747, 3045],
142.5–143.5° [997, 2004], 140° [2331];
^{1}H NMR [676, 997, 2004, 3320],
IR [676, 997, 2004, 3045].

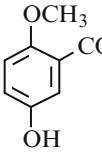
Methyl ester [59701-66-5] $C_{12}H_{14}O_5$ mol. wt. 238.24

-Obtained by treatment of the acid above with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 2.5 h (48 %) [1349].
-Also obtained by photo-Fries rearrangement of 4-methoxyphenyl methyl succinate (58 %) [2004].
-Also refer to: [997].

oil [997, 2004]; m.p. 41–42° [1349];
^{1}H NMR [997, 1349, 2004], IR [997, 1349, 2004].

4-(5-Hydroxy-2-methoxyphenyl)-4-oxo-1-butanoic acid

$C_{11}H_{12}O_5$ mol. wt. 224.21



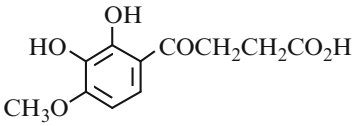
Synthesis

-Obtained (by-product) by reaction of succinic anhydride with hydroquinone dimethyl ether in the presence of aluminium chloride [696].

m.p. 135° [696].

4-(2,3-Dihydroxy-4-methoxyphenyl)-4-oxo-1-butanoic acid

[74882-03-4] $C_{11}H_{12}O_6$ mol. wt. 240.21



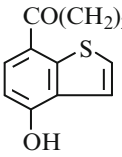
Synthesis

-Obtained (by-product) by reaction of succinic anhydride with 1,2,3-trimethoxybenzene in the presence of aluminium chloride in 1,1,2,2-tetrachloro-ethane at 0°. The red mixture was allowed to warm to ambient temperature, and after 16 h it was heated on a steam bath for 2 h [1209].

m.p. 174–176° [1209].

4-(4-Hydroxy-7-benzo[*b*]thiophene)-4-oxo-1-butanoic acid

$C_{12}H_{10}O_4S$ mol. wt. 250.28



Synthesis

-Refer to: [845].

Methyl ether [4878-81-3]

$C_{13}H_{12}O_4S$ mol. wt. 264.30

-Obtained by treatment of its methyl ester below with sodium hydroxide in refluxing dilute ethanol for 1 h (99 %) [845].

-Also refer to: [639].

m.p. 223.5° [845]; IR [639, 845].

Methyl ester of the methyl ether $C_{14}H_{14}O_4S$ mol. wt. 278.33

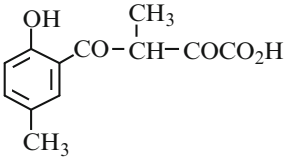
-Obtained by reaction of butanedioic acid, monochloride, methyl ester with 4-methoxy-benzo[*b*]thiophene (64.5 %) [845].

-Also refer to: [639].

b.p.$_{10}$ 255° [845]; m.p. 108° [845];
IR [639, 845].

4-(2-Hydroxy-5-methylphenyl)-3-methyl-2,4-dioxo-1-butanoic acid

$C_{12}H_{12}O_5$ mol. wt. 236.22



Synthesis

-Refer to: [193].

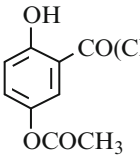
Ethyl ester

$C_{14}H_{16}O_5$ mol. wt. 264.28

-Obtained by treatment of 2-hydroxy-5-methylpropiophenone with diethyl oxalate in the presence of sodium [193].

4-[5-(Acetyloxy)-2-hydroxyphenyl]-4-oxo-1-butanoic acid

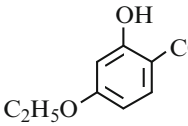
$C_{12}H_{12}O_6$ mol. wt. 252.22



Synthesis
-Refer to: [997].

4-(4-Ethoxy-2-hydroxyphenyl)-2,4-dioxo-1-butanoic acid

$C_{12}H_{12}O_6$ mol. wt. 252.22

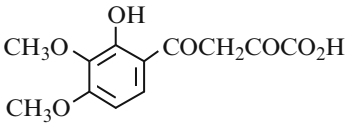


Syntheses
-Refer to: [1740, 1742].
Ethyl ester $C_{14}H_{16}O_6$ mol. wt. 280.28
-Refer to: [1740, 1742].

m.p. 99–100° [1742].

4-(2-Hydroxy-3,4-dimethoxyphenyl)-2,4-dioxo-1-butanoic acid

$C_{12}H_{12}O_7$ mol. wt. 268.22

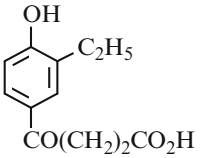


Synthesis
-Refer to: [810].
Ethyl ester
$C_{14}H_{16}O_7$ mol. wt. 296.28

-Obtained by reaction of diethyl oxalate with 2-hydroxy-3,4-dimethoxyacetophenone in the presence of granulous sodium [810].

4-(3-Ethyl-4-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Refer to: [845].
Methyl ether [3728-79-8]
$C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by treatment of its methyl ester below with sodium hydroxide in refluxing dilute ethanol for 1.5 h (86 %) [845].
-Also obtained by reaction of succinic anhydride with o-ethylanisole in the presence of aluminium chloride in nitrobenzene at r.t. for 24 h (80 %) [2727].
-Also refer to: [3038].

m.p. 151° [845], 149° [2727]; ^{1}H NMR [3038].

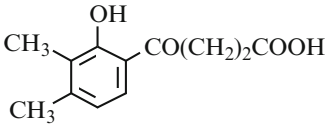
Methyl ester of the methyl ether [3728-78-7] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of butanedioic acid, monochloride, methyl ester with 2-ethylanisole (81.5 %) [845].

b.p.$_{17}$ 212–215° [845]; m.p. 45° [845].

4-(2-Hydroxy-3,4-dimethylphenyl)-4-oxo-1-butanoic acid

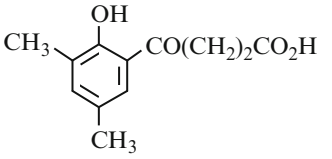
[83481-33-8] $C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Refer to: [693].
m.p. 188–189° [693].

4-(2-Hydroxy-3,5-dimethylphenyl)-4-oxo-1-butanoic acid

[7356-03-8] $C_{12}H_{14}O_4$ mol. wt. 222.24



Syntheses
-Obtained by treatment of 2,4-xylyl hydrogen succinate (m.p. 78°) with aluminium chloride,
*in nitrobenzene for 0.5 h at 140° (15 %) [694];
*in tetrachloroethane at 130° for 2.5 h (30 %) [1443].
-Also obtained (by-product) by Fries rearrangement of 2,4-xylyl succinate with aluminium chloride in tetrachloroethene at 125–135° [1443].
-Also refer to: [225, 269, 694, 997 (25 %)].

m.p. 149–151° [997], 147–148° [225, 269, 694], 147° [1443].
^{1}H NMR [997], IR [997].

Methyl ether $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by reaction of succinic anhydride with 2,4-dimethylanisole in the presence of aluminium chloride in benzene for 3 h, then at r.t. overnight (25 %) [691].
-Also refer to: [3272].

long needles [691]; m.p. 129–130° [691]; ^{1}H NMR [3272].

S-Benzylthiuronium salt [102457-90-9] $C_{20}H_{24}N_2O_4S$ mol. wt. 388.48

-Refer to: [269].

m.p. 151° [269].

2,4-Dimethylphenyl ester $C_{20}H_{22}O_4$ mol. wt. 326.39

-Obtained by Fries rearrangement of 2,4-xylyl succinate with aluminium chloride in tetrachloroethane at 125–135° [1443].

m.p. 130–132° [1443].

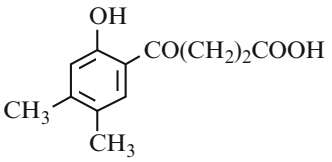
Methyl ester [123471-91-0] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Refer to: [997].

m.p. 60–65° [997]; ^{1}H NMR [997], IR [997].

4-(2-Hydroxy-4,5-dimethylphenyl)-4-oxo-1-butanoic acid

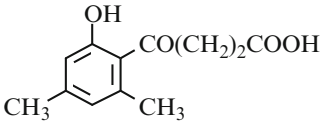
$C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Refer to: [225].
m.p. 153–154° [225].

4-(2-Hydroxy-4,6-dimethylphenyl)-4-oxo-1-butanoic acid

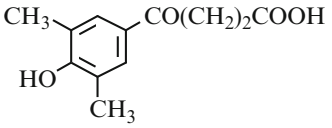
[96358-74-6] $C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Refer to: [397].
m.p. 117° [397]; ^{1}HNMR [397], IR [397].

4-(4-Hydroxy-3,5-dimethylphenyl)-4-oxo-1-butanoic acid

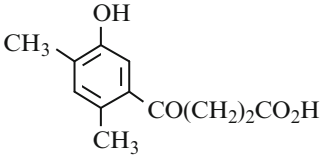
[52245-99-5] $C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Refer to: [669].
m.p. 168° [669].

4-(5-Hydroxy-2,4-dimethylphenyl)-4-oxo-1-butanoic acid

$C_{12}H_{14}O_4$ mol. wt. 222.24



Syntheses
-Obtained from its methyl ether [694, 695].
m.p. 139° [694].

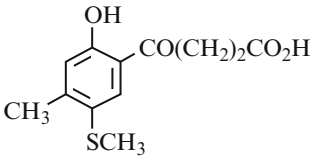
Methyl ether [78334-92-6]
$C_{13}H_{16}O_4$ mol. wt. 236.27

-Refer to: [187, 694, 695, 3272].

m.p. 52° [695], 50–51° [187]; ^{1}H NMR [3272].

4-(2-Hydroxy-4-methyl-5-methylthiophenyl)-4-oxo-1-butanoic acid

$C_{12}H_{14}O_4S$ mol. wt. 254.31



Synthesis
-Refer to: [2196].

Ethyl ether [41827-08-1]
$C_{14}H_{18}O_4S$ mol. wt. 282.36
2-Ethoxy-4-methyl-5-(methylthio)-γ-oxobenzenebutanoic acid.

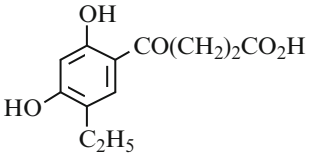
-Obtained by reaction of 3-methyl-4-methylthiophenetole with $CH_3O_2C(CH_2)_2COCl$ in the presence of stannic chloride in benzene first at 5°, then at r.t. for 1 h. After, the methylester obtained was warmed at 50° with a 5 % methanolic potassium hydroxide for 1 h [2196].

m.p. 117–118° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

4-(2,4-Dihydroxy-5-ethylphenyl)-4-oxo-1-butanoic acid

$C_{12}H_{14}O_5$ mol. wt. 238.24



Synthesis
-Refer to: [2196].

Dimethyl ether [100972-91-6]
$C_{14}H_{18}O_5$ mol. wt. 266.29
-Refer to: [115, 1450].

m.p. 141–142° [1450].

Diethyl ether [41827-04-7] $C_{16}H_{22}O_5$ mol. wt. 294.35

2,4-Diethoxy-5-ethyl-γ-oxobenzenebutanoic acid

-Obtained by heating a mixture of 4-ethylresorcinol diethyl ether and succinic acid monomethyl ester in the presence of PPA at 50–55° for 40 min. Ice-water was added to the mixture, the resulting aqueous mixture was diluted with acetic acid and heated at 80–90° for 50 min [2196].
-Also refer to: [115, 3037, 3039].

m.p. 153–155° [2196, 3037, 3039].

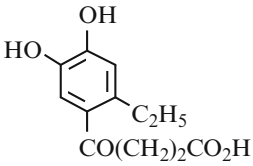
BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

2-Ethoxy-4-methoxy diether [129201-57-6] $C_{15}H_{20}O_5$ mol. wt. 280.32

-Refer to: [115].

4-(4,5-Dihydroxy-2-ethylphenyl)-4-oxo-1-butanoic acid

$C_{12}H_{14}O_5$ mol. wt. 238.24



Synthesis
-Refer to: [2196].

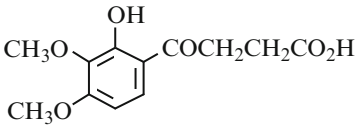
Dimethyl ether [100972-92-7]
$C_{14}H_{18}O_5$ mol. wt. 266.29

-Obtained by treatment of ethylveratrole with succinic anhydride in the presence of aluminium chloride in nitrobenzene for 24 h at r.t. (77.5 %) [2835].

white flakes [2835]; m.p. 123° [2835].

1-(2-Hydroxy-3,4-dimethoxyphenyl)-4-oxo-1-butanoic acid
γ-2-hydroxy-3,4-dimethoxyphenyl-γ-ketobutyric acid

[68486-75-9] $C_{12}H_{14}O_6$ mol. wt. 254.24



Syntheses
-Obtained by reaction of succinic anhydride with pyrogallol trimethyl ether in the presence of aluminium chloride,
*in tetrachloroethane (65 %) [2100], (32 %) [1981];
*in carbon disulfide [257, 258].
-Also refer to: [798, 1093, 1302 (30–40 %), 2463].

pale yellow needles [2463];
m.p. 154–156° [1302], 154–155° [2463], 153° [798], 152° [257, 258, 2100], 148° [1981].

Methyl ester [74882-02-3] $C_{13}H_{16}O_6$ mol. wt. 268.27

-Obtained by bubbling hydrogen chloride in 1-(2-hydroxy-3,4-dimethoxyphenyl)-4-oxo-1-butanoic acid in methanol for 1.5 h [257, 258].
-Also obtained from the title acid in refluxing methanol in the presence of 1 % concentrated sulfuric acid [1302].
-Also refer to: [798].

m.p. 110° [798], 106° [257, 258], 99–101° [1302].

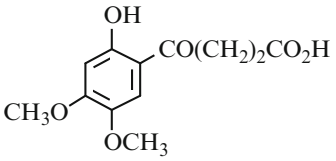
Ethyl ester $C_{14}H_{18}O_6$ mol. wt. 282.29

-Refer to: [798].

m.p. 58° [798].

4-(2-Hydroxy-4,5-dimethoxyphenyl)-4-oxo-1-butanoic acid
2-Hydroxy-4,5-dimethoxy-γ-oxubenzenebutanoic acid

[41827-12-7] $C_{12}H_{14}O_6$ mol. wt. 254.24



Syntheses
-Obtained by reaction of succinic anhydride with 3,4-dimethoxyphenol in the presence of aluminium chloride in carbon tetrachloride first at r.t., then at 70° for 2 h [2196].
-Also obtained by refluxing a mixture of 2,4,6-trimethoxybenzoylpropionic acid, potassium iodide and formic acid for 2 h (75 %) [2196].

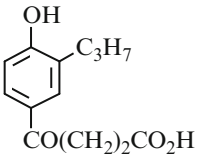
-Also refer to: [676, 2193, 3037].

m.p. 162–163° [2193, 2196, 3037], 152–155° [676];
^{1}H NMR [676], IR [676, 2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

1-(4-Hydroxy-3-propylphenyl)-4-oxo-1-butanoic acid

$C_{13}H_{16}O_4$ mol. wt. 236.37



Synthesis
-Refer to: [2728].

Methyl ether [100972-66-5]
$C_{14}H_{18}O_4$ mol. wt. 250.30

-Obtained by reaction of succinic anhydride with 2-propylanisole in the presence of aluminium chloride in nitrobenzene (50 %) [2728].

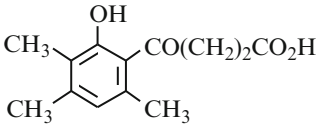
white needles [2728]; m.p. 139° [2728].

Ethyl ether [905590-12-7] $C_{15}H_{20}O_4$ mol. wt. 264.32

^{1}H NMR [3038].

4-(2-Hydroxy-3,4,6-trimethylphenyl)-4-oxo-1-butanoic acid

[84978-12-1] $C_{13}H_{16}O_4$ mol. wt. 236.27



Syntheses
-Obtained (by-product) by Fries rearrangement of 2,3,5-trimethylphenyl succinate with aluminium chloride in tetrachloroethane for 1.5 h at 140–150° (5 %) [2908].

-Also obtained by hydrolysis of its 2,3,5-trimethylphenyl ester below with aqueous methanolic potassium hydroxide (40 %) [2908].
-Also refer to: [2325].

m.p. 170–171° [2908], 168–171.5° [2325]; IR [2325].

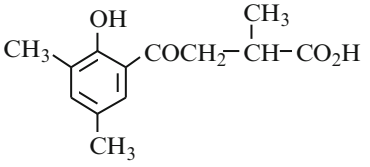
2,3,5-Trimethylphenyl ester $C_{22}H_{26}O_4$ mol. wt. 354.45

-Obtained (by-product) by Fries rearrangement of 2,3,5-trimethylphenyl succinate with aluminium chloride in tetrachloroethane for 1.5 h at 140–150° (6 %) [2908].

m.p. 134–135° [2908].

4-(2-Hydroxy-3,5-dimethylphenyl)-2-methyl-4-oxo-1-butanoic acid

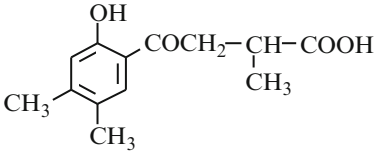
$C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Obtained by treatment of 2,4-dimethylphenyl 2-methylsuccinate (m.p. 112–113°) with aluminium chloride for 40 min at 140° (70 %) [694].
m.p. 122° [694].

4-(2-Hydroxy-4,5-dimethylphenyl)-2-methyl-4-oxo-1-butanoic acid

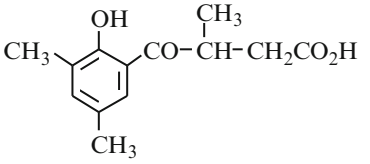
$C_{13}H_{16}O_4$ mol. wt. 236.27



Syntheses
-Refer to: [269, 694].
m.p. 158° [269, 694].

4-(2-Hydroxy-3,5-dimethylphenyl)-3-methyl-4-oxo-1-butanoic acid

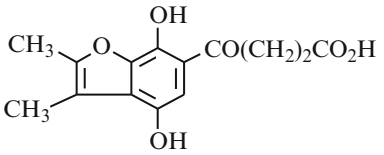
$C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Obtained by treatment of 2,4-dimethylphenyl 3-methylsuccinate (m.p. 65°) with aluminium chloride for 40 min at 140° [694].
m.p. 133° [694].

4-(4,7-Dihydroxy-2,3-dimethyl-6-benzofuranyl)-4-oxo-1-butanoic acid

$C_{14}H_{14}O_6$ mol. wt. 278.26



Synthesis
-Refer to: [1040].

Dimethyl ether
$C_{16}H_{18}O_6$ mol. wt. 306.32

-Refer to: [1040].

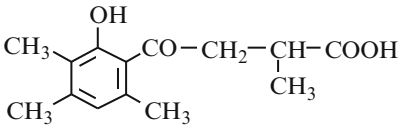
Methyl ester of the dimethyl ether $C_{17}H_{20}O_6$ mol. wt. 320.34

-Refer to: [1040 (51 %)].

m.p. 92° [1040]; LD_{50} [1040].

4-(2-Hydroxy-3,4,6-trimethylphenyl)-2-methyl-4-oxo-1-butanoic acid

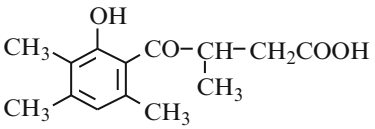
[34927-48-5] $C_{14}H_{18}O_4$ mol. wt. 250.29



Syntheses
-Refer to: [2150, 3275].
m.p. 182–184° [3275], 179–184° [2150];
^{1}H NMR [3275], IR [3275].

4-(2-Hydroxy-3,4,6-trimethylphenyl)-2-methyl-4-oxo-1-butanoic acid

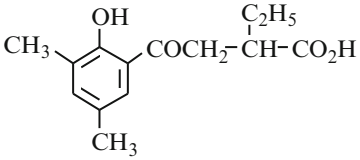
[34927-49-6] $C_{14}H_{18}O_4$ mol. wt. 250.29



Synthesis
-Refer to: [3275].
m.p. 138–139° [3275];
^{1}H NMR [3275], IR [3275].

4-(2-Hydroxy-3,5-dimethylphenyl)-2-ethyl-4-oxo-1-butanoic acid

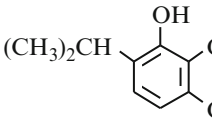
$C_{14}H_{18}O_4$ mol. wt. 250.29



Synthesis
-Obtained by Fries rearrangement of 2,4-dimethyl-phenyl 2-ethylsuccinate with aluminium chloride in nitrobenzene for 15 min at 140° (6 %) [694].
m.p. 140–141° [694].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-4-oxo-1-butanoic acid

[106591-86-0] $C_{14}H_{18}O_4$ mol. wt. 250.29

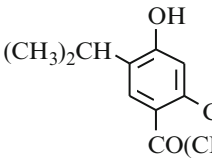


Synthesis
-Obtained by reaction of succinic acid with thymol in the presence of aluminium chloride on heating at reflux for 12 h (75 %) [2960].

m.p. 40° [2960].

4-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-4-oxo-1-butanoic acid

$C_{14}H_{18}O_4$ mol. wt. 250.29



Synthesis
-Refer to: [2649].
m.p. 117–120° [2649].

Methyl ether [101499-61-0] $C_{15}H_{20}O_4$ mol. wt. 264.32

-Refer to: [2649, 2934, 3050].

m.p. 93–94° [3050], 92–93° [2934], 92° [2649].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{21}H_{24}N_4O_7$ mol. wt. 444.44

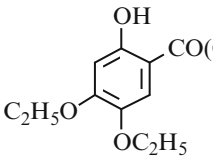
m.p. 144–145° [2934].

Phenylhydrazone of the methyl ether $C_{21}H_{26}N_2O_3$ mol. wt. 354.45

m.p. 144–145° [2934].

4-(4,5-Diethoxy-2-hydroxyphenyl)-4-oxo-1-butanoic acid

[63213-45-6] $C_{14}H_{18}O_6$ mol. wt. 282.29



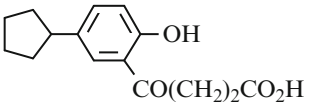
Synthesis
-Obtained by reaction of succinic anhydride with 3,4-diethoxyphenol in the presence of aluminium chloride in carbon tetrachloride first at r.t., then at 70° for 2 h [2196].

m.p. 142–144° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

4-(5-Cyclopentyl-2-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{15}H_{18}O_4$ mol. wt. 262.31



Synthesis
-Preparation by demethylation of its methyl ether [496].
m.p. 109° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether [874487-28-2] $C_{16}H_{20}O_4$ mol. wt. 276.33

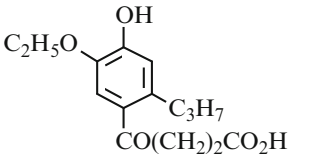
-Preparation by reaction of succinic anhydride with p-cyclopentylanisole in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 147° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-(5-Ethoxy-4-hydroxy-2-propylphenyl)-4-oxo-1-butanoic acid

$C_{15}H_{20}O_5$ mol. wt. 280.32



Synthesis
-Refer to: [2196].

Methyl ether [41826-99-7]
$C_{16}H_{22}O_5$ mol. wt. 294.35
Ethoxy-4-methoxy-γ-oxo-2-propylbenzene-butanoic acid

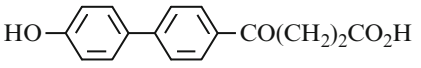
-Obtained by heating a mixture of 2-ethoxy-5-propylanisole and succinic acid monomethyl ester in the presence of PPA at 50–55° for 40 min. Ice-water was added to the mixture, the resulting aqueous mixture was diluted with acetic acid and heated at 80–90° for 50 min [2196].

m.p. 93° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

4-(4′-Hydroxybiphenyl)-4-oxo-1-butanoic acid

[74277-78-4] $C_{16}H_{14}O_4$ mol. wt. 270.28



Syntheses
-Obtained by demethylation of its methyl ether [496, 645, 986].

m.p. 218–220° [496]; UV [645].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether [36330-87-7] $C_{17}H_{16}O_4$ mol. wt. 284.31

-Obtained by condensation of 4-methoxydiphenyl with succinic anhydride in the presence of aluminium chloride in nitrobenzene in an ice bath. The mixture was stirred cold for 6 h at r.t. (24.5 %) [986], [645].
-Also refer to: [648, 649].

m.p. 201–202° [648, 649], 200–201° [986].

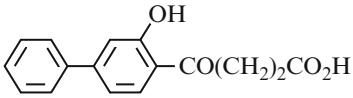
BIOLOGICAL ACTIVITY: Antiinflammatory [649].

Methyl ester of the methyl ether [54011-26-6] $C_{18}H_{18}O_4$ mol. wt. 298.34

m.p. 99–110° [986].

4-(5-Hydroxybiphenyl-4-yl)-4-oxo-1-butanoic acid

$C_{16}H_{14}O_4$ mol. wt. 270.28



Synthesis
-Also refer to: [986].

Methyl ether $C_{17}H_{16}O_4$ mol. wt. 284.31

-Obtained by condensation of 4-methoxydiphenyl with succinic anhydride in the presence of aluminium chloride in nitrobenzene in an ice bath. The mixture was stirred cold for 6 h at r.t. (60 %) [986].

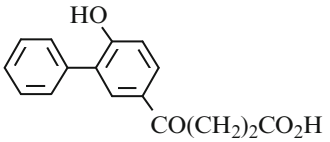
m.p. 155° [986].

Methyl ester $C_{18}H_{18}O_4$ mol. wt. 298.34

m.p. 48–49° [986].

4-(6-Hydroxybiphenyl-3-yl)-4-oxo-1-butanoic acid

[408336-52-7] $C_{16}H_{14}O_4$ mol. wt. 270.28



Synthesis
-Preparation by demethylation of its methyl ether with hydriodic acid in refluxing acetic anhydride for 20 min (84 %) [496].
m.p. 169–170° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether [408336-68-5] $C_{17}H_{16}O_4$ mol. wt. 284.31

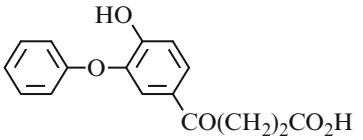
-Preparation by reaction of succinic anhydride with 2-methoxydiphenylmethane in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 131–132° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-(4-Hydroxy-3-phenoxyphenyl)-4-oxo-1-butanoic acid

$C_{16}H_{14}O_5$ mol. wt. 286.28



Synthesis
-Preparation by demethylation of its methyl ether [496].
m.p. 143° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether $C_{17}H_{16}O_5$ mol. wt. 300.31

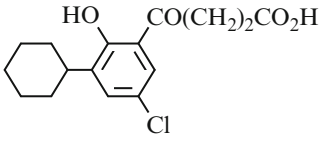
-Preparation by reaction of succinic anhydride with o-phenoxyanisole in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 158° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-(5-Chloro-3-cyclohexyl-2-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{16}H_{19}ClO_4$ mol. wt. 310.78



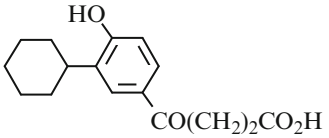
Synthesis
-Obtained by demethylation *in situ* in 5 % yield as the only product from the acylation of 2-cyclohexyl-4-chloro-anisole with succinic anhydride in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 174° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-(3-Cyclohexyl-4-hydroxyphenyl)-4-oxo-1-butanoic acid

[702701-04-0] $C_{16}H_{20}O_4$ mol. wt. 276.33



Synthesis
-Preparation by demethylation of its methyl ether [496].
m.p. 194° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether [412022-96-9] $C_{17}H_{22}O_4$ mol. wt. 290.36

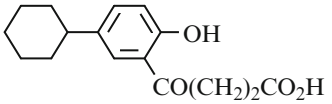
-Preparation by reaction of succinic anhydride with o-cyclohexylanisole in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 161° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-(5-Cyclohexyl-2-hydroxyphenyl)-4-oxo-1-butanoic acid

$C_{16}H_{20}O_4$ mol. wt. 276.33



Synthesis

-Preparation by demethylation of its methyl ether [496].

m.p. 126° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether [412033-83-1] $C_{17}H_{22}O_4$ mol. wt. 290.36

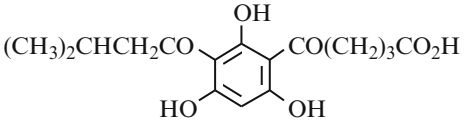
-Preparation by reaction of succinic anhydride with p-cyclohexylanisole in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 159–160° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

1-(3-Isovaleryl-2,4,6-trihydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{16}H_{20}O_7$ mol. wt. 324.33

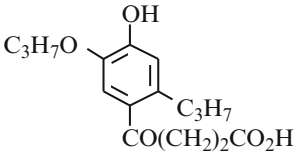


Synthesis

-Obtained by reaction of glutaric anhydride with 2-isovalerylphloroglucinol in the presence of boron trifluoride etherate at r.t. for 2 h (40–45 %) [338].

4-(4-Hydroxy-5-propoxy-2-propylphenyl)-4-oxo-1-butanoic acid

$C_{16}H_{22}O_5$ mol. wt. 294.35



Synthesis

-Refer to: [2196].

Methyl ether [41827-00-3]

$C_{17}H_{24}O_5$ mol. wt. 308.38

Methoxy-γ-oxo-5-propoxy-2-propylbenzene-butanoic acid

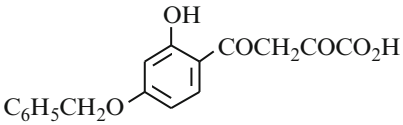
-Obtained by heating a mixture of 2-propoxy-5-propylanisole and succinic acid monomethyl ester in the presence of PPA at 50–55° for 40 min. Ice-water was added to the mixture, the resulting aqueous mixture was diluted with acetic acid and heated at 80–90° for 50 min [2196].

m.p. 70° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

4-(2-Hydroxy-4-(phenylmethoxy)phenyl)-2,4-dioxo-1-butanoic acid

$C_{17}H_{14}O_6$ mol. wt. 314.29



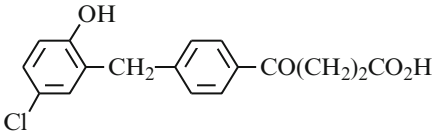
Synthesis
-Refer to: [1484].

Ethyl ester [860189-36-2]
$C_{19}H_{18}O_6$ mol. wt. 342.35

-Refer to: [1484]; m.p. 117.5–118° [1484].

4-[4-(5-Chloro-2-hydroxyphenylmethyl)phenyl]-4-oxo-1-butanoic acid

$C_{17}H_{15}ClO_4$ mol. wt. 318.76



Synthesis
-Preparation by demethylation of its dimethyl ether [496].
m.p. 200–201° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether $C_{18}H_{17}ClO_4$ mol. wt. 332.78

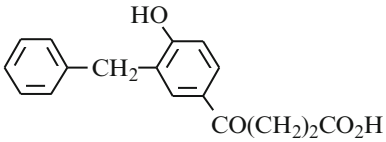
-Preparation by reaction of succinic anhydride with 5-Chloro-2-methoxydiphenylmethane in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 144–145° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-[3-(Phenylmethyl)-4-hydroxyphenyl]-4-oxo-1-butanoic acid

$C_{17}H_{16}O_4$ mol. wt. 284.31



Synthesis
-Preparation by demethylation of its methyl ether [496].
m.p. 185.5° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether $C_{18}H_{18}O_4$ mol. wt. 298.34

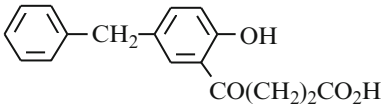
-Preparation by reaction of succinic anhydride with 2-methoxydiphenylmethane in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 133° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-[5-(Phenylmethyl)-2-hydroxyphenyl]-4-oxo-1-butanoic acid

$C_{17}H_{16}O_4$ mol. wt. 284.31



Synthesis
-Preparation by demethylation of its methyl ether [496].
m.p. 161° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether $C_{18}H_{18}O_4$ mol. wt. 298.34

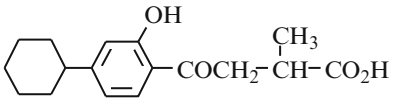
-Preparation by reaction of succinic anhydride with 4-methoxydiphenylmethane in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 121° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-(4-Cyclohexyl-2-hydroxyphenyl)-2-methyl-4-oxo-1-butanoic acid

$C_{17}H_{22}O_4$ mol. wt. 290.36



Synthesis
-Preparation by demethylation of its methyl ether [496].
m.p. 126° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether $C_{18}H_{24}O_4$ mol. wt. 304.39

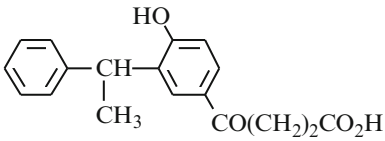
-Preparation by reaction of methylsuccinic anhydride (also named pyrotartaric anhydride) with p-cyclohexylanisole in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 151° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-[3-(1-Phenylethyl)-4-hydroxyphenyl]-4-oxo-1-butanoic acid

$C_{18}H_{18}O_4$ mol. wt. 298.34



Synthesis
-Refer to: [496].

Methyl ether

$C_{19}H_{20}O_4$ mol. wt. 312.37

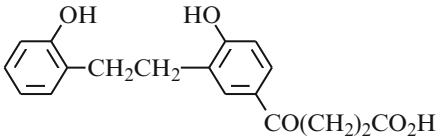
-Preparation by reaction of succinic anhydride with 2-(1-phenylethyl)anisole in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 150° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-[4-Hydroxy-3-(2-hydroxyphenetyl)phenyl]-4-oxo-1-butanoic acid

$C_{18}H_{18}O_5$ mol. wt. 314.34



Synthesis
-Preparation by demethylation of its dimethyl ether [496].
m.p. 147–148° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Dimethyl ether $C_{20}H_{22}O_5$ mol. wt. 342.39

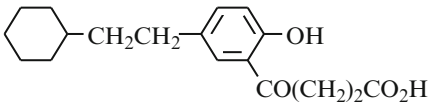
-Preparation by reaction of succinic anhydride with 2′,2″-dimethoxy-1,2-diphenylethane in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 143° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

4-[5-(2-Cyclohexylethyl)-2-hydroxyphenyl]-4-oxo-1-butanoic acid

$C_{18}H_{24}O_4$ mol. wt. 304.39



Synthesis
-Preparation by demethylation of its methyl ether [496].
m.p. 105.5° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Methyl ether $C_{19}H_{26}O_4$ mol. wt. 318.41

-Preparation by reaction of succinic anhydride with p-(β-cyclohexylethyl)anisole in the presence of aluminium chloride in nitrobenzene between 0 and 5° for 2 h [496].

m.p. 103° [496].

BIOLOGICAL ACTIVITY: Choleretic [496].

Chapter 3
Pentanones

1 Aromatic Hydroxyketones Derived from Pentanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-1,3-pentanedione

[35115-15-2] $C_{11}H_{12}O_3$ mol. wt. 192.21

Synthesis
-Refer to: [3083].
m.p. 60° [1297, 1298], ^{1}H NMR [2288].

Ethyl ether $C_{13}H_{16}O_3$ mol. wt. 220.27

-Obtained by reaction of 2-ethoxyacetophenone with ethyl propionate in the presence of sodium [3083].
-Also refer to: [2490].

m.p. 46° [2490], 44–45° [3083]; UV [3083].

Methyl ether $C_{12}H_{14}O_3$ mol. wt. 206.24

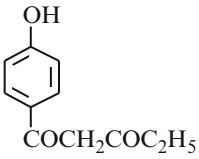
-Obtained by reaction of $CH_3CO(CH_2)_2COSeCH_3$ with anisole (20 %) [1750].

$b.p._{.0.8}$ 102° [1750]; ^{1}H NMR [1750], IR [1750], MS [1750].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_3

1-(4-Hydroxyphenyl)-1,3-pentanedione

[91143-26-9] $C_{11}H_{12}O_3$ mol. wt. 192.21



Synthesis
-Preparation from p-acetoxyacetophenone (59 %) [1538].
m.p. 43–44° [1538], 48° [675].

Copper salt $C_{22}H_{22}O_6Cu$ mol. wt. 447.53

m.p. 239–240° [1538].

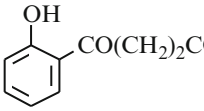
Methyl ether [54103-36-5] $C_{12}H_{14}O_3$ mol. wt. 206.24

-Obtained by reaction of $CH_3CO(CH_2)_2COSeCH_3$ with anisole (40 %) [1750].
-Also refer to: [1207, 2898].

$b.p._{\cdot 0.8}$ 102° [1750]; ^{1}H NMR [1750], IR [1750], MS [1750].

1-(2-Hydroxyphenyl)-1,4-pentanedione

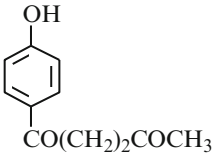
[16850-80-9] $C_{11}H_{12}O_3$ mol. wt. 192.21



Synthesis
-Refer to: [548].
m.p. 50° [548], ^{1}H NMR [548], IR [548], UV [548].

1-(4-Hydroxyphenyl)-1,4-pentanedione

$C_{11}H_{12}O_3$ mol. wt. 192.21



Synthesis
-Refer to: [1749].
m.p. 99–100° [3311], MS [2572].

Methyl ether [2108-54-5] $C_{12}H_{14}O_3$ mol. wt. 206.24

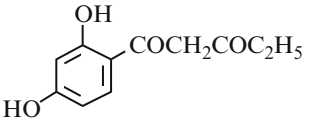
-Obtained by Friedel-Crafts acylation of anisole with $CH_3CO(CH_2)_2COSeMe$ during 3 min (60 %) [1749].
-Also obtained from acetaldehyde and 1-(4-methoxyphenyl)-2-propen-1-one (80 %) [2953].
-Also obtained by reaction of p-anisaldehyde with 3-buten-2-one in the presence of KOH and triethylamine in refluxing ethanol for 2 h (42.2 %) [2952].

-Also obtained by reaction of p-methoxyphenacyl bromide with ethyl acetoacetate in the presence of sodium metal in refluxing ethanol for 20 h (20.5 %) [1294].
-Refer to: [654, 1750, 1924, 2275, 2301, 2816 (46 %), 3358, 3392].

$b.p._{.0.6}$ 153–157° [2952], $b.p._{.0.8}$ 157–160° [2953], $b.p._{.4}$ 120–160° [1294];
m.p. 72° [2816], 58–59° [2952], 58° [2953], 55–57° [3358], 49–51° [3392], 46–48° [1294].
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [654, 1749, 1750, 1924, 2275, 2301, 2816, 2952, 2953, 3358],
^{13}C NMR [654, 3358, 3392],
IR [1294, 1749, 1750, 1924, 2275, 2301, 2816, 2952, 2953, 3358, 3392],
UV [1294, 2275], MS [2816].

1-(2,4-Dihydroxyphenyl)-1,3-pentanedione

$C_{11}H_{12}O_4$ mol. wt. 208.21



Synthesis
-Refer to: [3083].

Diethyl ether $C_{15}H_{20}O_4$ mol. wt. 264.32

-Obtained by reaction of 2,4-diethoxyacetophenone with ethyl propionate in the presence of sodium [3083].
-Refer to: [1741].

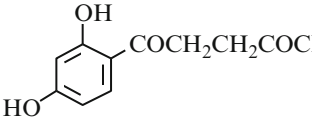
m.p. 74–75° [1741, 3083], UV [3083].

Dimethyl ether $C_{13}H_{16}O_4$ mol. wt. 236.27

m.p. 72° [1297].

1-(2,4-Dihydroxyphenyl)-1,4-pentanedione

$C_{11}H_{12}O_4$ mol. wt. 208.21



Synthesis
-Refer to: [2953].

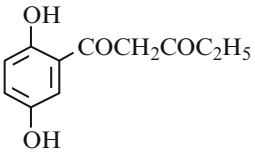
Dimethyl ether [67756-19-8]
$C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained from acetaldehyde and 1-(2,4-dimethoxyphenyl)-2-propen-1-one (73 %) [2953].

m.p. 63° [2953], ^{1}H NMR [2953], IR [2953].

1-(2,5-Dihydroxyphenyl)-1,3-pentanedione

$C_{11}H_{12}O_4$ mol. wt. 208.21



Synthesis
-Refer to: [3083].

Diethyl ether

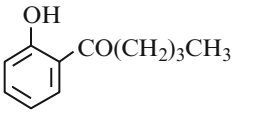
$C_{15}H_{20}O_4$ mol. wt. 264.32

-Obtained by reaction of 2,5-diethoxyacetophenone with ethyl propionate in the presence of sodium [3083].
-Refer to: [1741].

m.p. 49° [1741], 47–48° [3083], UV [3083].

1-(2-Hydroxyphenyl)-1-pentanone

[18430-91-6] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses
-Obtained by reaction of valeryl chloride with phenol in the presence of aluminium chloride at 125–130° for 1 h (56 %) [2700].
-Also obtained by reaction of valeric acid with phenol,
*in the presence of zinc chloride boiling for five min (by-product) [726];
*in the presence of zeolite [3266].
-Also obtained by treatment of 1-(2-hydroxyphenyl)-1-pentanol with manganese dioxide in methylene chloride for 7 h at r.t. (40 %) [77].
-Also obtained by photolysis of phenyl valerate in the presence of oxygen and β-cyclodextrin in aqueous solution for 1 h at 25° (20 %) [3216].
-Also obtained by Fries rearrangement of phenyl valerate with aluminium chloride,
*at 140° for 45 min (37 %) [932];
*in refluxing carbon disulfide for 2 h, then at 130–140° for 3 h, after solvent elimination [2587];
*in refluxing petroleum ether under nitrogen for 3 h (36 %) [3255].
-Also obtained [2478] by the method [2074].
-Also refer to: [1331, 1681, 3156, 3464].

colourless oil [77];
b.p.$_{0.1}$ 74° [932]; b.p.$_{10}$ 130° [2700]; b.p.$_{15}$ 138–141° [2478];
^{1}H NMR (Sadtler standard N° 38629M) [77, 3255], ^{13}C NMR [77],
IR (Sadtler standard N° 65678K) [77], UV [1996],
MS [77, 3255]; TLC [1994].

2,4-Dinitrophenylhydrazone [17744-53-5] $C_{17}H_{18}N_4O_5$ mol. wt. 358.35

m.p. 278–279° [524], 179° [2587], 178° [932].
N.B.: One of the reported melting point is obviously wrong.

Compound with β-cyclodextrin (1:1) [264615-37-4]

-Refer to: [3215].

^{1}H NMR [3215], UV [3215].

Acetate [97037-81-5] $C_{13}H_{16}O_3$ mol. wt. 220.27

-Obtained by action of butylmagnesium bromide with acetylsalicoyl chloride in ether at 0–5° [2587].
-Also refer to: [1037].

b.p.$_{0.5}$ 113° [1037]; ^{1}H NMR [1037], IR [1037].

Methyl ether [20359-54-0] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Preparation by addition of the appropriate substituted phenyl Grignard to valeronitrile [3254].
-Also obtained by adding n-butyllithium in ether to 2-methoxybenzaldehyde o-methyloxime in THF at 0° for 1 h (80 %) [1476].
-Also obtained by hydrolysis of alkenyl sulfides (35 %) [3040].
-Also obtained from 2-methoxybenzaldehyde (4 steps) (91 %) [264].
-Also refer to: [1036, 1084, 1117, 1378, 1626, 2068, 2094, 2343, 2848, 3156].

yellow oil [264];
b.p.$_{0.1}$ 82° [1036]; b.p.$_7$ 142° [3254];
^{1}H NMR [264, 1036, 1117, 1378, 1626, 2068, 2848],
^{13}C NMR [1378, 1626], IR [264, 1036, 1378, 2068],
UV [3254], MS [264, 1117, 1378, 3254];
ESR spectroscopy [3254], Phosphorescence spectroscopy [3254].

2,4-Dinitrophenylhydrazone of the methyl ether

[64957-70-6] $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 126.4–126.6° [2068].

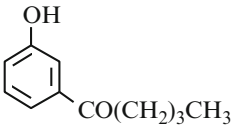
Benzyl ether [127154-56-7] $C_{18}H_{20}O_2$ mol. wt. 268.36

-Obtained by treatment of the potassium salt with benzyl chloride in refluxing methanol for 2 h (53 %) [3255].

white platelets [3255]; m.p. 26–28° [3255];
^{1}H NMR [3255], ^{13}C NMR [3255], IR [3255], UV [3255], MS [3255].

1-(3-Hydroxyphenyl)-1-pentanone

[62810-51-9] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses

-Synthesis of 3-hydroxyvalerophenone by means of organocadmium derivatives (75 %) [2586].

-Also obtained by treatment of its methyl ether with aluminium chloride in benzene by heating on a water bath for 2 h (80 %) [966].

-Also obtained in the same reaction that acetate below (25 %) [246].

-Also refer to: [1614, 1618].

b.p.$_{1.2}$ 165° [2586]; m.p. 67° [966, 2586]; ^{1}H NMR [1614, 1618].

Acetate [195393-34-1] $C_{13}H_{16}O_3$ mol. wt. 220.27

-Also obtained (**10**) by reaction of 1-acetoxy-5-pentanoyl-1,3-cyclohexadiene tricarbonyl-iron complex **8** with triethylamine N-oxide in DMA at r.t. for 1 h (57 %) [246].

b.p.$_1$ 132–134° [2586].

Methyl ether [20359-55-1] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Obtained by condensation of butylmagnesium bromide with m-methoxybenzamide in ethyl ether. The reaction was carried out at 60° for 48 h under hydrogen atmosphere (60–70 %) [966].

-Also obtained by addition of n-butylmagnesium bromide to m-methoxybenzonitrile [3254].

-To lithium 3-methoxybenzoate, n-butyllithium in hexane was added and the mixture stirred for 2 h [273].

-Also obtained by introduction of 3-methoxybenzoyl chloride into n-butyllithium in ether at −78°, previously added to cuprous iodide at 0°. After stirring 15 min at −78° methanol was added and the mixture allowed to reach ambient temperature (79 %) [273].

-Also refer to: [1023, 1201, 1202, 1204, 1614, 1618, 2759, 3252].

b.p.$_1$ 105–108° [273]; b.p.$_6$ 134° [3254], b.p.$_{30}$ 190° [966, 967];
^{1}H NMR [273, 1614, 1618], IR [273], UV [3254], MS [3254];
ESR spectroscopy [3254], Phosphorescence spectroscopy [3254].

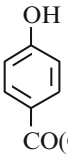
USE: In preparation of platelet activating factor antagonists [1203].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 147° [967].

1-(4-Hydroxyphenyl)-1-pentanone

[2589-71-1] $C_{11}H_{14}O_2$ mol. wt. 178.23



Syntheses

-Phenol was energetically mixed with finely divided aluminium chloride (1 mol) and heated to 100° (1 mol of hydrochloric acid is evolved); 1 mol of n-valeroyl chloride was then added and heated to 125–130° for 1 h (29 %) [2700].

-Also obtained by reaction of valeroyl chloride with phenol in the presence of aluminium chloride,
*in methylene chloride for 14 h at r.t. (45 %) [1910];
*in nitrobenzene [2923], first at 5–10°, then at r.t. overnight (87 %) [686], (72 %) [2970].
-Also obtained by reaction of valeric acid with phenol,
*in the presence of zinc chloride (5 %) [726];
*in the presence of polyphosphoric acid for 15 min on a water bath (47 %) [2240] or for 10 min at 100° (58 %) [2238].
-Also obtained by Fries rearrangement of phenyl valerate,
*in the presence of polyphosphoric acid for 10 min at 100° (40 %) [2238];
*in the presence of aluminium chloride at 140° for 45 min (41 %) [932], in nitrobenzene [1116, 2923] or in refluxing carbon disulfide for 2 h, then at 130–140° for 3 h, after solvent elimination (22 %) [2587].
-Also obtained [2478] by the method [2074].
-Also obtained by photolysis of phenyl valerate in the presence of oxygen and β-cyclodextrin in aqueous solution for 1 h at 25° (6.4 %) [3216].
-Also obtained by reaction of 4-iodophenol with n-Bu_3In in the presence of Pd $(PPh_3)_4$ in THF at 66° under atmospheric pressure of CO gas (64 %) [1851].
-Also refer to: [44, 62, 275, 556, 636, 868, 914, 1380, 1384, 1510, 1615–1617, 1936, 2043, 2732, 2861, 3165, 3254, 3379, 3454, 3471].

Isolation from natural sources

-Determination in coal extracts obtained from supercritical gas extraction by toluene [2330].

b.p.$_{0.6–0.8}$ 150–160° [686], b.p.$_{0.01}$ 156–158° [2970], b.p.$_1$ 160° [932];
b.p.$_{0.4}$ 167° [2587], b.p.$_{10}$ 197.5–198.5° [2700], b.p.$_{15}$ 210° [726]; b.p.$_{16}$ 213° [2478];
white solid [1910];
m.p. 77° [2240], 63–64° [2478], 63° (Sadtler standard N° 65672K) [2700], 62–64° [3254], 62–63° [726, 1910], 62° [932];
^{1}H NMR [1910], (Sadtler standard N° 38623M), ^{13}C NMR [1910], IR [1910], (Sadtler standard N° 65672K), UV [1995], MS [1910, 2330]; X-ray data [1936]; GC-MS [2330]; TLC [1910, 1994].
Cryoscopic study [182].
ESR spectroscopy [3254], Phosphorescence spectroscopy [3254].

USE: Preparation of pyrovalerone analogs as monoamine uptake inhibitors [2043]. Synthesis of nonsteroidal antiinflamatory and analgesic drugs by Beckmann rearrangement of oximes with zeolites and mesoporus molecular sieve catalysts [684].

BIOLOGICAL ACTIVITY: Inhibition of 17-β-hydroxysteroid dehydrogenase 3 [1910].

Oxime [864072-49-1] $C_{11}H_{15}NO_2$ mol. wt. 193.25

USE: Synthesis of nonsteroidal antiinflamatory and analgesic drugs by Beckmann rearrangement of oximes with zeolites and mesoporus molecular sieve catalysts [684].

2,4-Dinitrophenylhydrazone $C_{17}H_{18}N_4O_5$ mol. wt. 358.35

m.p. 182° [932].

Nicotinylhydrazone $C_{17}H_{19}N_3O_2$ mol. wt. 297.36

m.p. 152° [520, 521].

USE: In chemotherapy of leprosy [520, 521].

isoNicotinylhydrazone $C_{17}H_{19}N_3O_2$ mol. wt. 297.36

m.p. 206° [520, 521].

USE: In chemotherapy of leprosy [520, 521].

Compound with β-cyclodextrin (1:1) [264615-38-5]

-Refer to: [3215].

^{1}H NMR [3215], UV [3215].

Benzyl ether [35081-44-8] $C_{18}H_{20}O_2$ mol. wt. 268.36

-Preparation by reaction of benzyl chloride with p-hydroxyvalerophenone in the presence of potassium carbonate and potassium iodide in refluxing 90 % ethanol for 5 h (95 %) [556].

m.p. 65° [556].

Methyl ether [1671-76-7] $C_{12}H_{16}O_2$ mol. wt. 192.26

-Obtained by direct acylation of 4-bromoanisole with valeraldehyde by palladium catalysis (91 %) [2668].
-Also obtained by reaction of valeryl chloride with anisole [1853],
*in the presence of aluminium chloride (100 %) [742] in 1,2-ethylene chloride [2942], first at 0° for 40 min, then at r.t. for 8–15 h (73 %) [2243];

*in the presence of Si-Fe catalyst at 25° (25 %) [427].
-Also obtained by Et_2Zn-mediated rearrangement of a bromohydrin, the 2-bromo-1-(4-methoxy-phenyl)-1-pentanol (85 %) [1865].
-Also obtained by reaction of valeric anhydride with anisole,
*in the presence of aluminium chloride in boiling carbon disulfide for 30 min (85 %) [2297];
*in the presence of microcrystalline beta zeolite-II for 3 h at 130° under argon (89 %) [1594];
*in the presence of $SbCl_5$-$LiClO_4$ mixture in refluxing methylene chloride for 30 min (85 %) [2176].
-Also obtained by reaction of methyl iodide with 4-hydroxyvalerophenone in the presence of potassium carbonate in refluxing acetone [2043].
-Also obtained by reaction of dimethyl sulfate with 4-valerylphenol in the presence of aqueous sodium hydroxide for 4 h at reflux [2478].
-Preparation from 4-bromoanisole and valeric anhydride using cobalt catalysis [1656].
-Also obtained by reaction of 4-iodoanisole with n-Bu_3In in the presence of Pd $(PPh_3)_4$ in THF at 66° under atmospheric pressure of CO gas (77 %) [1851].
-Also obtained by oxidation of bis(4-methoxybenzyl)-1-butanol with bis (sym-collidine)bromine hexafluorophosphate (BBH) in methylene chloride at r.t. (83 %) [2659].
-Also obtained from N-methoxy-N-methyl-2-pyridyl urethane and p-methoxyphenylmagnesium bromide (96 %) [1850].
-Also obtained by reaction of 2-chloro-1-(trimethylsilyl)-1-pentanone with anisole in the presence of titanium tetrachloride (77 %) [1354].
-Also obtained by adding n-butyllithium in ether to 4-methoxybenzaldehyde o-methyloxime in THF at 0° for 1 h (76 %) [1476].
-Also obtained by reaction of n-butyllithium with 4-methoxybenzaldehyde in refluxing methylene chloride/toluene mixture for 16 h (56 %) [1329].
N.B.: Toluene was added to the mixture which was kept at −78° for 2 h after the addition of an aldehyde.
-Preparation from organocopper reagent with n-butyryl chloride and 4-iodoanisole (63 %) [2622].
-Also obtained by hydrolysis of alkenyl sulfides (55 %) [3040].
-Also obtained by reaction of 4-methoxyphenyl n-pentyl dithiolane with P_2I_4 in acetic anhydride for 9 h at r.t. (53 %) [2864].
-Also refer to: [531, 619, 667, 698 (68 %), 944, 950, 970, 1023, 1200, 1202, 1249, 1266, 1849, 1941, 2106, 2240, 2279, 2322, 2357 (84 %), 2723, 2862, 2980, 3214, 3247, 3248, 3252, 3262, 3264, 3265, 3456, 3472].

yellow oil [2243]; oil [742];
b.p.$_{0.5}$ 113° [1354]; b.p.$_{.2}$ 115° [1853]; b.p.$_{.6}$ 143° [531, 3254]; b.p.$_{.6}$ 150.5° [2297], b.p.$_{.12}$ 162° [2240], b.p.$_{.19}$ 175–178° [2478]; b.p.$_{.739}$ 300° [2297];
m.p. 28° [2240], 27–28° [3214], 26° [2901], 22–23.5° [1103];

^{1}H NMR [698, 1354, 1656, 1850, 1865, 2243, 2357, 2622],
^{13}C NMR [698, 1354, 1656, 2357, 2622],
IR [698, 1354, 1850, 2357, 2622], UV [2815, 3247, 3254],
MS [698, 1656, 3254]; GC/MS [2357].

USE: Preparation of high purity 4-n-pentylphenol [3456]; Rhodium-catalyzed allylation of aldehydes with homoallylic alcs. by retroallylation and isomerization to satd. ketones with conventional or microwave heating [2980]; Preparation of pyrovalerone analogs as monoamine uptake inhibitors [2043].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 154–155° [3214].

Propyl ether $C_{14}H_{20}O_2$ mol. wt. 220.31

-Obtained by reaction of valeryl chloride with phenyl propyl ether in the presence of zinc chloride at reflux for 30 min (44.5 %) [1237].

b.p.$_{.15}$ 193–198° [1237]; m.p. 20–21° [1237].

Oxime of the propyl ether $C_{14}H_{21}NO_2$ mol. wt. 235.33

m.p. 58° [1237].

Butyl ether [101100-66-7] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Refer to: [3352].

b.p.$_{.3}$ 178° [1235]; m.p. 20° [1235].

Pentyl ether [93156-87-7] $C_{16}H_{24}O_2$ mol. wt. 248.37

-Refer to: [3352].

b.p.$_{.1}$ 183° [1236]; m.p. 27° [1236].

Hexyl ether [93542-23-5] $C_{17}H_{26}O_2$ mol. wt. 262.39

-Refer to: [3351, 3352].

b.p.$_{.8}$ 210° [1236]; m.p. 19° [1236].

4-Hydroxyphenylethyl ether

[109720-03-8], (CA **107**, 175432x); [113279-26-8] $C_{19}H_{22}O_3$ mol. wt. 298.38

-Obtained by reaction of 1-bromo-2-[4-(trimethylsiloxy)phenyl]ethane with 4-hydroxy-valerophenone in the presence of potassium carbonate in refluxing acetone for 17 h [2732].
-Also refer to: [1853].

m.p. 95–96° [2732]; ^{1}H NMR [2732], IR [2732].

4-Methoxyphenylethyl ether

[109720-05-0], (CA **107**, 175432x); [113279-27-9] $C_{20}H_{24}O_3$ mol. wt. 312.40

-Obtained by reaction of 4′-methoxy-2-phenethyl bromide with 4-hydroxyvalerophenone in the presence of potassium carbonate in refluxing acetone for 17 h [2732].
-Also refer to: [1853].

m.p. 49–50° [2732]; ^{1}H NMR [2732], IR [2732].

Trifluoromethyl ether [79619-25-3] $C_{12}H_{13}F_3O_2$ mol. wt. 246.23

-Obtained by reaction of n-butylmagnesium bromide with p-(trifluoromethoxy) benzonitrile in ethyl ether at r.t. overnight [3251].

b.p.$_{4.5}$ 106–107° [3251]; ^{1}H NMR [3251], UV [3251], MS [3251].

N.B.: Electronic and phosphorescence spectrum and triplet energy [3251].

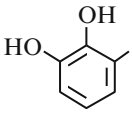
Ten various unsaturated ethers (photolysis of, triplet quenching in,) [3248].

3-Butenyl ether	[108919-69-3]	$C_{15}H_{20}O_2$	mol. wt. 232.32
5-Hexenyl ether	[108919-74-0]	$C_{17}H_{24}O_2$	mol. wt. 260.38
3-Methyl-3-butenyl ether	[108919-70-6]	$C_{16}H_{22}O_2$	mol. wt. 246.35
5-Methyl-4-hexenyl ether	[108919-68-2]	$C_{18}H_{26}O_2$	mol. wt. 274.40
4-Methyl-3-pentenyl ether	[108919-72-8]	$C_{17}H_{24}O_2$	mol. wt. 260.38
3-Pentenyl ether	[108919-67-1]	$C_{16}H_{22}O_2$	mol. wt. 246.35
3-Pentenyl ether (Z)	[108919-71-7]	$C_{16}H_{22}O_2$	mol. wt. 246.35
4-Pentenyl ether	[108919-73-9]	$C_{16}H_{22}O_2$	mol. wt. 246.35
2-Propenyl ether	[108919-66-0]	$C_{14}H_{18}O_2$	mol. wt. 218.30
10-Undecenyl ether	[108919-75-1]	$C_{22}H_{34}O_2$	mol. wt. 330.51
Benzoate	$C_{18}H_{18}O_3$		mol. wt. 282.33

m.p. 92° [2700].

1-(2,3-Dihydroxyphenyl)-1-pentanone

[862666-33-9] $C_{11}H_{14}O_3$ mol. wt. 194.23



Synthesis
-Obtained by deprotection of its dimethyl ether with boron tribromide in methylene chloride at 0°. Then, the mixture was stirred overnight at r.t. (68 %) [82].

brown solid [82]; m.p. 50° [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

USE: Reactant for preparation of lithium gallium/titanium ketone complexes [82].

Dimethyl ether [15122-00-6] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Obtained by treatment of 1-(2,3-dimethoxyphenyl)-1-pentanol in acetone with potassium dichromate in dilute sulfuric acid (Jones reagent) at r.t. for 3 h (23 %) [82].
-Obtained by oxidation of 1-(2,3-dimethoxyphenyl)-1-pentanol with sodium dichromate in dilute sulfuric acid (73–83 %) [2747].
-Also refer to: [82, 2747].

colourless oil [82]; pale yellow viscous oil [2747]; b.p.$_{0.08\text{-}0.1}$ 90.5–93.5° [2747];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

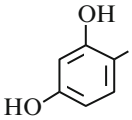
2,4-Dinitrophenylhydrazone of the dimethyl ether

[15116-05-9] $C_{19}H_{22}N_4O_6$ mol. wt. 402.41

m.p. 138–139° [2747].

1-(2,4-Dihydroxyphenyl)-1-pentanone

[15116-13-9] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Preparation by reaction of valeric acid with resorcinol, *in the presence of boron trifluoride [2382] for 2 h at 70° (79 %) [2312];

*in the presence of zinc chloride [(51 %) 2294, (68–78 %) 2501, 2702, (82 %) 2747, (60 %) 2889].
-Also refer to: [22, 893, 1628, 1629, 2114, 2842, 3127].

yellow viscous oil [2747];
b.p.$_{0.2}$ 111–114° [2747], b.p.$_{6\text{-}7}$ 190–192° [893, 2842];
m.p. 63° [2114, 2294, 2312], 62° [2889], 58.5–60° [893, 2842];
^{1}H NMR [2889], IR [2382], UV [2382]; pK_a 5.39 [2889].

USE: As antioxidant for vitamin A [1628, 1629]; As fungicide for soy sauce [1053]; Antiseptic and germicidal product [2734]; Antifungal activity [2114]; In detn. of uranium by spectrophotometry [2891].

Oxime *(DHVOX)* [57991-55-6] $C_{11}H_{15}NO_3$ mol. wt. 209.25

white solid [2890]; m.p. 170° [2890].

Metal complexes of 2,4-dihydroxyvalerophenone oxime [2890].

$Pd(C_{11}H_{14}NO_3)_2$	yellow	m.p. 250° (d)	IR, UV
$Cu(C_{11}H_{14}NO_3)_2$	buff	m.p. 245° (d)	IR, UV
$Ni(C_{11}H_{14}NO_3)_2$	light green	m.p. 230° (d)	IR, UV
$Co(C_{11}H_{14}NO_3)_2$	dark brown	m.p. 241° (d)	IR, UV
$Mn(C_{11}H_{14}NO_3)_2$	brownish black	m.p. 165° (d)	IR, UV
$VO(C_{11}H_{14}NO_3)_2$	black	m.p. 100° (d)	IR, UV
$UO_2(C_{11}H_{14}NO_3)_2$	orange	m.p. 180° (d)	IR, UV
$MoO_2(C_{11}H_{14}NO_3)_2$	orange yellow	m.p. 175° (d)	IR, UV

Semicarbazone $C_{12}H_{17}N_3O_3$ mol. wt. 251.29

m.p. 175° [2294].

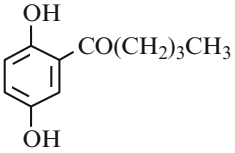
Dimethyl ether [854659-33-9] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Obtained by treatment of the title ketone with methyl iodide [2294].
-Also obtained by hydrolysis of 4,6-dimethoxy-3-butylidenephthalide in acetone with concd. HCl, followed by the decarboxylation with Cu dust [2294].

m.p. 38.5° [2294].

1-(2,5-Dihydroxyphenyl)-1-pentanone

[4693-17-8] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Obtained by Friedel-Crafts acylation of hydroquinone with valeryl chloride in the presence of aluminium chloride [1442].
-Also obtained by reaction of valeric acid with hydroquinone in the presence of zinc chloride (Nencki reaction) (17 %) [150].

-Also refer to: [1325, 2102, 2540, 2896, 2955, 3204, 3394].

$b.p._{.3}$ 161–162° [1325], $b.p._{.4}$ 161–163° [150]; $b.p._{.2}$ 174–176° [2955];
$b.p._{.15}$ 180–185° [1442];
m.p. 62° [3204], 61–62.5° [2102].

Semicarbazone $C_{12}H_{17}N_3O_3$ mol. wt. 251.29

m.p. 189–190° [150].

2-Acetate $C_{13}H_{16}O_4$ mol. wt. 236.27

-Refer to: [1, 900].

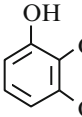
Dimethyl ether [38843-82-2] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Obtained by reaction of valeric acid with p-dimethoxybenzene, in the presence of polyphosphoric acid. The resulting deep was heated on the steam bath for 3 h (30 %) [2878].
-Also obtained by reaction of valeroyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [3073],
*in methylene chloride at r.t. for 1 h (30 %) [2878];
*in carbon disulfide at 20–25° for 2.5 h (70 %) [2234].
-Also refer to: [2874, 2896].

pale amber oil [2878]; pale yellow liquid [2234];
b.p.$_{0.6}$ 142° [2234], b.p.$_{20}$ 185° [2874], b.p.$_{20}$ 188–192° [2878];
m.p. 63° [2874]; IR [2234, 2878].

1-(2,6-Dihydroxyphenyl)-1-pentanone

[63411-80-3] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Obtained from 2,6-dihydroxyacetophenone (54 %) [385].
-Also obtained by treatment of 4-methyl-7-hydroxy-8-n-valerylcoumarin with a 16 % aqueous sodium hydroxide solution at reflux for 4 h under nitrogen (88 %) [26].

-Also refer to: [32, 329].

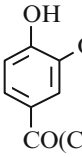
m.p. 85–86° [26, 32], 85° [329], 78–79° [385].

Dimethyl ether $C_{13}H_{18}O_3$ mol. wt. 222.28

b.p.$_{15}$ 172–175° [329].

1-(3,4-Dihydroxyphenyl)-1-pentanone

[2525-01-1] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Obtained by Fries rearrangement of guaiacol valerate with aluminium chloride in nitrobenzene (by-product) [726].
-Also obtained by Fries rearrangement of pyrocatechol divalerate with aluminium chloride in the presence of pyrocatechol for 4.5 h at 135–140° (50 %) [2075].

-Also obtained by Fries rearrangement of pyrocatechol valerate [3056].
-Also refer to: [27, 946, 1262].

b.p.$_{.4}$ 210–220° [2075], b.p.$_{.15}$ 230–240° [726], b.p.$_{.10}$ 245–255° [3056];
m.p. 143–144° [726], 100–101° (dilute dioxane) or 93–94° (benzene) [2075], 99–100° [27], 97° [946, 1262].
N.B.: One of the reported melting point is obviously wrong.

O-Methyloxime [474668-86-5] $C_{12}H_{17}NO_3$ mol. wt. 223.27

-Refer to: [3177].

Dimethyl ether [66053-97-2] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Obtained by Friedel-Crafts acylation of 3,4-dimethoxybenzene with pentanoic acid anhydride, Lewis acids and silver salts as catalysts [2180].
-Also obtained by reaction of valeryl chloride with veratrole in the presence of zinc chloride in refluxing carbon disulfide at 60° for 4 h (51.8 %) [2837].
-Also obtained from 3,4-dimethoxybenzaldehyde (4 steps) (92 %) [264].
-Also refer to: [1249, 1277, 1947, 2043, 2172, 2174, 2175, 2183, 2997, 2999].

viscous liquid [2837];
b.p.$_{0.05}$ 131° [1947]; b.p.$_{1}$ 160° [2837];
^{1}H NMR [264, 1249, 1947, 2999], ^{13}C NMR [1249, 2999],
IR [264, 1249, 2999], MS [264].

USE: Preparation of pyrovalerone analogs as monoamine uptake inhibitors [2043].

Oxime of the dimethyl ether [100619-32-7] $C_{13}H_{19}NO_3$ mol. wt. 237.30

-Refer to: [2183, 2837].

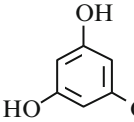
viscous oil [2837]; ^{1}H NMR [2182], ^{13}C NMR [2182].

Semicarbazone of the dimethyl ether [101778-12-5] $C_{14}H_{21}N_3O_3$ mol. wt. 279.34

colourless needles [2837]; m.p. 179° [2837].

1-(3,5-Dihydroxyphenyl)-1-pentanone

[70627-61-1] $C_{11}H_{14}O_3$ mol. wt. 194.23



Syntheses
-Obtained by treatment of its diacetate with 5 % sodium hydroxide at reflux for 4.5 h (63 %) [1406].
-Also obtained by treatment of its dimethyl ether with pyridinium chloride at 220° for 15 min (66 %) [2318].
-Also obtained by reaction of 3,5-diacetoxybenzoyl chloride with dibutylcadmium, followed by hydrolysis [227].

-Also obtained by reaction of n-butylmagnesium bromide with 3,5-bis-trimethylsilyloxy-benzamide in the presence of a crystal of iodine in refluxing ethyl ether for 48 h under nitrogen atmosphere (85 %) [259].
-The 3,5-dihydroxyphenyl *n*-butyl ketone was synthesized by the known method [1406] in four steps starting from 3,5-dihydroxybenzoic acid [3180].
-Also refer to: [1873 (Chinese paper)].

Isolation from natural sources

-From the roots and stems of *Ardisia virens* Kurz (Myrsinaceae) [607].

m.p. 119° [1406], 118° [3180], 116–117° [2318]; ^{1}H NMR [2318], IR [2318].

2,4-Dinitrophenylhydrazone [101593-70-8] $C_{17}H_{18}N_4O_6$ mol. wt. 374.35

m.p. 247° (d) [1406].

Diacetate [101103-45-1] $C_{15}H_{18}O_5$ mol. wt. 278.30

-Preparation by reaction of dibutylcadmium with 3,5-diacetoxybenzoyl chloride in refluxing benzene for 1 h (82 %) [1406].

b.p.$_{0.1}$ 146–153° [1406], b.p.$_{0.5}$ 178–182° [1406];
$n_D^{20} = 1.5097$ [1406].

2,4-Dinitrophenylhydrazone of the diacetate

[112441-56-2] $C_{21}H_{22}N_4O_8$ mol. wt. 458.43

m.p. 163° [1406].

Dimethyl ether [5333-29-9] $C_{13}H_{18}O_3$ mol. wt. 222.28

-Provided by reductive alkylation (zinc amalgam) of 3,5-dimethoxybenzamide [1873 (Chinese paper)].
-A reaction of 3,5-dimethoxybenzoic acid with lithium hydride gave a salt, which was acylated by butyllithium to synthesize 1-(3,5-dimethoxyphenyl)-1-pentanone [3357], in 83–85 % yield [227, 3356].
-Also obtained by reaction of n-butylmagnesium bromide with N-trimethylsilyl 3,5-dimethoxy-benzamide in the presence of a crystal of iodine in refluxing ethyl ether for 72 h under nitrogen atmosphere (low yield) [259].
-Also obtained by treatment of ethyl 3,5-dimethoxybenzoylpropylacetate with 6 % sulfuric acid for 1 h at 195° (82 %) [149].
-Preparation by reaction of butylmagnesium bromide with 3,5-dimethoxybenzamide in refluxing ethyl ether for 5 h (80 %) [2990].
-Also obtained by treatment of 3,5-dimethoxybenzoic acid with n-butyllithium at r.t. (95 %) [2900].
-Also obtained by treatment of "methyläther-lobaritonsäure" with bronze in quinoline for 5 min at 215° [150].

-Preparation: n-butyl bromide was added to Li metal and a crystal of iodine in ether at 0°. Then, N,N-diethyl-3,5-dimethoxybenzamide in ether was added at −25°, then maintained the temperature at −10° for 2 h, and 5 h at 0° then at r.t. for 11 h (60.4 %) [1119].
-Oxidation potential of [33].
-Preparation from 1,3-dimethoxybenzene (92 %) [2792].

-Also refer to: [213 (19 %), 273 (84 %), 983, 1119, 1764, 1988 (11 %), 2209, 2575, 2793 (96 %), 2990, 3340, 3341].

pale yellow solid [2793];
b.p.$_{.3}$ 140–142° [213], b.p.$_{0.3}$ 150° [273]; b.p.$_{.11}$ 175–177° [2990];
m.p. 53° [2990], 42.5° [2990], 42–44° [227], 42–43° [33, 149, 150], 39–41° [1988], 38–39° [1119], 37–40° [259], 34–36° [273];
^{1}H NMR [227, 259, 273, 983, 2209, 2793, 2900],
^{13}C NMR [2209], IR [227, 983, 1119, 2209], MS [983].

USE: Preparation of cannabinoid derivatives as cannabinoid receptor agonists or antagonists [983].

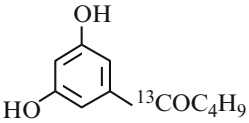
Dimethyl ether-1-^{14}C
(Dimethoxy-3,5-phenyl)-1-pentanone-(^{14}C-1)

[54109-33-0] $C_{12}{}^{(14)}CH_{18}O_3$ mol. wt. 224.27

-Refer to: [2265]; ^{1}H NMR [2265], MS [2265].

1-(3,5-Dihydroxyphenyl)-1-pentanone-1-^{13}C

$C_{10}{}^{(13)}CH_{14}O_3$ mol. wt. 195.22



Synthesis
-Refer to: [2507].

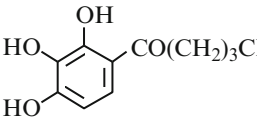
Dimethyl ether [98631-68-6]
$C_{12}{}^{(13)}CH_{16}O_3$ mol. wt. 222.28

-Obtained by reaction of [carboxy-^{13}C]-3,5-dimethoxybenzoic acid with n-butyllithium (98 %) [2507].
-Also refer to: [149].

m.p. 42–43° [149], 39–41° [2507].

1-(2,3,4-Trihydroxyphenyl)-1-pentanone

[43043-25-0] $C_{11}H_{14}O_4$ mol. wt. 210.23



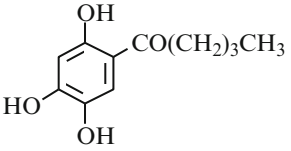
Syntheses
-Obtained by reaction of valeric acid with pyrogallol in the presence,
*of zinc chloride [214, 2678], at 140–145° for 4 h (70 %) [506];

*of boron trifluoride in ethyl ether at 0° for 1 h (88 %) [540].
-Also refer to: [1260].

yellow needles [1260]; b.p.$_{14}$ 202–204° [506];
m.p. 108° [214, 2678], 84–84.5° [1260], 82° [540]; UV [540].

1-(2,4,5-Trihydroxyphenyl)-1-pentanone

[62060-62-2] $C_{11}H_{14}O_4$ mol. wt. 210.23



Syntheses
-Obtained by reaction of valeryl chloride with 1,2,4-trihydroxybenzene in the presence of aluminium chloride in nitrobenzene at r.t. for several hrs. and heated 0.5 h at 65° [290].
-Also refer to: [771, 1508].

m.p. 151–153° [290]; ^{13}C NMR [1508].

USE: Antioxidant in fats and oils [290].

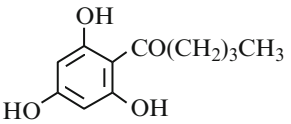
Trimethyl ether [90834-05-2] $C_{14}H_{20}O_4$ mol. wt. 252.31

-Obtained by reaction of pentanoyl chloride with 1,2,4-trimethoxybenzene in the presence of aluminium chloride (60–74 %) [771].
-Also obtained by reaction of valeric acid with 1,2,4-trimethoxybenzene in the presence of polyphosphoric acid for 4 h at 45–50° [2695].
-Also obtained by reaction of valeric anhydride with 1,2,4-trimethoxybenzene in the presence of aluminium chloride in methylene chloride at 60° for 1 h (60 %) [772].
-Also refer to: [2696].

white powder [772];
m.p. 62–64° [772], 62–63° [2695];
^{1}H NMR [772, 2695], ^{13}C NMR [772], IR [772, 2695], MS [772, 2695].

1-(2,4,6-Trihydroxyphenyl)-1-pentanone
(Phlorovalerophenone)

[2999-18-0] $C_{11}H_{14}O_4$ mol. wt. 210.23



Syntheses
-Obtained by reaction of pentanoyl chloride with phloroglucinol in the presence of aluminium chloride,
*in nitrobenzene for 3 days at r.t. (60–70 %) [421];

*in nitrobenzene and carbon disulfide mixture (58 %) [2113];
*in nitrobenzene and methylene chloride mixture [2580].
-Also obtained by adding valeronitrile to a mixture of phloroglucinol and zinc chloride in ether at 0°, hydrogen chloride fed 7–8 h, and the mixture kept overnight at r.t. [2110, 2111, 2531].

-Also obtained by reaction of valeric anhydride with phloroglucinol in the presence of boron trifluoride etherate (70–80 %) [2014].
-Also obtained by acid hydrolysis of its 2-β-D-glucopyranoside in methanol in the presence of 1 N HCl at reflux for 4 h [209].
-Also refer to: [56, 708, 1026, 1375, 1439, 1917, 1942, 1992, 3202, 3297].

Isolation from natural sources

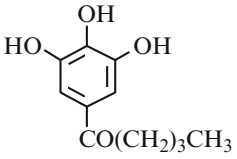
-In bud exudate of *Populus cathayana* (Salicaceae) [1163].
-In bud exudate of *Populus koreana*, *Populus maximowiczii* and *Populus suaveolens* (Salicaceae) [1164].

m.p. 155–157° [209], 152° [2113], 149–150° [1439], 149° [421, 3297];
^{1}H NMR [209, 421], IR [421], MS [209, 421];
GLC [2531]; GC-MS [1163, 1164].

BIOLOGICAL ACTIVITY: Antifungal [2113].

1-(3,4,5-Trihydroxyphenyl)-1-pentanone

$C_{11}H_{14}O_4$ mol. wt. 210.23



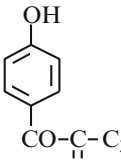
Synthesis
-Refer to: [151].
Trimethyl ether [114085-80-2]
$C_{14}H_{20}O_4$ mol. wt. 252.31

-Obtained by oxidation of 1-(3,4,5-trimethoxyphenyl)-1-pentanol (81 %) [917].
-Also obtained by reaction of butylmagnesium bromide with 3,4,5-trimethoxybenzoyl chloride in the presence of zinc chloride in benzene at 20° for 12 h (90 %) [211, 212].
-Also refer to: [149, 151, 1426].

yellow oil [917];
b.p.$_{0.4}$ 152° [211], b.p.$_4$ 174–175° [151], b.p.$_4$ 174° [149];
m.p. 27° [151];
^{1}H NMR [211, 917], ^{13}C NMR [917], MS [917].

1-(4-Hydroxyphenyl)-2-methylene-1-pentanone

$C_{12}H_{14}O_2$ mol. wt. 190.24



Synthesis
-Refer to: [742].
Methyl ether [101375-34-2]
$C_{13}H_{16}O_2$ mol. wt. 204.27
-Obtained by treatment of 4-methoxyvalerophenone with N,N,N′, N′-tetramethylmethanediamine (93 %) [742].

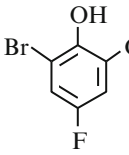
-Also obtained from 2-bromo-1-(4-methoxyphenyl)-2-methyl-1-propanone [742].

liquid (93 %) [742]; ^{1}H NMR [742].

1.2 Substituted Hydroxyketones

1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-pentanone

[1813-21-4] $C_{11}H_{12}BrFO_2$ mol. wt. 275.12



Synthesis
-Obtained by Fries rearrangement of 2-bromo-4-fluoro-phenyl valerate with aluminium chloride at 130–140° for 3 h (70 %) [1550].
b.p.$_{4.5}$ 145–150° [1550].

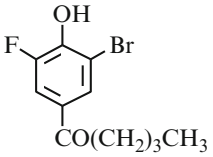
2,4-Dinitrophenylhydrazone [1644-98-0] $C_{17}H_{16}BrFN_4O_5$ mol. wt. 455.24

-Refer to: [1550].

m.p. 183–184° [1550].

1-(3-Bromo-5-fluoro-4-hydroxyphenyl)-1-pentanone

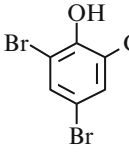
[455-53-8] $C_{11}H_{12}BrFO_2$ mol. wt. 275.12



Synthesis
-Obtained by reaction of bromine with 3-fluoro-4-hydroxy-valerophenone in acetic acid [516].
m.p. 87° [516].

1-(3,5-Dibromo-2-hydroxyphenyl)-1-pentanone

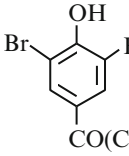
[22362-69-2] $C_{11}H_{12}Br_2O_2$ mol. wt. 336.02



Syntheses
-Refer to: [647, 2002].
m.p. 76° (Sadtler standard N° 65680K), 74.5° [647];
^{1}H NMR (Sadtler standard N° 38631M),
IR (Sadtler standard N° 65680K).

1-(3,5-Dibromo-4-hydroxyphenyl)-1-pentanone

[5408-44-6] $C_{11}H_{12}Br_2O_2$ mol. wt. 336.02

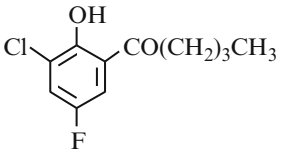


Syntheses
-Obtained by reaction of bromine with 4-hydroxy-valerophenone [1995].
-Also refer to: [516].
m.p. 75° [516], 70° (Sadtler standard N° 65676K);

^{1}H NMR (Sadtler standard N° 38627M), IR (Sadtler standard N° 65676K).

1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-pentanone

[1813-22-5] $C_{11}H_{12}ClFO_2$ mol. wt. 230.67



Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-fluorophenyl valerate with aluminium chloride at 130–140° for 3 h (78 %) [1550].
b.p.$_1$ 140–141° [1550].

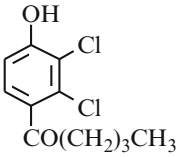
2,4-Dinitrophenylhydrazone [2193-04-6] $C_{17}H_{16}ClFN_4O_5$ mol. wt. 410.79

-Refer to: [1550].

m.p. 159° [1550].

1-(2,3-Dichloro-4-hydroxyphenyl)-1-pentanone

[55507-79-4] $C_{11}H_{12}Cl_2O_2$ mol. wt. 247.12



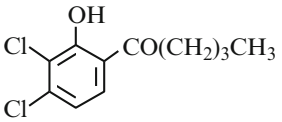
Syntheses
-Refer to: [7, 8, 342, 739].
m.p. 107–110° [739].
Methyl ether [101375-31-9]
$C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15

-Preparation by reaction of valeroyl chloride with 2,3-dichloroanisole in the presence of aluminium chloride (84 %) [742].
-Also refer to: [342, 343].

m.p. 61–63° [742]; ^{1}H NMR [742].

1-(3,4-Dichloro-2-hydroxyphenyl)-1-pentanone

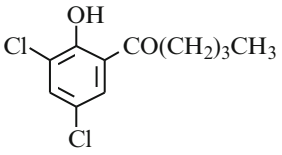
[196307-75-2] $C_{11}H_{12}Cl_2O_2$ mol. wt. 247.12



Synthesis
-Refer to: [949].
^{13}C NMR [949].

1-(3,5-Dichloro-2-hydroxyphenyl)-1-pentanone

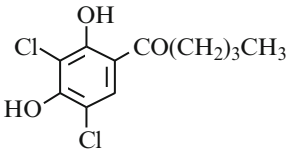
$C_{11}H_{12}Cl_2O_2$ mol. wt. 247.12



Synthesis
-Obtained by Fries rearrangement of 2,4-dichlorophenyl valerate with aluminium chloride at 170° for 40 min (72 %) [646].
m.p. 46–47° [646].

1-(3,5-Dichloro-2,4-dihydroxyphenyl)-1-pentanone

$C_{11}H_{12}Cl_2O_3$ mol. wt. 263.12

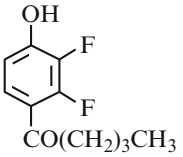


Synthesis
-Refer to: [1052].

BIOLOGICAL ACTIVITY: Bactericide [1052]; As fungicide for soy sauce [1053].

1-(2,3-Difluoro-4-hydroxyphenyl)-1-pentanone

$C_{11}H_{12}F_2O_2$ mol. wt. 214.21

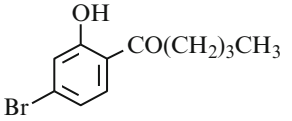


Synthesis
-Refer to: [1161].

Methyl ether [134364-70-8]
$C_{12}H_{14}F_2O_2$ mol. wt. 228.24
-Refer to: [1161].

1-(4-Bromo-2-hydroxyphenyl)-1-pentanone

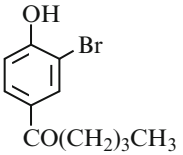
[189875-21-6] $C_{11}H_{13}BrO_2$ mol. wt. 257.13



Synthesis
-Refer to: [2340].

1-(3-Bromo-4-hydroxyphenyl)-1-pentanone

[67548-61-2] $C_{11}H_{13}BrO_2$ mol. wt. 257.13



Syntheses
-Obtained (by-product) by reaction of valeryl chloride with 2-bromoanisole in the presence of aluminium chloride (**XX**) [1334].
-Also refer to: [1673, 1798].

m.p. 101° [1334], 100–101° [1673].

BIOLOGICAL ACTIVITY: Nematocide [1798].

Methyl ether [859968-25-5] $C_{12}H_{15}BrO_2$ mol. wt. 271.15

-Preparation by reaction of valeryl chloride with 2-bromoanisole in the presence of aluminium chloride (**XI**) [1334].
-Also refer to: [1160].

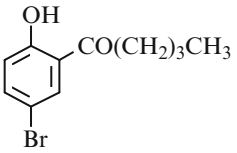
m.p. 56–57° [1160], 49° [1334].

Phenylhydrazone of the methyl ether $C_{18}H_{21}BrN_2O$ mol. wt. 361.28

m.p. 124° [1334].

1-(5-Bromo-2-hydroxyphenyl)-1-pentanone

[67548-62-3] $C_{11}H_{13}BrO_2$ mol. wt. 257.13



Syntheses
-Obtained by Fries rearrangement of 4-bromophenyl valerate in the presence of aluminium chloride [1701, 2797], in tetrachloroethane at 120° for 30 min (45 %) [2026].
-Also refer to: [1798, 2202].

needles [2026]; m.p. 30° [2026];
b.p.$_1$ 120–121° [2026], b.p.$_2$ 127–136° [1701]; TLC [2026].

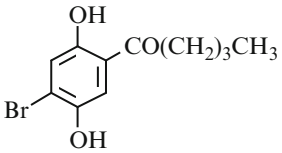
BIOLOGICAL ACTIVITY: Nematocide [1798].

2,4-Dinitrophenylhydrazone [101876-10-2] $C_{17}H_{17}BrN_4O_5$ mol. wt. 437.25

m.p. 231° [2026].

1-(4-Bromo-2,5-dihydroxyphenyl)-1-pentanone

[52376-25-7] $C_{11}H_{13}BrO_3$ mol. wt. 273.13



Synthesis
-Obtained by Fries rearrangement of 2-bromohydroquinone divalerate with aluminium chloride, first at 170° for 2 h, then at 180° for 10 min [1105].
m.p. 70–71° [1105].

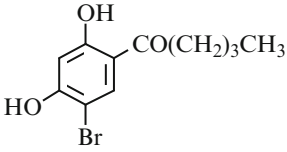
Semicarbazone [52376-26-8] $C_{12}H_{16}BrN_3O_3$ mol. wt. 330.18

-Refer to: [1105].

m.p. 208–209° [1105].

1-(5-Bromo-2,4-dihydroxyphenyl)-1-pentanone

$C_{11}H_{13}BrO_3$ mol. wt. 273.13



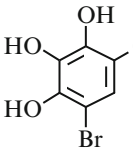
Syntheses
-Refer to: [2416, 2417].

Oxime [235103-27-2]
$C_{11}H_{14}BrNO_3$ mol. wt. 288.08

USE: Gravimetric reagent for Ni(II) and Cu(II) and spectrophotometric study of the complexes [2416]; Gravimetric reagent for Pd(II) and Mn(II) and spectrophotometric study of the complexes [2417].

1-(5-Bromo-2,3,4-trihydroxyphenyl)-1-pentanone

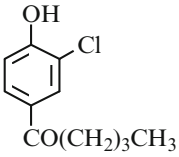
$C_{11}H_{13}BrO_4$ mol. wt. 289.13



Synthesis
-Obtained by reaction of bromine with 4-valeroyl-pyrogallol in acetic acid [506].
m.p. 123–124° [506].

1-(2-Chloro-4-hydroxyphenyl)-1-pentanone

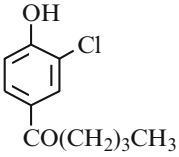
$C_{11}H_{13}ClO_2$ mol. wt. 212.68



Synthesis
-Refer to: [3335].
b.p.$_2$ 190–192° [3335].

1-(3-Chloro-4-hydroxyphenyl)-1-pentanone

[34190-36-8] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



Syntheses
-Obtained (by-product) by reaction of valeryl chloride with 2-chloroanisole in the presence of aluminium chloride (**XVII**) [1334].
-Also refer to: [1673, 3335].

b.p.$_4$ 180–184° [3335]; m.p. 97–98° [3335], 97° [1334], 96–97° [1673].

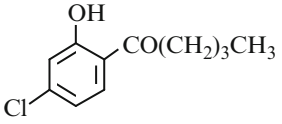
Methyl ether $C_{12}H_{15}ClO_2$ mol. wt. 226.70

-Refer to: [1160].

m.p. 58–59° [1160].

1-(4-Chloro-2-hydroxyphenyl)-1-pentanone

[27581-18-6] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



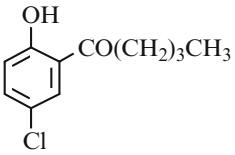
Syntheses
-Preparation by Fries rearrangement of m-chlorophenyl valerate with aluminium chloride,
*for 3 h at 140–150° (90 %) [2432];
*for 1 h at 165° (50 %) [3335].

-Also refer to: [2428, 2429].

b.p.$_{12}$ 160–164° [3335], b.p.$_{20}$ 165° [2432];
^{1}H NMR [2432], IR [2432].

1-(5-Chloro-2-hydroxyphenyl)-1-pentanone

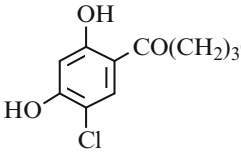
[209462-25-9] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



Syntheses
-Obtained by Fries rearrangement of 4-chlorophenyl valerate with aluminium chloride [3170].
-Also refer to: [1702, 1945, 3283].
b.p.$_{0.9}$ 107° [3170], b.p.$_{2}$ 120–125° [1702];
m.p. 28° [3170]; UV [3170].

1-(5-Chloro-2,4-dihydroxyphenyl)-1-pentanone

[101043-59-8] $C_{11}H_{13}ClO_3$ mol. wt. 228.68

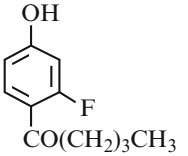


Synthesis
-Refer to: [1479].

USE: Recording material contg. encapsulated electron donating dye and, as colour developer [1479].

1-(2-Fluoro-4-hydroxyphenyl)-1-pentanone

$C_{11}H_{13}FO_2$ mol. wt. 196.22

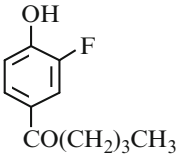


Synthesis
-Refer to: [2437].

Methyl ether [80222-35-1]
$C_{12}H_{15}FO_2$ mol. wt. 210.25
-Refer to: [2437].

1-(3-Fluoro-4-hydroxyphenyl)-1-pentanone

[350-26-5] $C_{11}H_{13}FO_2$ mol. wt. 196.22



Syntheses
-Obtained by refluxing 3-fluoro-4-methoxyvalerophenone with pyridinium chloride for 15 min [516].
-Also refer to: [3150].
m.p. 49° [516].

isoNicotinylhydrazone [449-31-0] $C_{17}H_{18}FN_3O_2$ mol. wt. 315.35

m.p. 228° [520, 521].

USE: In chemotherapy of leprosy [520, 521].

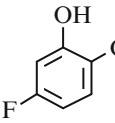
Methyl ether [586-20-9] $C_{12}H_{15}FO_2$ mol. wt. 210.25

-Obtained by Friedel-Crafts acylation of 2-fluoroanisole with valeroyl chloride in the presence of aluminium chloride in carbon disulfide (75–85 %) [516].
-Also refer to: [2437, 3260].

liquid [516]; b.p.$_{32}$ 198–201° [516]; $n_D^{28} = 1.5350$ [516].

1-(4-Fluoro-2-hydroxyphenyl)-1-pentanone

$C_{11}H_{13}FO_2$ mol. wt. 196.22

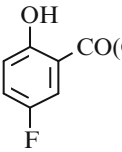


Synthesis
-Refer to: [2437].
Methyl ether [80222-34-0]
$C_{12}H_{15}FO_2$ mol. wt. 210.25

-Refer to: [2437].

1-(5-Fluoro-2-hydroxyphenyl)-1-pentanone

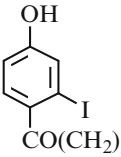
[319-30-2] $C_{11}H_{13}FO_2$ mol. wt. 196.22



Synthesis
-Obtained by Fries rearrangement of 4-fluorophenyl valerate with aluminium chloride at 150° [2991].
b.p.$_{14}$ 131–135° [2991]; m.p. 7–9° [2991].

1-(4-Hydroxy-2-iodophenyl)-1-pentanone

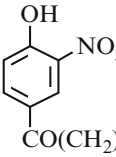
$C_{11}H_{13}IO_2$ mol. wt. 304.12



Synthesis
-Refer to: [608].
Methyl ether [447439-58-9]
$C_{12}H_{15}IO_2$ mol. wt. 318.15
-Refer to: [608, 2573].

1-(4-Hydroxy-3-nitrophenyl)-1-pentanone

$C_{11}H_{13}NO_4$ mol. wt. 223.23



Synthesis
-Obtained by reaction of valeryl chloride with 2-nitrophenol in the presence of aluminium chloride in nitrobenzene, first at 55–60° for 2.5 h, then at r.t. overnight (34 %) [465].
m.p. 27.4–28.2° [465].

2,4-Dinitrophenylhydrazone $C_{17}H_{17}N_5O_7$ mol. wt. 403.35

-Refer to: [465].

m.p. 167.8–168.4° [465].

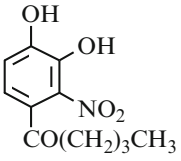
Methyl ether [1032174-12-1] $C_{12}H_{15}NO_4$ mol. wt. 237.25

-Obtained by adding potassium nitrate to an ice-cold solution of 4-methoxyvalerophenone in sulfuric acid, then the reaction was run at r.t. for 8–15 h (63 %) [2243].
-Also refer to: [3451].

white crystalline solid [2243]; m.p. 81–82° [2243];
^{1}H NMR [2243].

1-(3,4-Dihydroxy-2-nitrophenyl)-1-pentanone

[383383-01-5] $C_{11}H_{13}NO_5$ mol. wt. 239.23

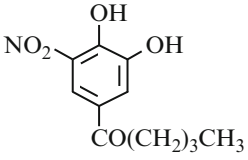


Synthesis
-Refer to: [1842].

USE: As COMT inhibitor for treatment of central and peripheral nervous system disorders [1842].

1-(3,4-Dihydroxy-5-nitrophenyl)-1-pentanone

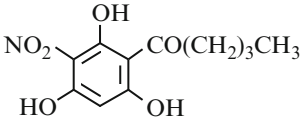
[125628-93-5] $C_{11}H_{13}NO_5$ mol. wt. 239.23



Syntheses
-Refer to: [322, 323, 429].
pK_a [429].

1-(2,4,6-Trihydroxy-3-nitrophenyl)-1-pentanone

[119691-95-1] $C_{11}H_{13}NO_6$ mol. wt. 255.23



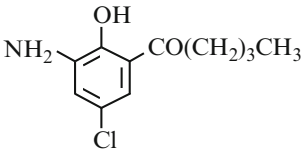
Synthesis
-Obtained by adding hexane, then a mixture of concentrated sulfuric acid and fuming nitric acid at 0° to a solution of 1-(2,4,6-trihydroxyphenyl)-1-pentanone in concentrated sulfuric acid below 0° (70–80 %) [3114].

bright yellow needles [3114]; m.p. 81–84° [3114];
^{1}H NMR [3114], IR [3114], MS [3114].

BIOLOGICAL ACTIVITY: Germination inhibition [3114]; PET inhibition [3114].

1-(3-Amino-5-chloro-2-hydroxyphenyl)-1-pentanone

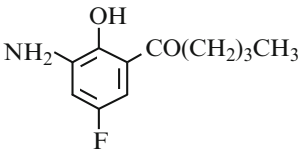
$C_{11}H_{14}ClNO_2$ mol. wt. 227.69



Synthesis
-Refer to: [2105].

1-(3-Amino-5-fluoro-2-hydroxyphenyl)-1-pentanone

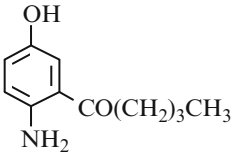
$C_{11}H_{14}FNO_2$ mol. wt. 211.24



Synthesis
-Refer to: [2105].

1-(2-Amino-5-hydroxyphenyl)-1-pentanone

$C_{11}H_{15}NO_2$ mol. wt. 193.25

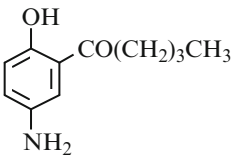


Synthesis
-Refer to: [710].

Methyl ether [90033-66-2]
$C_{12}H_{17}NO_2$ mol. wt. 207.27
-Refer to: [710].

1-(5-Amino-2-hydroxyphenyl)-1-pentanone

[497934-63-1] $C_{11}H_{15}NO_2$ mol. wt. 193.25

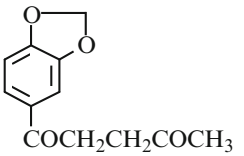


Syntheses
-Obtained by treatment of paracetamol valerate with Lewis acid catalyst in organic solvent, then deacetylating the 4-hydroxy-3-valeroylacetamide obtained with an inorganic acid at refluxing temperature [3464].

-Also refer to: [3281].

1-(3,4-Methylenedioxyphenyl)-1,4-pentanedione

[61363-13-1] $C_{12}H_{12}O_4$ mol. wt. 220.22

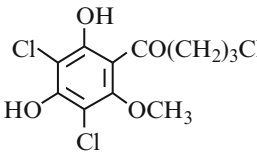


Synthesis
-Obtained by reaction of piperonal with 3-buten-2-one in the presence of KOH and triethylamine in refluxing ethanol for 2 h (40.4 %) [2952].
b.p.$_{0.4\text{-}0.5}$ 157° [2952];

m.p. 85–86° [2952]; ^{1}H NMR [2952], IR [2952].

1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-pentanone

[118191-27-8] $C_{12}H_{14}Cl_2O_4$ mol. wt. 293.15

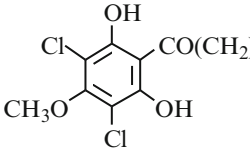


Synthesis
-Obtained by reaction of chlorine with 2,4-dihydroxy-6-methoxyvalerophenone in water [2012].
^{1}H NMR [2012], MS [2012].

BIOLOGICAL ACTIVITY: Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-pentanone
(DIF-1) [-1]

[113411-16-8] $C_{12}H_{14}Cl_2O_4$ mol. wt. 293.15



Syntheses
-Preparation by adding a solution of sulfuryl chloride (1.5 equiv.) in ethanol to a solution of 2,6-dihydroxy-4-methoxyvalerophenone in chloroform at r.t.; then, the solution was stirred for 1 h at r.t. [1129].

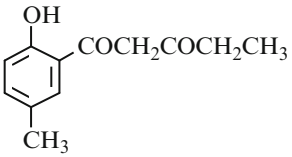
-Also obtained by reaction of chlorine with 2,6-dihydroxy-4-methoxyvalerophenone in water [2012].
-Also refer to: [1653, 1772, 1773, 1804, 2011, 3153].

yellow amorphous solid [1129];
^{1}H NMR [2012], MS [1129, 2012]; GC [2154].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Differentiation-inducing factor-1 and -2 function also as modulators for Dictyostelium chemotaxis [1804]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129]; Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012]; Cell differentiation regulation by, in *Dictyostelium discoideum* [1653]; Differentiation-inducing factor, from *Dictyostelium discoideum*, characterization of, [2011].

1-(2-Hydroxy-5-methylphenyl)-1,3-pentanedione

[104516-35-0] $C_{12}H_{14}O_3$ mol. wt. 206.24



Syntheses

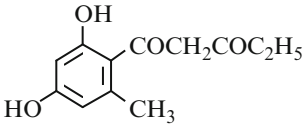
-Obtained by heating a mixture of 2-acetyl-4-methylphenol, ethyl propionate (b.p. 98.5–100°) and powdered sodium on the steam bath for 30 min (57 %) [235].

-Also refer to: [1011, 2745, 2746].

colourless, thick, rectangular prisms [235]; m.p. 75–76° [235].

1-(2,4-Dihydroxy-6-methylphenyl)-1,3-pentanedione

$C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis

-Obtained by refluxing a mixture of orcacetophenone, propionic anhydride and sodium propionate at 180–190° for 9 h [2814].

dark brown viscous oil [2814].

Dimethyl ether [62036-47-9] $C_{14}H_{18}O_4$ mol. wt. 250.29

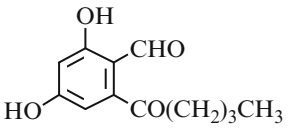
-Obtained by Claisen condensation of 2,4-dimethoxy-6-methylacetophenone with ethyl propionate (11 %) [49].

-Refer to: [2003, 2814].

oil [49]; $b.p._{2\text{-}4}$ 185–190° [2814].

2,4-Dihydroxy-6-(1-oxopentyl)benzaldehyde

$C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis

-Refer to: [1986].

Dimethyl ether

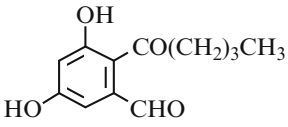
$C_{14}H_{18}O_4$ mol. wt. 250.29

-Refer to: [1986].

^{1}H NMR [1986], MS [1986].

3,5-Dihydroxy-2-(1-oxopentyl)benzaldehyde

$C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Refer to: [1986].

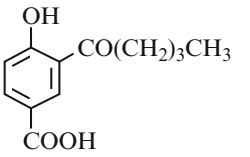
Dimethyl ether
$C_{14}H_{18}O_4$ mol. wt. 250.29

-Refer to: [1986].

^{1}H NMR [1986].

4-Hydroxy-3-valeroylbenzoic acid

[20031-96-3] $C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Obtained by hydrolysis of its ethyl ester [967].
m.p. 190° [1], 184° [967].

Acetate $C_{14}H_{16}O_5$ mol. wt. 264.28

-Obtained by acetylation of 4-hydroxy-3-valeroylbenzoic acid [967].

m.p. 101° [967].

Methyl ether $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by methylation of 4-hydroxy-3-valeroylbenzoic acid [967].

m.p. 154° [967].

Methyl ester [20035-78-3] $C_{13}H_{16}O_4$ mol. wt. 236.27

m.p. 86–87° [1], 78–80° [900].

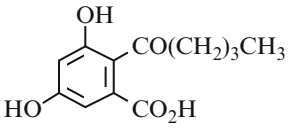
Ethyl ester $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of valeroyl chloride with ethyl 4-hydroxybenzoate in the presence of aluminium chloride in tetrachloroethane, then the reaction mixture was heated at 120° for 3–4 h [967].

b.p.$_{30}$ 190° [967]; $n_D^{34} = 1.5220$ [967]; $d_{28} = 1.108$ [967].

3,5-Dihydroxy-2-(1-oxopentyl)benzoic acid

$C_{12}H_{14}O_5$ mol. wt. 238.24



Synthesis
-Refer to: [1986].

Dimethyl ether [944558-07-0]
$C_{14}H_{18}O_5$ mol. wt. 266.29

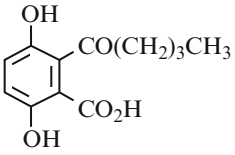
-Refer to: [1986, 2294].

m.p. 99–100° [1986], 98° [2294]; ^{1}H NMR [1986], MS [1986].

BIOLOGICAL ACTIVITY: Ecotoxicology [1986].

3,6-Dihydroxy-2-(1-oxopentyl)benzoic acid

$C_{12}H_{14}O_5$ mol. wt. 238.24



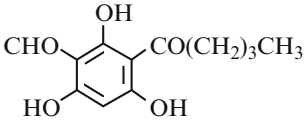
Synthesis
-Refer to: [2294].

Dimethyl ether $C_{14}H_{18}O_5$ mol. wt. 266.29
-Obtained by heating a mixture of 3,5-dimethoxyphthalic anhydride, valeric anhydride and sodium valerate on the oil bath at 185–210° for 2 h [2294].

m.p. 134° [2294].

2,4,6-Trihydroxy-3-(1-oxopentyl)benzaldehyde

[96573-31-8] $C_{12}H_{14}O_5$ mol. wt. 238.24



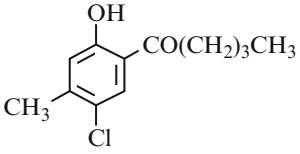
Synthesis
-Obtained by reaction of ethyl orthoformate with 2,4,6-trihydroxyvalerophenone in the presence of aluminium chloride in methylene chloride with cooling in an ice bath for 30 min (70 %) [421].

m.p. 135–137° [421]; ^{1}H NMR [421], IR [421], MS [421].

BIOLOGICAL ACTIVITY: As photosynthetic electron transport (PET) [3405].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-pentanone

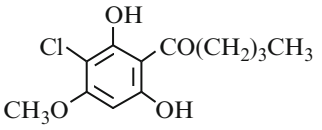
$C_{12}H_{15}ClO_2$ mol. wt. 226.70



Synthesis
-Refer to: [3138].
Fluorescence [3138].

1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-1-pentanone
(DIF-3) (-1)

[120529-47-7] $C_{12}H_{15}ClO_4$ mol. wt. 258.70



Syntheses
-Preparation by adding a solution of sulfuryl chloride (1.5 equiv.) in ethanol to a solution of 2,6-dihydroxy-4-methoxyvalerophenone in chloroform at r.t.; then, the solution was stirred for 1 h at r.t. [1129].

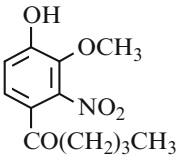
-Also refer to: [1772, 2153].

colourless amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(4-Hydroxy-3-methoxy-2-nitrophenyl)-1-pentanone

[383383-10-6] $C_{12}H_{15}NO_5$ mol. wt. 253.25

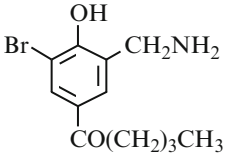


Synthesis
-Refer to: [1842].

USE: As COMT inhibitor for treatment of central and peripheral nervous system disorders [1842].

1-[3-(Aminomethyl)-5-bromo-4-hydroxyphenyl]-1-pentanone

$C_{12}H_{16}BrNO_2$ mol. wt. 286.16



Synthesis
-Refer to: [3373].

O-Methyloxime [104129-16-0]
$C_{13}H_{19}BrN_2O_2$ mol. wt. 315.21

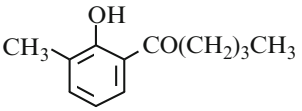
-As diuretic and antihypertensive [3373].

Oxime [104145-15-5] $C_{12}H_{17}BrN_2O_2$ mol. wt. 301.22

-As diuretic and antihypertensive [3373].

1-(2-Hydroxy-3-methylphenyl)-1-pentanone

[189875-29-4] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Obtained by Fries rearrangement of 2-methylphenyl valerate in the presence of aluminium chloride at 160–180° for 30 min (46 %) [726].

-Also obtained by acylation of organometallic reagents (94 %) [1627].

-Also refer to: [2340].

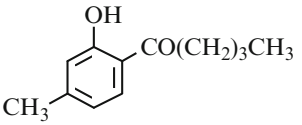
colourless oil [1627]; b.p.$_{15}$ 143–145° [726]; m.p. 18° [726]; ^{1}H NMR [1627], ^{13}C NMR [1627].

Phenylhydrazone $C_{18}H_{22}N_2O$ mol. wt. 282.38

m.p. 116–118° [726].

1-(2-Hydroxy-4-methylphenyl)-1-pentanone

[173851-66-6] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Preparation by Fries rearrangement of 3-methylphenyl valerate in the presence of aluminium chloride,

*without solvent at 160° for 2 h (85 %) [726] or at 120–140° for 10–20 min (80 %) [243];

*in nitrobenzene at 25° for 24 h (67 %) [243] or at 25–30° for 24 h (70 %) [244].

-Also obtained by Fries rearrangement of 3-methylphenyl valerate in the presence of boron trifluoride etherate at 110° under nitrogen for 4 h (85 %) [1118].

b.p.$_3$ 121–125° [243, 244], b.p.$_3$ 122–123° [1118], b.p.$_{15}$ 152–154° [726]; m.p. 16° [726, 1118]; ^{1}H NMR [244, 1118].

Methyl ether [173851-69-9] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of pentanoic acid with 3-methylanisole in the presence of trifluoroacetic anhydride under nitrogen at r.t. for 3.5 h (22 %) [656].

-Also obtained by reaction of dimethyl sulfate with 2-hydroxy-4-methylvalerophenone in the presence of potassium carbonate in refluxing acetone for 2 h (97 %) [1118].

oil [1118]; ^{1}H NMR [1118], IR [1118].

Phenylhydrazone $C_{18}H_{22}N_2O$ mol. wt. 282.38

m.p. 138–139° [243].

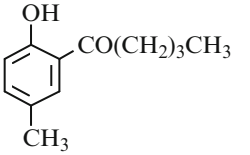
2,4-Dinitrophenylhydrazone $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

-Refer to: [243].

m.p. 138–139° [243].

1-(2-Hydroxy-5-methylphenyl)-1-pentanone

[150033-77-5] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Obtained by Fries rearrangement of 4-methylphenyl valerate with aluminium chloride at 160° for 2 h (65 %) [726].

-Also obtained by reaction of valeric acid (0.95 mmol) with p-cresol (0.95 mmol) in the presence of ferric chloride (0.32 mmol) under microwave irradiation (600 W) (85 %) [2213].

-Also obtained by reaction of valeric acid with p-cresol in the presence of,

*zinc chloride under microwave irradiation with 500 W for 3.3 min (98 %) [2211];

*stannic chloride under microwave irradiation with 700 W for 2 min at 50° and atmospheric pressure conditions (95 %) [2212];

*boron trifluoride etherate under microwave irradiation for 2 min at r.t. (98 %) [2210].

-Also refer to: [2340].

oil [2210–2212];
b.p.$_{15}$ 144–145° [726]; m.p. 32–33° [726];
^{1}H NMR [2210–2213], IR [2210–2213];
TLC [2210, 2211, 2213].

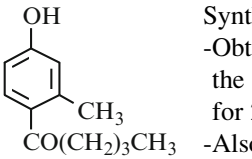
Methyl ether $C_{13}H_{18}O_2$ mol. wt. 206.28

-Preparation by reaction of valeroyl chloride with 4-methylanisole in the presence of aluminium chloride in carbon disulfide (52 %) [515].

colourless oil [515]; b.p.$_{13}$ 161–162° [515];
$n_D^{21} = 1.5240$ [515].

1-(4-Hydroxy-2-methylphenyl)-1-pentanone

[173851-67-7] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Obtained by Fries rearrangement of 3-methylphenyl valerate in the presence of aluminium chloride in nitrobenzene at 25–30° for 24 h (14 %) [244].

-Also obtained by Fries rearrangement of 3-methylphenyl valerate in the presence of boron trifluoride etherate at 110° under nitrogen for 4 h (2 %) [1118].

colourless needle prisms [244]; m.p. 88–89° [244, 1118].

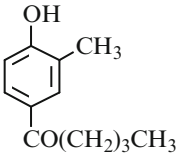
Methyl ether [173851-65-5] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of pentanoic acid with 3-methylanisole in the presence of trifluoroacetic anhydride under nitrogen at r.t. for 3.5 h (77 %) [656], (51 %) [1118].

colourless crystals [1118]; m.p. 52–53° [1118];
^{1}H NMR [1118], IR [1118], MS [1118].

1-(4-Hydroxy-3-methylphenyl)-1-pentanone

$C_{12}H_{16}O_2$ mol. wt. 192.26



Synthesis
-Obtained by Fries rearrangement of 2-methylphenyl valerate in the presence of aluminium chloride at 160–180° for 30 min (30 %) [726].
b.p.$_{15}$ 205° [726]; m.p. 103–104° [726].

Methyl ether [5394-88-7] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of valeric anhydride with 2-methylanisole in the presence of aluminium chloride in boiling carbon disulfide for 30 min (83 %) [2297].
-Also refer to: [660, 1249, 2172, 2174, 2175, 2997, 2999].

b.p.$_4$ 151.5° [2297], b.p.$_5$ 151–155° [660], b.p.$_{744}$ 308.7° [2297];
m.p. 31–33° [2297];
^{1}H NMR [1249, 2999], ^{13}C NMR [1249, 2999], IR [1249, 2999].

Phenylhydrazone $C_{18}H_{22}N_2O$ mol. wt. 282.38

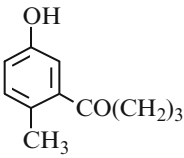
m.p. 120–121° [726].

Benzoate $C_{19}H_{20}O_3$ mol. wt. 296.36

m.p. 72–73° [726].

1-(5-Hydroxy-2-methylphenyl)-1-pentanone

$C_{12}H_{16}O_2$ mol. wt. 192.26



Synthesis
-Refer to: [574].
Methyl ether [74571-50-9]
$C_{13}H_{18}O_2$ mol. wt. 206.28

-Refer to: [574 (45 %)].

b.p.$_{0.002}$ 110–120° [574];
^{1}H NMR [574], IR [574], UV [574], MS [574].

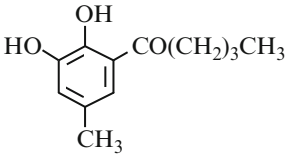
2,4-Dinitrophenylhydrazone of the methyl ether

[74571-52-1] $C_{19}H_{22}N_4O_5$ mol. wt. 386.41

m.p. 75–76° [574].

1-(2,3-Dihydroxy-5-methylphenyl)-1-pentanone

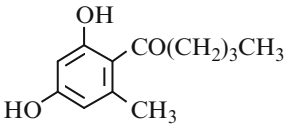
$C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis
-Obtained from creosol (66 %) [784].
yellow crystals [784];
m.p. 85–86° [784].

1-(2,4-Dihydroxy-6-methylphenyl)-1-pentanone

[154921-41-2] $C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis
-Obtained from 2-difluoroboryloxy-4-hydroxy-6-methylvalerophenone by refluxing in dilute ethanol (72 %) [2938]. 2-Difluoroboryloxy-4-hydroxy-6-methyl-valerophenone, still named: Difluoro[1-(2,4-dihydroxy-6-methylphenyl)-1-valeronato-O,O′] boron (72 %, m.p. 134°, IR).

m.p. 132° [2938]; IR [2938], UV [2938].

Dimethyl ether $C_{14}H_{20}O_3$ mol. wt. 236.31

^{1}H NMR [554].

Dimethyl ether (D) [92120-60-0] $C_{14}H_{18}D_2O_3$ mol. wt. 238.29

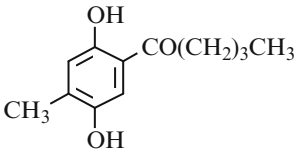
1-[2,4-Dihydroxy-6-(methyl-*d*)phenyl]-1-pentanone

-Obtained by adding n-butyllithium in hexane to a solution of ethyl 2,4-dimethoxy-6-methyl-benzoate in THF under nitrogen and cooled at −78°. Then, D_2O in THF was added (71 %) [554].
N.B.: The compound was found to be deuterated on the methylene next to the ketone.

oil [554]; b.p.$_{0.01}$ 100° [554];
^{1}H NMR [554], IR [554], UV [554], MS [554].

1-(2,5-Dihydroxy-4-methylphenyl)-1-pentanone

$C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis
-Refer to: [1755].

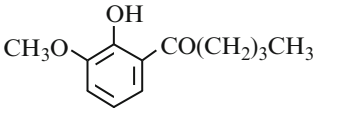
Dimethyl ether [83893-22-5]
$C_{14}H_{20}O_3$ mol. wt. 236.31

-Prepared by Friedel-Crafts acylation (95 %) [1755].

b.p. $_3$ 140–143° [1755]; m.p. 33.5–34° [1755];
^{1}H NMR [1755], IR [1755].

1-(2-Hydroxy-3-methoxyphenyl)-1-pentanone

[15116-08-2] $C_{12}H_{16}O_3$ mol. wt. 208.26

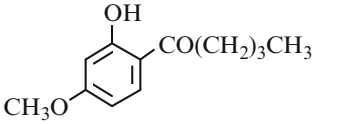


Synthesis
-Obtained by partial demethylation of its methyl ether with aluminium chloride in toluene (60–90 %) [2747].

oil [2747]; b.p.$_{0.08\text{-}0.1}$ 87–89.5° [2747].

1-(2-Hydroxy-4-methoxyphenyl)-1-pentanone

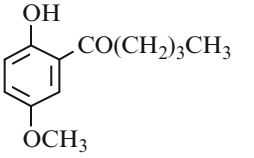
[372486-18-5] $C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis
-Preparation by partial methylation of 2,4-dihydroxy-valerophenone with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 4–6 h (85–90 %) [2501].

1-(2-Hydroxy-5-methoxyphenyl)-1-pentanone

[57314-80-4] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses
-Obtained by reaction of valeroyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156], (51 %) [770],
*in methylene chloride at r.t. for 1 h (9 %) [2878];

*in refluxing carbon disulfide for 4 h, and the mixture left overnight (77 %) [1113].
-Also obtained by Fries rearrangement of 4-methoxyphenyl valerate in the presence of aluminium chloride [156].

-Also obtained by heating 4-methoxyphenyl valerate with aluminium chloride on the steam bath for 6 h (49 %) [770].

pale yellow needles [770];
$b.p._{.0.1}$ 135–145° [1113], $b.p._{.0.2}$ 146–154° [770];
m.p. 62–62.5° [2878], 62° [770, 1113]; UV [2878].

Oxime [140943-12-0] $C_{12}H_{17}NO_3$ mol. wt. 223.27

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

2,4-Dinitrophenylhydrazone $C_{18}H_{20}N_4O_6$ mol. wt. 388.38

m.p. 186° [770], 185° [1113].

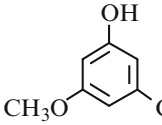
Acetate $C_{14}H_{18}O_4$ mol. wt. 250.29

-Acetylation of 2-hydroxy-5-methoxyvalerophenone by means of acetic anhydride in pyridine solution [1113].

m.p. 72–73° [1113].

1-(3-Hydroxy-5-methoxyphenyl)-1-pentanone

$C_{12}H_{16}O_3$ mol. wt. 208.26

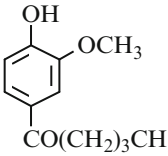


Synthesis
-Refer to: [607].
Isolation from natural sources
-From the roots and stems of *Ardisia virens* Kurz (Myrsinaceae) [607].

colourless needles [607], m.p. 66–67° [607],
^{1}H NMR [607], ^{13}C NMR [607], IR [607], UV [607], MS [607].

1-(4-Hydroxy-3-methoxyphenyl)-1-pentanone

[114515-51-4] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses
-Obtained by Fries rearrangement of 2-methoxyphenyl valerate in the presence of aluminium chloride in nitrobenzene (50 %) [726].
-Also obtained by hydrolysis of its benzoate (90 %) [1377].
-Also obtained by adding DDQ to 1-(4-hydroxy-3-methoxyphenyl)-1-pentanol in benzene and the reaction mixture stirred for 4 h at r.t. [2989].

-Also obtained by hydrolysis and conversion of fractionated glycoside aroma precursors in neutral grapes by Saccharomyces cerevisiae [981].

b.p.$_{15}$ 195–197° [726]; m.p. 62.9° [1377], 61° [2989], 60–62° [726]; ^{1}H NMR [2989].

BIOLOGICAL ACTIVITY: Choleretic [2989].

Benzoate $C_{19}H_{20}O_4$ mol. wt. 312.36

-Obtained by oxidation of α-(4-benzoyloxy-3-methoxyphenyl)-n-butyl carbinol with potassium dichromate in acetic acid and dilute sulfuric acid, first 10 min at r.t., then at 85° (92 %) [1377].

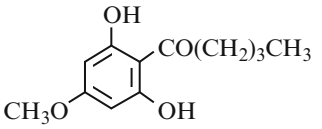
m.p. 88.1° [1377], 85–87° [726].

Phenylhydrazone of the benzoate $C_{25}H_{26}N_2O_3$ mol. wt. 402.49

m.p. 163° [1377].

1-(2,6-Dihydroxy-4-methoxyphenyl)-1-pentanone
(Desaspidinol Y)

[69480-05-3] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses

-Preparation by reaction of pentanoyl chloride with phloroglucinol monomethyl ether in the presence of aluminium chloride in methylene chloride at r.t. [1129].

-Also refer to: [3301].

Isolation from natural sources

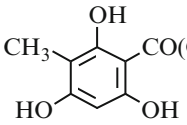
-In bud exudate of *Populus nigra* L [1162].
-Of *Populus tritis* bud exudate [955].
-In bud exudate of *Populus cathayana* (Salicaceae) [1163].
-In bud exudate of *Populus koreana*, *Populus maximowiczii* and *Populus suaveolens* (Salicaceae) [1164].
-From *Ctenitis apiciflora* [3295].
-From *Ctenitis nidus* [3295].

colourless amorphous solid [1129]; m.p. 96–98° [3301]; MS [1129]; GLC [2531]; GC-MS [1162–1164].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2,4,6-Trihydroxy-3-methylphenyl)-1-pentanone

[49583-26-8] $C_{12}H_{16}O_4$ mol. wt. 224.26

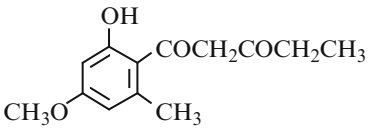


Syntheses
-Refer to: [1917, 2531, 3297, 3301].
Isolation from natural sources
-From *Dryopteris bissetiana* [3299].

m.p. 166–167° [3301], 149–151° [1917, 3297];
MS [1917]; GC-MS [2531]; GLC [2531].

1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1,3-pentanedione

[62036-46-8] $C_{13}H_{16}O_4$ mol. wt. 236.27



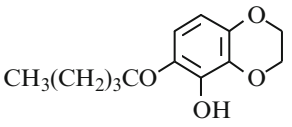
Syntheses
-Obtained by reaction of ethyl propionate with 2-hydroxy-4-methoxy-6-methylacetophenone in the presence of pulverized sodium. Then, the reaction mixture was heated for 1 h on a boiling water bath (38 %) [49].

-Also refer to: [1097].

colourless needles [49]; m.p. 124–125° [49, 1097].

5-Hydroxy-6-(1-oxopentyl)-1,4-benzodioxane

$C_{13}H_{16}O_4$ mol. wt. 236.27

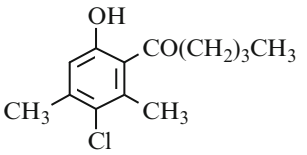


Synthesis
-Obtained by Fries rearrangement of 5-valeryloxy-1,4-benzodioxane in the presence of aluminium chloride in nitrobenzene at 20° (73 %) [801].

$b.p._{0.1}$ 165–167° [801]; m.p. 98–99° [801]; UV [801].

1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-pentanone

[100607-74-7] $C_{13}H_{17}ClO_2$ mol. wt. 240.73



Synthesis
-Preparation by Fries rearrangement of 4-chloro-3,5-dimethylphenyl valerate with aluminium chloride in carbon disulfide at 80° for 2 h, then at 110° for 2 h after solvent elimination (73 %) [3114].

m.p. 63° [3114].

Semicarbazone [100794-83-0] $C_{14}H_{20}ClN_3O_2$ mol. wt. 297.78

m.p. 200° [3114].

Allyl ether [102075-11-6] $C_{16}H_{21}ClO_2$ mol. wt. 280.79

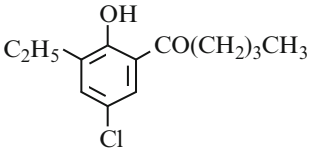
-Obtained by reaction of allyl bromide with the title ketone in the presence of potassium carbonate in refluxing acetone for 6 h (98 %) [3114].

b.p.$_{.3}$ 160° [3114].

USE: Insecticide [3114].

1-(5-Chloro-3-ethyl-2-hydroxyphenyl)-1-pentanone

[53347-27-6] $C_{13}H_{17}ClO_2$ mol. wt. 240.73

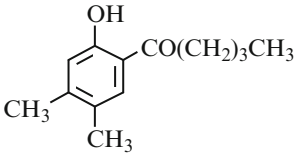


Synthesis
-Obtained by Fries rearrangement of 4-chloro-2-ethylphenyl valerate in the presence of aluminium chloride at 120° for 1.5 h (80.6 %) [2763].

b.p.$_{0.2}$ 111–112° [2763]; $n_D^{20} = 1.5416$ [2763].

1-(2-Hydroxy-4,5-dimethylphenyl)-1-pentanone

[149696-17-3] $C_{13}H_{18}O_2$ mol. wt. 206.28



Synthesis
-Obtained by reaction of valeric acid with 3,4-dimethyl-phenol in the presence of boron trifluoride etherate (78 %) [2939].
m.p. 41–42° [2939];

^{1}H NMR [2939], IR [2939], UV [2939].

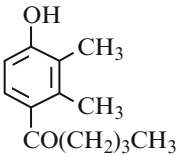
Methyl ether [159847-59-3] $C_{14}H_{20}O_2$ mol. wt. 220.31

^{1}H NMR [533], ^{13}C NMR [533], IR [533], MS [533].

-Formation in allylation of benzamide deriv. [533].

1-(4-Hydroxy-2,3-dimethylphenyl)-1-pentanone

$C_{13}H_{18}O_2$ mol. wt. 206.28



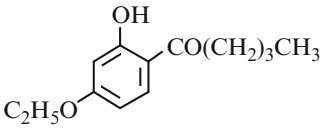
Synthesis
-Refer to: [742].
Methyl ether [101375-32-0]
$C_{14}H_{20}O_2$ mol. wt. 220.31

-Preparation by reaction of valeroyl chloride with 2,3-dimethylanisole in the presence of aluminium chloride (96 %) [742].

m.p. 68–69° [742].

1-(4-Ethoxy-2-hydroxyphenyl)-1-pentanone

$C_{13}H_{18}O_3$ mol. wt. 222.28

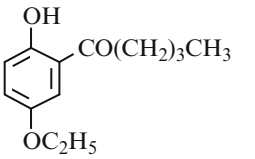


Synthesis
-Refer to: [2221].
Oxime [928769-73-7]
$C_{13}H_{19}NO_3$ mol. wt. 237.30

USE: As an analytical reagent for molybdenum (VI) determination by spectrophotometry [2221].

1-(5-Ethoxy-2-hydroxyphenyl)-1-pentanone

[140943-31-3] $C_{13}H_{18}O_3$ mol. wt. 222.28



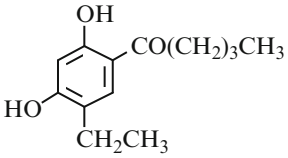
Synthesis
-Refer to: [285].
Oxime [140943-18-6]
$C_{13}H_{19}NO_3$ mol. wt. 237.30

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-(5-Ethyl-2,4-dihydroxyphenyl)-1-pentanone

$C_{13}H_{18}O_3$ mol. wt. 222.28



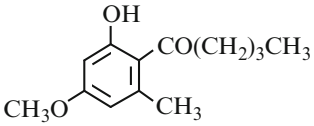
Synthesis
-Obtained by Fries rearrangement of 4-ethylresorcinol divalerate with aluminium chloride in nitrobenzene at 50–60° or without solvent at 40–50° [2651].
b.p.$_9$ 220° [2651]; m.p. 92° [2651].

2,4-Dinitrophenylhydrazone $C_{19}H_{22}N_4O_6$ mol. wt. 402.41

-Refer to: [2651]; m.p. 125–126° [2651].

1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1-pentanone
(Evernipentanone)

$C_{13}H_{18}O_3$ mol. wt. 222.28

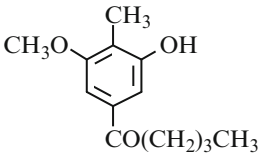


Synthesis
-To a solution of ethyl everninate (1 mol) in THF at −78° was added a cold n-BuLi (7 mol) in hexane. The reaction mixture was kept for 1 h at −78° and then for 18 h at r.t. (80 %) [871].

m.p. 59–63° [871];
^{1}H NMR [871], UV [871], MS [871]; TLC [871].

1-(3-Hydroxy-5-methoxy-4-methylphenyl)-1-pentanone

$C_{13}H_{18}O_3$ mol. wt. 222.28

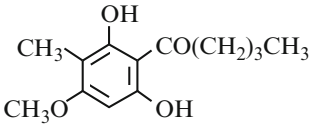


Isolation from natural sources
-From the roots of *Ardisia cornudentata* Mez. (Myrsinaceae) [604].
colourless needles [604];
m.p. 84–86° [604];

^{1}H NMR [604], ^{13}C NMR [604], IR [604], UV [604], MS [604].

1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-1-pentanone
(Aspidinol V)

[57765-52-3] $C_{13}H_{18}O_4$ mol. wt. 238.28

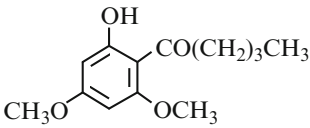


Syntheses
-Refer to: [2531, 3297].
Isolation from natural sources
-From *Ctenitis apiciflora* [3295].
-From *Ctenitis nidus* [3295].

m.p. 138–140° [3297]; GLC [2531].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-pentanone

[80986-13-6] $C_{13}H_{18}O_4$ mol. wt. 238.28

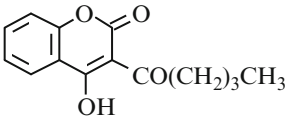


Syntheses
-Obtained by reaction of dimethyl sulfate with phlorovalerophenone in the presence of potassium carbonate in refluxing acetone for 30–40 min (80–90 %) [2014].
-Also obtained by methylation of 2,4,6-trihydroxyvalerophenone [56] according to [1375].
-Also refer to: [56, 1986].

^{1}H NMR [1986].

4-Hydroxy-3-(1-oxopentyl)-2*H*-1-benzopyran-2-one

[36953-87-4] $C_{14}H_{14}O_4$ mol. wt. 246.26

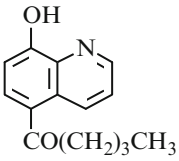


Syntheses
-Obtained by reaction of valeryl chloride with 4-hydroxy-coumarin in pyridine containing one drop of piperidine for 3 h on a water bath (39 %) [3174].
-Also refer to: [2306, 3144].

m.p. 99° [3174].

1-(8-Hydroxy-5-quinolinyl)-1-pentanone

$C_{14}H_{15}NO_2$ mol. wt. 229.28



Synthesis
-Refer to: [1335].

N-methylcarbamate
$C_{16}H_{18}NO_3$ mol. wt. 272.32

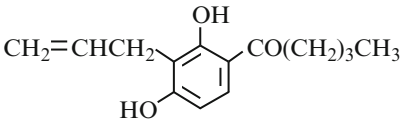
-Refer to: [1335 (62 %)].

m.p. 105–107° [1335].

BIOLOGICAL ACTIVITY: Fungicide [1335].

1-[2,4-Dihydroxy-3-(2-propenyl)phenyl]-1-pentanone

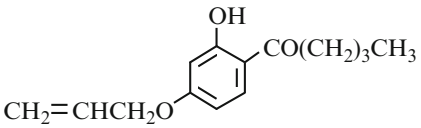
[194792-60-4] $C_{14}H_{18}O_3$ mol. wt. 234.30



Synthesis
-Refer to: [22].

1-[2-Hydroxy-4-(2-propenyloxy)phenyl]-1-pentanone

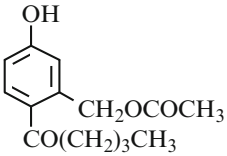
[194792-59-1] $C_{14}H_{18}O_3$ mol. wt. 234.30



Synthesis
-Refer to: [22].

1-[2-(Acetoxymethyl)-4-hydroxyphenyl]-1-pentanone

$C_{14}H_{18}O_4$ mol. wt. 250.29



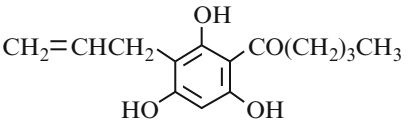
Synthesis
-Refer to: [1118].

Methyl ether [173851-71-3]
$C_{15}H_{20}O_4$ mol. wt. 264.32
-Obtained by reaction of valeric acid with 3-acetoxymethyl-anisole in the presence of trifluoroacetic acid at r.t. for 72 h under nitrogen (28 %) [1118].

white crystals [1118]; m.p. 42.5–43° [1118];
^{1}H NMR [1118], IR [1118], MS [1118].

1-[2,4,6-Trihydroxy-3-(2-propenyl)phenyl]-1-pentanone
2-Valeryl-4-(propen-2-yl)phloroglucinol (**19**) [1026].

[74477-99-9] $C_{14}H_{18}O_4$ mol. wt. 250.29



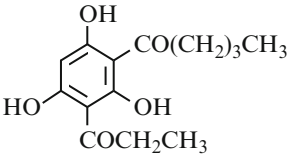
Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and allyl chloride to a solution of phlorovalerophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].
-Also obtained by reaction of allyl chloride with phlorovalerophenone in an alkaline two-phase (aqueous-ether) system and catalyzed by CuCl [838, 3193].

m.p. 123–126° [3193];
^{13}C NMR [839, 1026, 3193], IR [1026].

BIOLOGICAL ACTIVITY: Bactericidal and fungicidal [1026, 3193].

1-(3-Propionyl-2,4,6-trihydroxyphenyl)-1-pentanone

$C_{14}H_{18}O_5$ mol. wt. 266.29

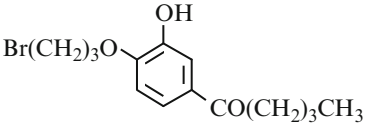


Synthesis
-Preparation [3405] according to the method [421].

BIOLOGICAL ACTIVITY: As photosynthetic electron transport (PET) [3405]; This compound was assayed for its inhibition of the Hill reaction using chloroplasts isolated from the leaves of *Spinacia oleracea*; pl 50 = 4.9 [3405].

1-[4-(3-Bromopropoxy)-3-hydroxyphenyl]-1-pentanone

$C_{14}H_{19}BrO_3$ mol. wt. 315.20

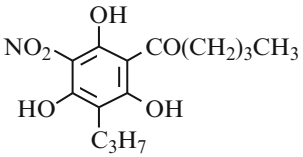


Synthesis
-Refer to: [2965].
Methyl ether [133455-19-3]
$C_{15}H_{21}BrO_3$ mol. wt. 329.23

-Obtained by reaction of 1,3-dibromopropane with 4-hydroxy-3-methoxyvalerophenone [2962].
-Also refer to: [2963–2967].

1-(2,4,6-Trihydroxy-3-nitro-5-propylphenyl)-1-pentanone

[119692-01-2] $C_{14}H_{19}NO_6$ mol. wt. 297.31



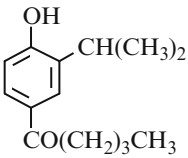
Synthesis
-Obtained by adding a mixture of fuming nitric acid and acetic acid to the solution of 1-(2,4,6-trihydroxy-3-propyl-phenyl)-1-pentanone in acetic acid at 60° for 30 min (30–40 %) [3114].

m.p. 51–52° [3114]; ^{1}H NMR [3114], IR [3114], MS [3114].

BIOLOGICAL ACTIVITY: Germination inhibition [3114]; PET inhibition [3114].

1-[4-Hydroxy-3-(1-methylethyl)phenyl]-1-pentanone

[95102-37-7] $C_{14}H_{20}O_2$ mol. wt. 220.31

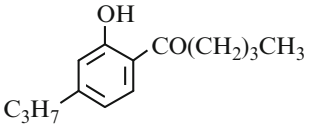


Syntheses
-Refer to: [1595, 2704].

USE: Colour developer, for thermal recording materials [1595].

1-(2-Hydroxy-4-propylphenyl)-1-pentanone

$C_{14}H_{20}O_2$ mol. wt. 220.31

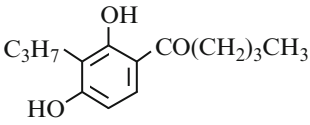


Synthesis
-Obtained by reaction of valeric acid with 3-propylphenol in the presence of zinc chloride (Nencki reaction) (30–40 %) [728].

b.p.$_{0.7}$ 84–85° [728], b.p.$_{18}$ 127–129° [728].

1-(2,4-Dihydroxy-3-propylphenyl)-1-pentanone

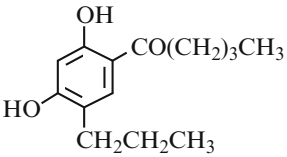
[194792-61-5] $C_{14}H_{20}O_3$ mol. wt. 236.31



Synthesis
-Refer to: [22].

1-(2,4-Dihydroxy-5-propylphenyl)-1-pentanone

$C_{14}H_{20}O_3$ mol. wt. 236.31

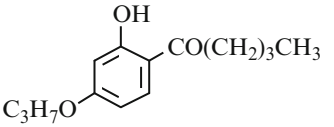


Synthesis
-Obtained by Fries rearrangement of 4-propylresorcinol divalerate with aluminium chloride in nitrobenzene at 50–60° or without solvent at 40–50° [2651].

b.p.$_{9.5}$ 205° [2651]; m.p. 85° [2651].

1-(2-Hydroxy-4-propoxyphenyl)-1-pentanone

$C_{14}H_{20}O_3$ mol. wt. 236.31

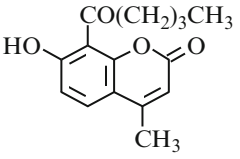


Synthesis
-Refer to: [2222].
Oxime [161171-55-3]
$C_{14}H_{21}NO_3$ mol. wt. 251.33

-Iron complex; stability const. and free energy of formation and molar absorptivity [2222].
-As a spectrophotometric reagent for iron (III) [2222].

7-Hydroxy-4-methyl-8-(1-oxopentyl)-2*H*-1-benzopyran-2-one

[6324-54-5] $C_{15}H_{16}O_4$ mol. wt. 260.29

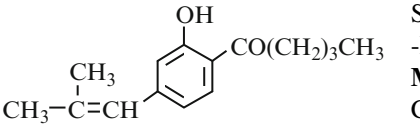


Syntheses
-Obtained by treatment of 4-methyl-7-n-valeroxycoumarin with aluminium chloride at 150° for 1 h (68 %) [1275].
-Also refer to: [329].
pale yellow needles [1275];

m.p. 106° [329], 98–103° [1275].

1-[2-Hydroxy-4-(2-methyl-1-propenyl)phenyl]-1-pentanone

$C_{15}H_{20}O_2$ mol. wt. 232.32

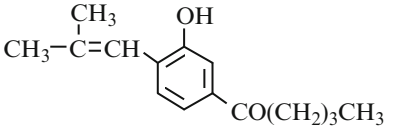


Synthesis
-Refer to: [2323].
Methyl ether [146923-05-9]
$C_{16}H_{22}O_2$ mol. wt. 246.35

-Refer to: [2323].

1-[3-Hydroxy-4-(2-methyl-1-propenyl)phenyl]-1-pentanone

$C_{15}H_{20}O_2$ mol. wt. 232.32

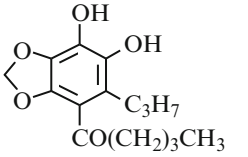


Synthesis
-Refer to: [2323].
Methyl ether [146923-06-0]
$C_{16}H_{22}O_2$ mol. wt. 246.35

-Refer to: [2323].

1-(6,7-Dihydroxy-5-propyl-1,3-benzodioxol-4-yl)-1-pentanone

$C_{15}H_{20}O_5$ mol. wt. 280.32



Synthesis
-Refer to: [2179].
Dimethyl ether [82652-25-3]
(Valeryl dihydrodillapiole)
$C_{17}H_{24}O_5$ mol. wt. 308.37

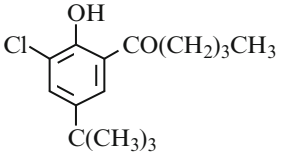
-Obtained by reaction of valeryl chloride with dihydrodillapiole in the presence of fused zinc chloride in methylene chloride for 3–4 h in an ice bath (70 %) [2179].

colourless solid [2179]; ^{1}H NMR [2179], IR [2179].

USE: Synergistic insecticidal activity with pyrethrum [2179].

1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-pentanone

[102003-73-6] $C_{15}H_{21}ClO_2$ mol. wt. 268.78



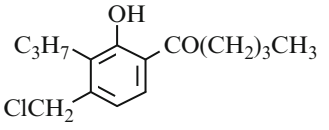
Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-tert-butyl-phenyl valerate with aluminium chloride at 110° (75 %) [3119].
b.p.$_{20}$ 154° [3119].

2,4-Dinitrophenylhydrazone [102596-47-4] $C_{21}H_{25}ClN_4O_5$ mol. wt. 448.91

-Refer to: [3119]; m.p. 185° [3119].

1-[4-(Chloromethyl)-2-hydroxy-3-propylphenyl]-1-pentanone

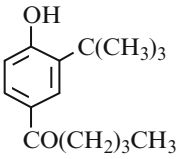
[97582-39-3] $C_{15}H_{21}ClO_2$ mol. wt. 268.78



Synthesis
-Refer to: [877].

1-[3-(1,1-Dimethylethyl)-4-hydroxyphenyl]-1-pentanone

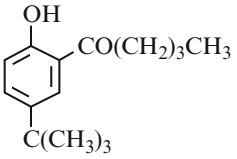
[95185-63-0] $C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis
-Refer to: [2704].

1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-pentanone

[75060-52-5] $C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis
-Obtained by treatment of 2-methoxy-5-tert-butylvalerophenone with 47 % hydrobromic acid /57 % hydriodic acid mixture in refluxing acetic acid for 2 h (45 %) [1475].

^{1}H NMR [1475], IR [1475]; TLC [1475].

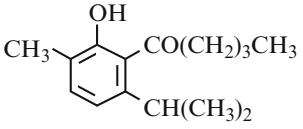
Methyl ether [75060-45-6] $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by reaction of valeryl chloride with 4-tert-butylanisole in the presence of aluminium chloride in methylene chloride under nitrogen, first at 0°, then at 20° for 30 min (100 %) [1475].

TLC [1475].

1-[2-Hydroxy-3-methyl-6-(1-methylethyl)phenyl]-1-pentanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



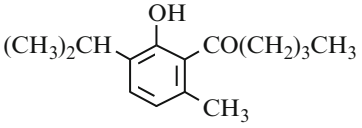
Synthesis
-Obtained by Fries rearrangement of carvacryl valerate with aluminium chloride at 120° (66 %) [2798].
b.p.$_3$ 154° [2798].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

-Refer to: [2798]; m.p. 136° [2798].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-pentanone

[859786-47-3] $C_{15}H_{22}O_2$ mol. wt. 234.34



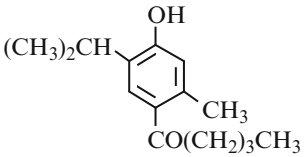
Synthesis
-Obtained by Fries rearrangement of thymyl valerate with aluminium chloride at 120° (77 %) [2803].
b.p.$_2$ 164° [2803].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_5$ mol. wt. 414.45

-Refer to: [2803]; m.p. 170° [2803].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-pentanone

[80356-11-2] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses

-Obtained by photo-Fries rearrangement of thymyl pentanoate in methanol for 6 h at 25° under nitrogen (32 %) (**2a**) [2421].

-Also obtained from its methyl ether by boiling in pyridinium chloride (205–215°) for 105 min (**XXIV**) (19 %) [2660].

-Also refer to: [2704].

b.p.$_{16}$ 200° [2660]; m.p. 86° [2421], 84° [2660];
^{1}H NMR [2421], IR [2421].

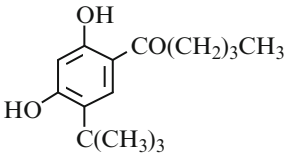
Methyl ether (**V**) $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by reaction of valeryl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (62 %) [2660].

b.p.$_{15}$ 185–187° [2660].

1-[2,4-Dihydroxy-5-(1,1-dimethylethyl)phenyl]-1-pentanone

$C_{15}H_{22}O_3$ mol. wt. 250.34



Synthesis

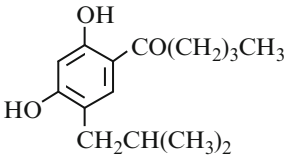
-Refer to: [2704].

m.p. 153° [2704].

USE: As colour developer [2704].

1-[2,4-Dihydroxy-5-(2-methylpropyl)phenyl]-1-pentanone

[798559-94-1] $C_{15}H_{22}O_3$ mol. wt. 250.34



Synthesis

-Obtained by treatment of its dimethyl ether with boron tribromide in methylene, first at −78°, then at 40° [816].

^{1}H NMR [816], ^{13}C NMR [816], IR [816].

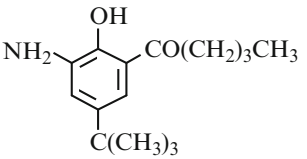
Dimethyl ether [798559-82-7] $C_{17}H_{26}O_3$ mol. wt. 278.39

-Preparation by reaction of pentanoyl chloride with 4-isobutylresorcinol dimethyl ether in the presence of titanium tetrachloride in methylene chloride at 0° (94 %) [816].

m.p. 78–80° [816];
^{1}H NMR [816], ^{13}C NMR [816], IR [816].

1-[3-Amino-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-pentanone

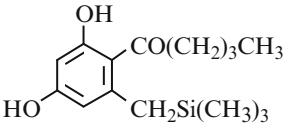
$C_{15}H_{23}NO_2$ mol. wt. 249.35



Synthesis
-Refer to: [2105].

1-[2,4-Dihydroxy-6-[(trimethylsilyl)methyl]phenyl]-1-pentanone

$C_{15}H_{24}O_3Si$ mol. wt. 280.44



Synthesis
-Refer to: [554].

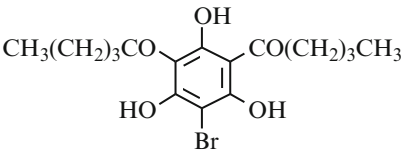
Dimethyl ether [92120-78-0]
$C_{17}H_{28}O_3Si$ mol. wt. 308.49

-Obtained by adding n-butyllithium in hexane to a solution of ethyl 2,4-dimethoxy-6-trimethyl-silyl-methylbenzoate in THF under argon and cooled at −78°. Then, D_2O in THF was added (58 %) [554].
N.B.: The compound was found to be deuteriated on the methylene next to the ketone $C_{17}H_{27}DO_3Si$ mol. wt. 309.19

oil [554];
^{1}H NMR [554], IR [554], UV [554], MS [554].

1,1′-(5-Bromo-2,4,6-trihydroxy-1,3-phenylene)bis-1-pentanone

[3136-48-9] $C_{16}H_{21}BrO_5$ mol. wt. 373.24



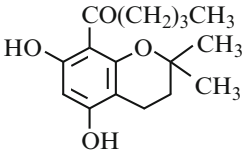
Synthesis
-Refer to: [933].
m.p. 89–91° [457, 2911].

4-Trichloromethane sulfenate [30509-74-1] $C_{17}H_{20}BrCl_3O_5S$ mol. wt. 522.67

-Refer to: [933].

1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-1-pentanone

[35049-65-1] $C_{16}H_{22}O_4$ mol. wt. 278.35

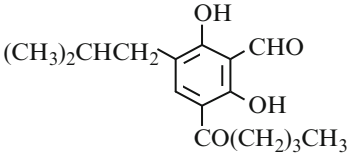


Syntheses
-Obtained from 2-pentanoylcyclohexane-1,3,5-trione [709].
-Also obtained (by-product) by reaction of 2-methyl-2-buten-1-ol with phlorovalerophenone in the presence of Amberlite IR-120 resin (H^+ form) in dioxane at r.t. for 0.5 h. Then, the mixture was refluxed for 24 h (4–5 %) [708]. (Alkenylation of 2-valeroyl-cyclohexane-1,3,5-trione).

m.p. 102° [708, 709];
^{1}H NMR [709], IR [709], UV [709].

2,6-Dihydroxy-3-(2-methylpropyl)-5-(1-oxopentyl)benzaldehyde

[798559-92-9] $C_{16}H_{22}O_4$ mol. wt. 278.35



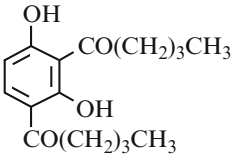
Synthesis
-Preparation by oxidation of 1-[2,4-dihydroxy-3-(hydroxymethyl)-5-(2-methylpropyl)phenyl]-1-pentanone with manganese dioxide (quantitative yield) [816].

^{1}H NMR [816], ^{13}C NMR [816], IR [816].

BIOLOGICAL ACTIVITY: Antiangiogenic [816].

1,1′-(2,4-Dihydroxy-1,3-phenylene)bis-1-pentanone

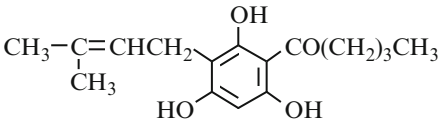
$C_{16}H_{22}O_4$ mol. wt. 278.35



Synthesis
-Obtained by Fries rearrangement of resorcinol divalerate with aluminium chloride (>2 mol) at 130–135° [2651].
b.p.$_{20}$ 196° [2651].

1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-pentanone
(2-Valeryl-4-(3-methylbuten-2-yl)phloroglucinol) (**4**) [1026].

[69916-09-2] $C_{16}H_{22}O_4$ mol. wt. 278.35



Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and prenyl bromide to a solution of phlorovalerophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

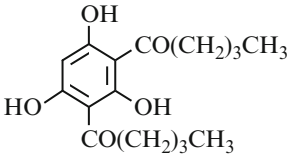
-Also prepared by adding prenyl bromide to a suspension of the sodium salt of phlorovalero-phenone in benzene, then the mixture obtained was refluxed for 3 h [1026, 2111].
-Also obtained by reaction of prenyl chloride with phlorovalerophenone in an alkaline two-phase (aqueous-ether) system and catalyzed by CuCl [838, 3193].
-Also prepared by adding at 5° a solution of sodium methoxide in methanol, followed by isopentenyl bromide in ethyl ether to a solution of phlorovalerophenone in benzene and ethyl ether; then the mixture was stirred at r.t. for 6 h (22 %) [2110, 2113].

m.p. 145° [2113], 126–127° [3193];
N.B.: One of the reported melting point is obviously wrong.
^{13}C NMR [839, 1026, 3193], IR [1026].

BIOLOGICAL ACTIVITY: Antifungal against *Trichophyton* species [2113]; Antifungal [2113]; Min. inhibitory *Trichophyton interdigitale, Candida albicans, Staphylococcus aureus*, etc. [2110]; Bactericidal and fungicidal [1026, 3193].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-pentanone
(Divaleryl phloroglucinol)

[3118-32-9] $C_{16}H_{22}O_5$ mol. wt. 294.35



Syntheses
-Refer to: [457, 644, 2190, 2911, 3405].
m.p. 104–106° [457, 2911].

BIOLOGICAL ACTIVITY: As photosynthetic electron transport (PET) [3405]; Antiviral towards the replication of vesicular stomatitis virus in HEL cell cultures [644]; Inhibited aldose reductase in swines [2190]; Inhibition of the Hill reaction using chloroplasts isolated from the leaves of *Spinacia oleracea* [3405].

Na salt m.p. 140–180° [2911].

Tri-Na salt [5862-26-0] $C_{16}H_{19}O_5Na_3$ mol. wt. 361.32

-Refer to: [457].

m.p. 180° (d) [457].

Mg salt [24070-03-9].

-Refer to: [457, 2911].

m.p. >200° [457, 2911], 200° (d) [457].

Piperazine salt [4963-67-1] $C_{16}H_{22}O_5*C_4H_{10}N_2$ mol. wt. 380.48

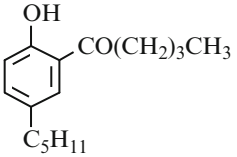
m.p. 80–85° [457, 2911].

1,3,5-Tris-trichloromethane sulfenate [30509-76-3].

-Refer to: [933].

1-(2-Hydroxy-5-pentylphenyl)-1-pentanone

[63494-45-1] $C_{16}H_{24}O_2$ mol. wt. 248.37



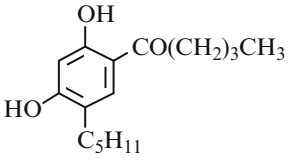
Synthesis

-Obtained by reaction of pentanoic acid with 4-pentylphenol in the presence of boron trifluoride at 25–30° for 45 min, then at 140° for 12 min and at 140–150° for 1 h (77 %) [142].

$b.p._{.1}$ 122–127° [142].

1-(2,4-Dihydroxy-5-pentylphenyl)-1-pentanone

$C_{16}H_{24}O_3$ mol. wt. 264.36



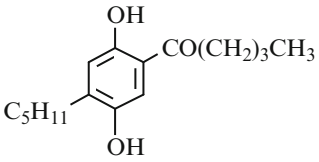
Syntheses

-Refer to: [1628, 1629].

USE: As antioxidant for vitamin A [1628, 1629].

1-(2,5-Dihydroxy-4-pentylphenyl)-1-pentanone

$C_{16}H_{24}O_3$ mol. wt. 264.36



Synthesis
-Refer to: [2234].

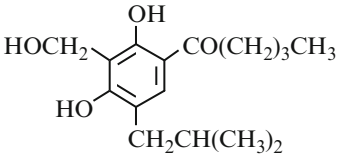
Dimethyl ether [38844-02-9]
$C_{18}H_{28}O_3$ mol. wt. 292.42

-Obtained by reaction of valeryl chloride with 1,4-dimethoxy-2-pentylbenzene in the presence of aluminium chloride in carbon disulfide (71 %) [2234].

colourless liquid [2234]; b.p.$_{0.6}$ 155–160° [2234].

1-[2,4-Dihydroxy-3-(hydroxymethyl)-5-(2-methylpropyl)phenyl]-1-pentanone

[798559-83-8] $C_{16}H_{24}O_4$ mol. wt. 280.36



Synthesis
-Obtained by reaction of formaldehyde with 1-[2,4-dihydroxy-5-(2-methylpropyl)phenyl]-1-pentanone in the presence of KOH and $CaCl_2$ in methanol (62 %) [816].

m.p. 90–92° [816];
^{1}H NMR [816], ^{13}C NMR [816], IR [816].

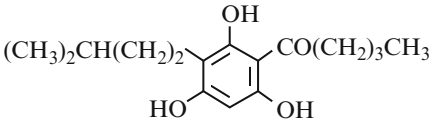
Dimethyl ether [798559-84-9] $C_{18}H_{28}O_4$ mol. wt. 308.42

-Obtained by treatment of the title ketone with methyl iodide in the presence of potassium carbonate in propanone (72 %) [816].

^{1}H NMR [816], ^{13}C NMR [816], IR [816].

1-[2,4,6-Trihydroxy-3-(3-methylbutyl)phenyl]-1-pentanone

[74477-98-8] $C_{16}H_{24}O_4$ mol. wt. 280.36



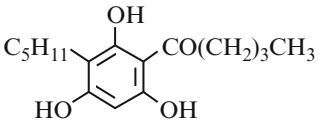
Synthesis
-Obtained by hydrogenation of 1-[2,4,6-tri-hydroxy-3-(3-methyl-2-butenyl)phenyl]-1-pentanone in the presence of PtO_2 in methanol under a hydrogen atmosphere at r.t. for 1 h (88 %) [2113].

m.p. 169° [2113].

BIOLOGICAL ACTIVITY: Antifungal [2113].

1-(2,4,6-Trihydroxy-3-pentylphenyl)-1-pentanone

[69916-12-7] $C_{16}H_{24}O_4$ mol. wt. 280.36



Synthesis

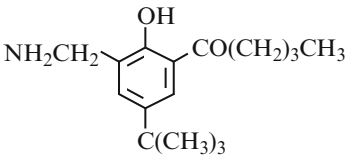
-Obtained by adding a solution of pentanoyl chloride in nitrobenzene to a suspension, of 2,4,6-trihydroxypentyl-benzene and aluminium chloride in carbon disulfide at r.t., then stirring the mixture for 6 h at 30–35° (40 %) [2113].

m.p. 134° [2113].

BIOLOGICAL ACTIVITY: Antifungal [2113].

1-[(3-Aminomethyl)-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-pentanone

[75060-95-6] $C_{16}H_{25}NO_2$ mol. wt. 263.38



Synthesis

-Refer to: [1475].

Hydrochloride [75060-70-7]

$C_{16}H_{25}NO_2$, HCl mol. wt. 299.84

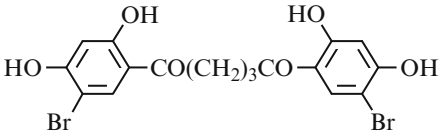
-Obtained by treatment of 1-[3-(N-chloroacetylaminomethyl)-5-(1,1-dimethylethyl)-2-hydroxy-phenyl]-1-pentanone with conc. hydrochloric acid in refluxing ethanol for 20 h (68 %) [1475].

white amorphous crystals [1475]; m.p. 187–190° [1289, 1475]; ^{1}H NMR [1475], IR [1475]; TLC [1475].

BIOLOGICAL ACTIVITY: As inflammation inhibitor [1475].

1,5-Bis(5-bromo-2,4-dihydroxyphenyl)-1,5-pentanedione

[16093-32-6] $C_{17}H_{14}Br_2O_6$ mol. wt. 474.10



Syntheses

-Obtained by treatment of its tetramethyl ether below with 40 % hydrobromic acid in refluxing acetic acid for 15 h (67 %) [592].

-Also obtained by condensation of 4-bromoresorcinol with glutaryl chloride in the presence of aluminium chloride in nitrobenzene [592].

m.p. 214–215° [592].

Di-2,4-dinitrophenylhydrazone [16093-33-7] $C_{29}H_{22}Br_2N_8O_{12}$ mol. wt. 834.35

m.p. 262° [592].

Tetramethyl ether [16093-34-8] $C_{21}H_{22}Br_2O_6$ mol. wt. 530.21

-Obtained by reaction of glutaryl chloride with 4-bromoresorcinol dimethyl ether in the presence of aluminium chloride in nitrobenzene at 0° for 13 h (21 %) [592].

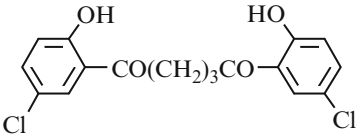
m.p. 193° [592].

Dioxime of the tetramethyl ether [16093-35-9] $C_{21}H_{24}Br_2N_2O_6$ mol. wt. 560.24

m.p. 205° [592].

1,5-Bis(5-chloro-2-hydroxyphenyl)-1,5-pentanedione

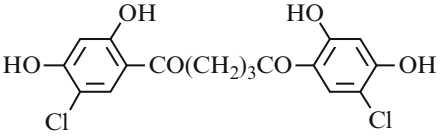
[52016-63-4] $C_{17}H_{14}Cl_2O_4$ mol. wt. 353.20



Syntheses
-Refer to: [1291].
m.p. 156–157° [670], 156° [1291], 97° [1783]; ^{1}H NMR [1783], IR [1783].

1,5-Bis(5-chloro-2,4-dihydroxyphenyl)-1,5-pentanedione

[16093-26-8] $C_{17}H_{14}Cl_2O_6$ mol. wt. 385.20



Syntheses
-Also obtained by condensation of 4-chloro-resorcinol with glutaryl chloride in the presence of aluminium chloride in nitrobenzene [592].
-Also refer to: [586].

m.p. 284° [586], 223° [592].

Dioxime [16093-27-9] $C_{17}H_{16}Cl_2N_2O_6$ mol. wt. 415.23

m.p. 321° [592].

Di-2,4-dinitrophenylhydrazone [96809-09-5] $C_{29}H_{22}Cl_2N_8O_{12}$ mol. wt. 745.45

m.p. 290° [586].

Tetramethyl ether [16093-28-0] $C_{21}H_{22}Cl_2O_6$ mol. wt. 441.31

-Obtained by reaction of glutaryl chloride with 4-chlororesorcinol dimethyl ether in the presence of aluminium chloride in nitrobenzene [592].

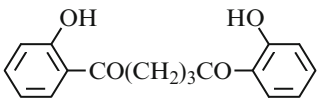
m.p. 198° [592].

Dioxime of the tetramethyl ether [16093-29-1] $C_{21}H_{24}Cl_2N_2O_6$ mol. wt. 471.34

m.p. 208° [592].

1,5-Bis(2-hydroxyphenyl)-1,5-pentanedione
(1,3-Disalicycloylpropane)

[4945-79-3] $C_{17}H_{16}O_4$ mol. wt. 284.31



Syntheses
-Obtained by Fries rearrangement of phenyl glutarate with aluminium chloride (15–20 %) [1576], (11 %) [1400],
-in the presence of solvents:
*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];
*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].
-Also obtained by alkaline hydrolysis of dicoumarol [723, 941 (66 %), 2324, 3293 (98–99 %)].
-Also refer to: [1575, 2118, 2936].

m.p. 102° [902, 941, 1575, 1576], 101–102° [2936], 100–102° [1400];
^{1}H NMR [2324], UV [2118]; pK_a [2118].

Dimethyl ether [190248-05-6] $C_{19}H_{20}O_4$ mol. wt. 312.36

-Obtained by reaction of methyl iodide with the title ketone in the presence of silver oxide at reflux for 1 h (50 %) [1400].
-Also obtained by reaction of dimethyl sulfate with the title bisphenol in the presence of potassium hydroxide in ethanol (87 %) [3293].
-Also refer to: [2936].

m.p. 86–88° [1400, 2936]; UV [1400].

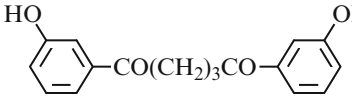
Dimethanesulfonate $C_{19}H_{20}O_8S_2$ mol. wt. 440.50

-Obtained by reaction of MsCl with 1,5-bis(2-hydroxyphenyl)-1,5-pentanedione in the presence of triethylamine in methylene chloride at r.t. for 1.5 h under nitrogen atmosphere (87.7 %) [2324].

m.p. 68–69° [2324]; ^{1}H NMR [2324], IR [2324]; TLC [2324].

1,5-Bis(3-hydroxyphenyl)-1,5-pentanedione

[10365-53-4] $C_{17}H_{16}O_4$ mol. wt. 284.31

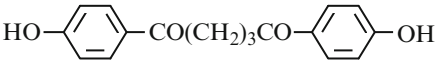


Syntheses
-Obtained by diazotization of 1,5-bis (3-aminophenyl)-1,5-pentanedione (40–50 %) [1576].
-Also refer to: [1575].

m.p. 152° [1575, 1576].

1,5-Bis(4-hydroxyphenyl)-1,5-pentanedione

[20837-35-8] $C_{17}H_{16}O_4$ mol. wt. 284.31



Syntheses
-Obtained by Fries rearrangement of phenyl glutarate with aluminium chloride [1400],

-in the presence of solvents:
*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];
*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].
-Also obtained by reaction of hydrobromic acid with its dimethyl ether in acetic acid for 2 h at 120° [902].

m.p. 222–225° [1148], 220–221° [902]; IR [588].

Diacetate [102474-24-8] $C_{21}H_{20}O_6$ mol. wt. 368.39

-Obtained by reaction of acetic anhydride with 1,5-bis(4-hydroxyphenyl)-1,5-pentanedione [902].

m.p. 122° [902].

Dimethyl ether [4609-11-4] $C_{19}H_{20}O_4$ mol. wt. 312.36

Syntheses
-Obtained by reaction of dimethyl sulfate with 1,5-bis(4-hydroxyphenyl)-1,5-pentanedione in the presence of 2 N NaOH [902].
-Also obtained by reaction of glutaryl dichloride with anisole in the presence of aluminium chloride [2644], (80–90 %) [1576],
*in carbon disulfide (78 %) [2495];
*in nitrobenzene/tetrachloroethane mixture (1:4) [588];
*in methylene chloride [2329].
-Also obtained by reaction of glutaric anhydride with anisole in the presence of aluminium chloride in tetrachloroethane/nitrobenzene (1:2) at 0–5° [588].
-Also obtained by oxidation (ozonization) of 1,2-bis-(p-methoxyphenyl) cyclopentene [2169].
-Also refer to: [1890 (40 %)].

Isolation from natural sources

-In the New Zealand manuka honey [790].

m.p. 101° [588, 2694], 99.8–100.2° [2169], 99.5–100.5° [2644], 99–101° [2329], 99–100° [1148], 99° [902, 1575, 1576, 1890, 3288], 97–98° [1155], 95–96° [1867];
^{1}H NMR [1867], ^{13}C NMR [1867], IR [588, 1867]; GC-MS [790].

Di-2,4-dinitrophenylhydrazone of the dimethyl ether $C_{31}H_{28}N_8O_{10}$ mol. wt. 672.61

m.p. 245–246° [2169].

Diethyl ether [101684-67-7] $C_{21}H_{24}O_4$ mol. wt. 340.42

-Refer to: [1890 (35 %), 2466, 2469, 3288].

m.p. 133° [3288], 112.5° [1890].

Dipropyl ether [101684-68-8] $C_{23}H_{28}O_4$ mol. wt. 368.47

-Refer to: [1890 (30 %), 2466, 2469].

m.p. 88° [1890].

Dibutyl ether [101684-69-9] $C_{25}H_{32}O_4$ mol. wt. 396.53

-Obtained by reaction of glutaryl dichloride with phenyl butyl ether in the presence of aluminium chloride in methylene chloride [2329].
-Also refer to: [1890, 2466 (44 %)].

m.p. 95–97° [2329], 85° [1890].

Dipentyl ether [101684-71-3] $C_{27}H_{36}O_4$ mol. wt. 424.58

-Refer to: [1890 (37 %), 2466].

m.p. 75° [1890].

Dihexyl ether [104192-31-6] $C_{29}H_{40}O_4$ mol. wt. 452.63

-Refer to: [1890 (33 %), 2468].

m.p. 93–95° [2468], 85° [1890].

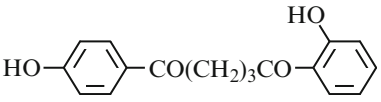
Diphenyl ether $C_{29}H_{24}O_4$ mol. wt. 436.51

-Obtained by reaction of glutaryl dichloride with diphenyl oxide in the presence of aluminium chloride in methylene chloride [2329].

m.p. 99–101° [2329].

1-(2-Hydroxyphenyl)-5-(4-hydroxyphenyl)-1,5-pentanedione

[101597-59-5] $C_{17}H_{16}O_4$ mol. wt. 284.31



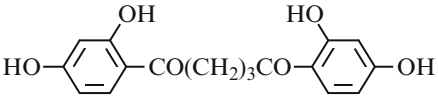
Syntheses
-Obtained by Fries rearrangement of phenyl glutarate with aluminium chloride,
-in the presence of solvents,

*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];
*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].

m.p. 141° [902].

1,5-Bis(2,4-dihydroxyphenyl)-1,5-pentanedione

[16093-22-4] $C_{17}H_{16}O_6$ mol. wt. 316.31



Syntheses
-Obtained by condensation of resorcinol with glutaryl chloride in the presence of aluminium chloride in nitrobenzene [592].
-Also refer to: [586].

m.p. 225° [592], 201–202° [586].

Dioxime [16093-23-5] $C_{17}H_{18}N_2O_6$ mol. wt. 346.34

m.p. 238° [592].

Di-2,4-dinitrophenylhydrazone [96273-02-8] $C_{29}H_{24}N_8O_{12}$ mol. wt. 676.56

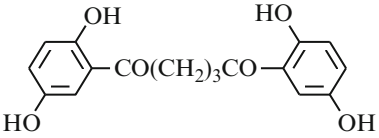
m.p. 290° [586].

Tetramethyl ether [95002-59-8] $C_{21}H_{24}O_6$ mol. wt. 372.42

-Refer to: [586]; m.p. 115° [586].

1,5-Bis(2,5-dihydroxyphenyl)-1,5-pentanedione

[91453-24-6] $C_{17}H_{16}O_6$ mol. wt. 316.31



Synthesis
-Obtained by treatment of 1,5-bis(2-hydroxy-5-methoxyphenyl)-1,5-pentanedione with boron tribromide in methylene chloride (80 %) [2103].

yellow solid [2103]; m.p. 211–213° [2103].

Tetramethyl ether [10365-22-7] $C_{21}H_{24}O_6$ mol. wt. 372.42

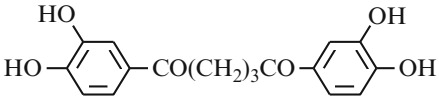
-Obtained by reaction of glutaric acid dichloride (1 mol) with hydroquinone dimethyl ether (2.5 mol) in the presence of aluminium chloride (1 mol) (64 %) [1575].

-Also obtained by reaction of glutaric acid dichloride with hydroquinone dimethyl ether in the presence of aluminium chloride in carbon disulfide or methylene chloride (53–56 %) [1402]; in carbon disulfide for 3 h at 0°, then 13 h at r.t. (67 %) [2159].
-Also refer to: [1575].

m.p. 66° [1575], 64–65° [2159]; IR [2159].

1,5-Bis(3,4-dihydroxyphenyl)-1,5-pentanedione

$C_{17}H_{16}O_6$ mol. wt. 316.31



Synthesis
-Refer to: [592].
Tetramethyl ether [1248-88-0]
$C_{21}H_{24}O_6$ mol. wt. 372.42

-Obtained by condensation of veratrole with glutaryl chloride in the presence of aluminium chloride in tetrachloroethane [592] or in carbon disulfide (12 %) [2376].
-Also obtained by condensation of veratrole with glutaric acid in the presence of boron trifluoride at 80–90° for 2 h (15 %) [2376].
-Also obtained by condensation of veratrole with glutaric anhydride [2524].
-Also refer to: [1014 (85 %)].

m.p. 144–146° [2524], 124° [592], 121° [2376], 120–121° [1014].

Dioxime of the tetramethyl ether $C_{21}H_{26}N_2O_6$ mol. wt. 402.44

m.p. 146° [2376], 112–114° [1014].

Di-methyloxime of the tetramethyl ether

[50766-27-3] $C_{23}H_{30}N_2O_6$ mol. wt. 430.50

m.p. 112–114° [1014].

Di-2,4-dinitrophenylhydrazone of the tetramethyl ether

[16148-93-9] $C_{33}H_{32}N_8O_{12}$ mol. wt. 732.66

m.p. 200–202° [2524], 150° [592].

Tetrabutyl ether [123387-95-1] $C_{33}H_{48}O_6$ mol. wt. 540.74

-Refer to: [97].

^{1}H NMR [97].

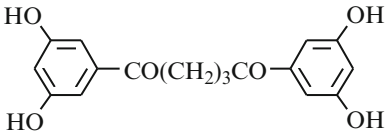
Tetradecyl ether [123387-96-2] $C_{57}H_{96}O_6$ mol. wt. 877.38

-Refer to: [97].

^{1}H NMR [97].

1,5-Bis(3,5-dihydroxyphenyl)-1,5-pentanedione

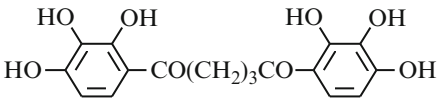
$C_{17}H_{16}O_6$ mol. wt. 316.31



Synthesis
-Refer to: [1316].
m.p. 205–208° [1316].

1,5-Bis(2,3,4-trihydroxyphenyl)-1,5-pentanedione

$C_{17}H_{16}O_8$ mol. wt. 348.31



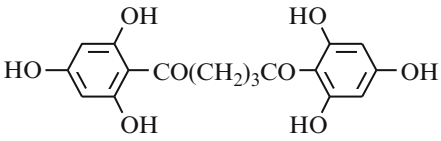
Synthesis
-Refer to: [1574].
Hexamethyl ether [10475-16-8]
$C_{23}H_{28}O_8$ mol. wt. 432.47

-Obtained by reaction of dimethyl sulfate with 1,5-bis(2-hydroxy-3,4-dimethoxyphenyl)-1,5-pentanedione the presence of 30 % sodium hydroxide (65–90 %) [1574].
-Also refer to: [1575].

m.p. 84° [1574, 1575].

1,5-Bis(2,4,6-trihydroxyphenyl)-1,5-pentanedione

[16093-48-4] $C_{17}H_{16}O_8$ mol. wt. 348.31



Syntheses
-Obtained by reaction of glutaryl chloride with phloroglucinol in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture [592].

-Also refer to: [3374].

m.p. 288° [592], 286–286.5° (d) [3374].

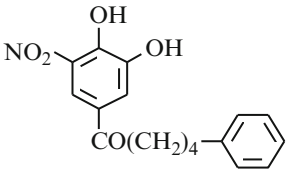
Di-2,4-dinitrophenylhydrazone

[16093-15-5] $C_{29}H_{24}N_8O_{14}$ mol. wt. 708.56

m.p. 276° [592].

1-(3,4-Dihydroxy-5-nitrophenyl)-5-phenyl-1-pentanone

$C_{17}H_{17}NO_5$ mol. wt. 315.33

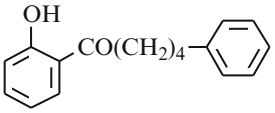


Syntheses
-Obtained by cleavage of 3-methyl ether,
*with 48 % hydrobromic acid in boiling acetic acid [1843];
*using aluminium chloride and pyridine in warm ethyl acetate (90–99 %) [1843].

m.p. 109–111° [1843];
^{1}H NMR [1843], ^{13}C NMR [1843], IR [1843]; HPLC [1843].

1-(2-Hydroxyphenyl)-5-phenyl-1-pentanone

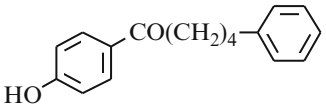
[37765-93-8] $C_{17}H_{18}O_2$ mol. wt. 254.33



Synthesis
-Refer to: [84].
b.p.$_{1.7}$ 157–158° [84]; m.p. 36.5–37.5° [84].

1-(4-Hydroxyphenyl)-5-phenyl-1-pentanone
(Daphnolon)

$C_{17}H_{18}O_2$ mol. wt. 254.33

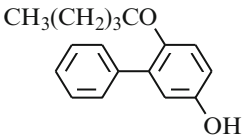


Isolation from natural product
-From Callus cells of *Daphne Giraldii* [3263].

BIOLOGICAL ACTIVITY: Cytotoxic [3263].

1-[1,1′-Biphenyl]-2-yl-5-hydroxy-1-pentanone

$C_{17}H_{18}O_2$ mol. wt. 254.33



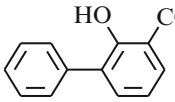
Synthesis
-Refer to: [239].
Methyl ether [1093860-17-3]
$C_{18}H_{20}O_2$ mol. wt. 268.36

-Refer to: [239].

USE: Preparation of aminobiphenylcyclopentanecarboxamide derivs. for use as renin inhibitors [239].

1-[1,1′-Biphenyl]-3-yl-2-hydroxy-1-pentanone

$C_{17}H_{18}O_2$ mol. wt. 254.33



Syntheses
-Obtained by Fries rearrangement of 2-(valeroyloxy)-biphenyl with aluminium chloride at 160° for 30–45 min (20 %) [1257].

-Also refer to: [661].

b.p.$_{.5}$ 200–210° [661, 1257].

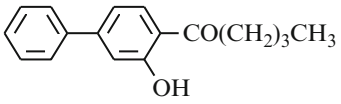
Methyl ether $C_{18}H_{20}O_2$ mol. wt. 268.36

-Refer to: [504, 661, 1257].

b.p.$_{.4}$ 202–204° [661, 1257], b.p.$_{.27}$ 275–280° [504];
$n_D^{27} = 1.5857$ [504].

1-(1,1′-Biphenyl)-4-yl-3-hydroxy-1-pentanone

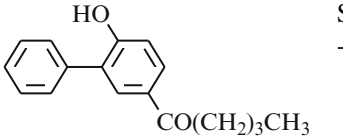
[792706-16-2] $C_{17}H_{18}O_2$ mol. wt. 254.33



Synthesis
-Refer to: [2553].

1-[1,1′-Biphenyl]-5-yl-2-hydroxy-1-pentanone

[95102-33-3] $C_{17}H_{18}O_2$ mol. wt. 254.33



Syntheses
-Obtained by Fries rearrangement of 2-(valeroyloxy)-biphenyl with aluminium chloride at 160° for 30–45 min (40 %) [1257].
-Also obtained by treatment of its methyl ether with pyridinium chloride for 1 h at reflux [504].

-Also refer to: [661, 1595].

Fine colourless needles [504]; m.p. 104° [661, 1257], 75° [504].

USE: Colour developer, for thermal recording materials [2704].

Methyl ether [854659-36-2] $C_{18}H_{20}O_2$ mol. wt. 268.36

-Obtained by reaction of valeroyl chloride (or valeroyl anhydride [1334]) with 2-methoxydiphenyl in the presence of aluminium chloride in carbon disulfide for 4 h at r.t. (85 %) or for 2 h at reflux (40 %) [1257].

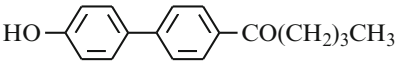
pale yellow oil [504]; b.p.$_{.4}$ 202–204° [1257], b.p.$_{.27}$ 275–280° [504];
$n_D^{27} = 1.5857$ [504].

Semicarbazone of the methyl ether $C_{19}H_{23}N_3O_2$ mol. wt. 325.41

m.p. 141° [504].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-pentanone

[219513-03-8] $C_{17}H_{18}O_2$ mol. wt. 254.33



Synthesis
-Refer to: [1518].

USE: For preparation of biphenylyl sulfamates as steroid sulfatase inhibitors for estrogen-dependent diseases [1518].

Acetate [214534-24-4] $C_{19}H_{20}O_3$ mol. wt. 296.36

-Obtained by reaction of pentanoyl chloride with 4-acetoxybiphenyl in the presence of aluminium chloride in methylene chloride at 0–5° for 6 h (63.1 %) [2344].

Methyl ether [56116-77-9] $C_{18}H_{20}O_2$ mol. wt. 268.36

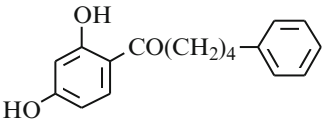
-Refer to: [847].

Octyl ether [56117-37-4] $C_{25}H_{34}O_2$ mol. wt. 366.54

USE: Lamellar liquid crystals comprising [920].

1-(2,4-Dihydroxyphenyl)-5-phenyl-1-pentanone

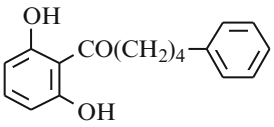
[20038-59-9] $C_{17}H_{18}O_3$ mol. wt. 270.33



Synthesis
-Refer to: [1010].
m.p. 80–83° [1010].

1-(2,6-Dihydroxyphenyl)-5-phenyl-1-pentanone

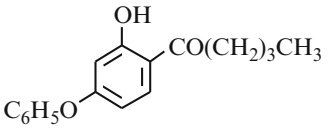
$C_{17}H_{18}O_3$ mol. wt. 270.33



Synthesis
-Refer to: [1389].
^{1}H NMR [1389], IR [1389].

1-(2-Hydroxy-4-phenoxyphenyl)-1-pentanone

[307000-44-8] $C_{17}H_{18}O_3$ mol. wt. 270.32

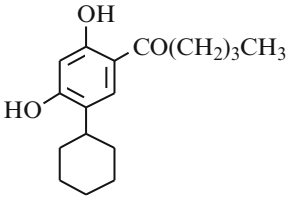


Synthesis
-Refer to: [1345].

USE: Preparation of hydroxydiphenyl ethers as antimicrobials [1345].

1-(5-Cyclohexyl-2,4-dihydroxyphenyl)-1-pentanone

[159977-39-6] $C_{17}H_{24}O_3$ mol. wt. 276.38

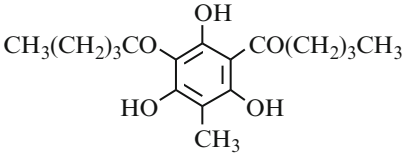


Synthesis
-Obtained (**XIX**) by reaction of valeric acid with 4-cyclohexylresorcinol in the presence of boron trifluoride etherate at 105–108° for 15 min, the hydrolysis of the BF_2-chelate (**IX**) obtained [2382].
m.p. 134–135° [2382]; IR [2382], UV [2382].

BF2-chelate (**IX**) $C_{17}H_{23}BF_2O_3$ mol. wt. 324.17 (61 %) [2382].
m.p. 106–107° [2382]; IR [2382].

1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-pentanone

[3118-33-0] $C_{17}H_{24}O_5$ mol. wt. 308.37

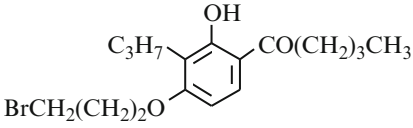


Syntheses
-Refer to: [457, 600, 2911].
m.p. 98–100° [457, 2911].

BIOLOGICAL ACTIVITY: For treatment of immune dysfunction associated with human immunodeficiency virus infection [600]; Anthelmintic [457].

1-[4-(3-Bromopropoxy)-2-hydroxy-3-propylphenyl]-1-pentanone

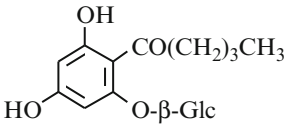
[194792-62-6] $C_{17}H_{25}BrO_3$ mol. wt. 357.28



Synthesis
-Refer to: [22].

1-[2-(β-D-Glucopyranosyloxy)-4,6-dihydroxyphenyl]-1-pentanone

[853913-75-4] $C_{17}H_{25}O_9$ mol. wt. 373.15



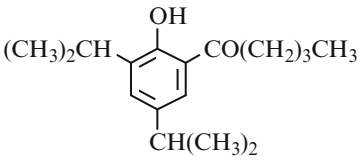
Isolation from natural sources
-From the whole plant of *Indigofera heterantha* (Leguminosae) [209].
colourless gummy solid [209];

^{1}H NMR [209], ^{13}C NMR [209], IR [209], UV [209], MS [209].

BIOLOGICAL ACTIVITY: Lipoxygenase enzyme inhibitor [209].

1-[2-Hydroxy-3,5-di(1-methylethyl)phenyl]-1-pentanone

[73991-79-4] $C_{17}H_{26}O_2$ mol. wt. 262.39



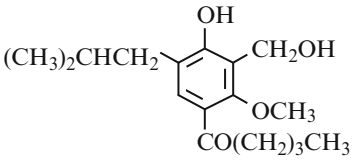
Synthesis
-Obtained by reaction of n-butylmagnesium bromide with 3,5-diisopropylsalicylic acid in the presence of nickel [1970].
^{1}H NMR [1970] IR [1970], MS [1970], ESR spectrum [1970].

ion(1-), radical ion (1-) [57133-44-5].

-Formation of, in reaction of diisopropylsalicylic acid with butylmagnesium bromide, ESR spectrum of [1970].

1-[4-Hydroxy-3-(hydroxymethyl)-2-methoxy-5-(2-methylpropyl)phenyl]-1-pentanone

[798559-89-4] $C_{17}H_{26}O_4$ mol. wt. 294.39



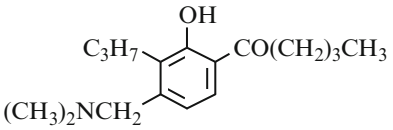
Syntheses
-Preparation by chemoselective protection of 1-[2,4-dihydroxy-3-(hydroxymethyl)-5-(2-methyl-propyl)phenyl]-1-pentanone by treatment of this with p-toluenesulfonic acid in propanone. The intermediate obtained (93 %) was methylated by reaction with methyl iodide in the presence of potassium carbonate in propanone at 57°, followed by deprotection of the acetal (60 %) [816].

-The synthesis of this ketone was accomplished in eight steps and 33 % overall yield [2310] in accordance to [816].

m.p. 60–61° [816];
^{1}H NMR [816], ^{13}C NMR [816], IR [816].

1-[4-[(Dimethylamino)methyl]-2-hydroxy-3-propylphenyl]-1-pentanone

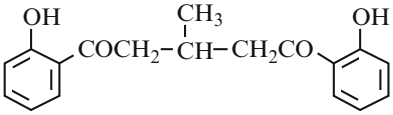
[97582-34-8] $C_{17}H_{27}NO_2$ mol. wt. 277.41



Synthesis
-Refer to: [877].

1,5-Bis(2-hydroxyphenyl)-3-methyl-1,5-pentanedione

[52852-89-8] $C_{18}H_{18}O_4$ mol. wt. 298.34

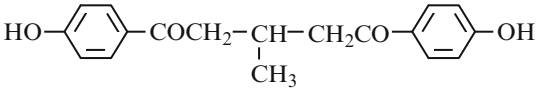


Syntheses
-Refer to: [941 (79 %), 2118, 2925].
m.p. 112° [941]; pK_a [2118];

^{1}H NMR [2925], ^{13}C NMR [2925], IR [2925], UV [2118].

1,5-Bis(4-hydroxyphenyl)-3-methyl-1,5-pentanedione

$C_{18}H_{18}O_4$ mol. wt. 298.34



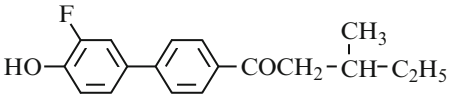
Synthesis
-Refer to: [1890].

Dimethyl ether $C_{20}H_{22}O_4$ mol. wt. 326.39

-Refer to: [1890, 3288].

1-(3′-Fluoro-4′-hydroxy[1,1′-biphenyl]-4-yl)-3-methyl-1-pentanone

$C_{18}H_{19}FO_2$ mol. wt. 286.35



Synthesis
-Refer to: [2107].

Heptyl ether (S) [112780-60-6] $C_{25}H_{33}FO_2$ mol. wt. 384.53

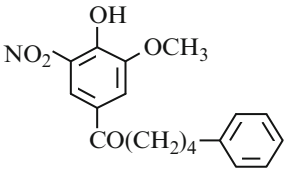
USE: Liq.-crystal compns. contg., for display devices [2107].

Octyl ether (S) [112780-61-7] $C_{26}H_{35}FO_2$ mol. wt. 398.56

USE: Liq.-crystal compns. contg., for display devices [2107].

1-(4-Hydroxy-3-methoxy-5-nitrophenyl)-5-phenyl-1-pentanone

$C_{18}H_{19}NO_5$ mol. wt. 329.35

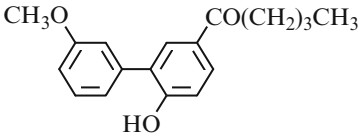


Synthesis

-Obtained by regioselective nitration under mild conditions of 1-(4-hydroxy-3-methoxyphenyl)-5-phenyl-1-pentanone with 70 % nitric acid in acetic acid (67–77 %) [1843].

1-(6-Hydroxy-3′-methoxy[1,1′-biphenyl]-3-yl)-1-pentanone

[565203-88-5] $C_{18}H_{20}O_3$ mol. wt. 284.35



Synthesis

-Obtained by treatment of its methyl ether with boron tribromide in methylene chloride [1885].

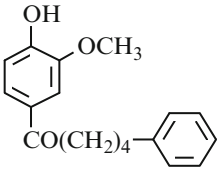
Methyl ether [565203-85-2] $C_{19}H_{22}O_3$ mol. wt. 298.38

1-(3′,6-Dimethoxy[1,1′-biphenyl]-3-yl)-1-pentanone

-Obtained treatment of the mixture of 3-iodo-4-methoxyvalerophenone and 3-methoxyphenyl-boronic acid with $Pd(PPh_3)_4$ [1885].

1-(4-Hydroxy-3-methoxyphenyl)-5-phenyl-1-pentanone

$C_{18}H_{20}O_3$ mol. wt. 284.35



Synthesis

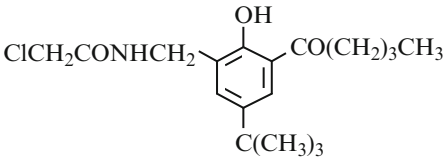
-Selective deprotection of the benzyl-protecting group proceeded smoothly under acidic conditions (excess 30 % HBr in acetic acid and methylene chloride) at r.t. for 2 h (75–87 %) or more conveniently by catalytic hydrogen transfer using ammonium formate as hydrogen donor and palladium catalysis to provide the phenol (84–92 %) [1843].

Benzyl ether $C_{25}H_{26}O_3$ mol. wt. 374.48

-Obtained from 1-(4-benzyloxy-3-methoxyphenyl)-5-phenyl-1-pentanol by Oppenauer oxidation using sodium tert-butoxide as base and cyclohexanone as hydrogen acceptor in warm toluene (87–94 %) [1843].

1-[3-(N-Chloroacetylaminomethyl)-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-pentanone

$C_{18}H_{26}ClNO_3$ mol. wt. 339.86



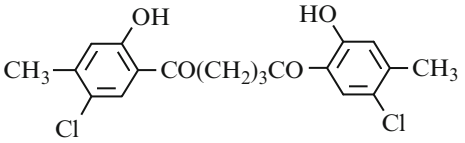
Synthesis

-Obtained by adding N-hydroxymethylchloro-acetamide to 2-valeryl-4-tert-butylphenol dissolved in acetic acid and conc. sulfuric acid mixture at r.t. and stirred at 60° for 2 h (60 %) [1475].

^{1}H NMR [1475], IR [1475]; TLC [1475].

1,5-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,5-pentanedione

[4609-08-9] $C_{19}H_{18}Cl_2O_4$ mol. wt. 381.26



Synthesis

-Obtained by reaction of glutaric anhydride with 4-chloro-3-methyl-phenol in the presence of aluminium chloride in tetrachloro-ethane/nitrobenzene mixture (1:1) [588].

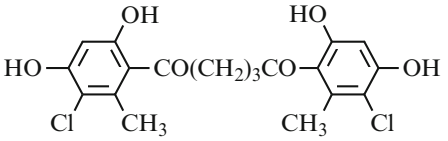
m.p. 160° [588]; IR [588].

Dioxime [4609-09-0] $C_{19}H_{20}Cl_2N_2O_4$ mol. wt. 411.28

m.p. 210° [588].

1,5-Bis(5-chloro-2,4-dihydroxy-6-methylpheny)l-1,5-pentanedione

$C_{19}H_{18}Cl_2O_6$ mol. wt. 413.25



Synthesis

-Also refer to: [592].

Tetramethyl ether [16148-68-8]

$C_{23}H_{26}Cl_2O_6$ mol. wt. 469.36

-Obtained by condensation of 4-chloroorcinol dimethyl ether with glutaryl chloride in the presence of aluminium chloride [592].

m.p. 145° [592].

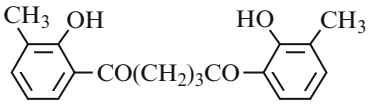
Di-2,4-dinitrophenylhydrazone of the tetramethyl ether

[16093-49-5] $C_{35}H_{34}Cl_2N_8O_{12}$ mol. wt. 829.61

m.p. 176° [592].

1,5-Bis(2-hydroxy-3-methylphenyl)-1,5-pentanedione

[10365-65-8] $C_{19}H_{20}O_4$ mol. wt. 312.36



Syntheses

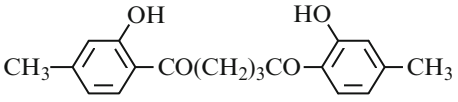
-Obtained by Fries rearrangement of o-cresol glutarate with aluminium chloride (15–20 %) [1576].

-Also refer to: [1575].

m.p. 105° [1575, 1576].

1,5-Bis(2-hydroxy-4-methylphenyl)-1,5-pentanedione

[10571-10-5] $C_{19}H_{20}O_4$ mol. wt. 312.36



Syntheses

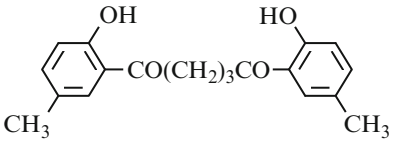
-Obtained by Fries rearrangement of m-cresol glutarate with aluminium chloride (70–80 %) [1576].

-Also refer to: [1575].

m.p. 180° [1575, 1576].

1,5-Bis(2-hydroxy-5-methylphenyl)-1,5-pentanedione

[4649-03-0] $C_{19}H_{20}O_4$ mol. wt. 312.36



Syntheses

-Obtained by Fries rearrangement of di (4-methyl-phenyl) glutarate with aluminium chloride,

*in refluxing chlorobenzene for 6 h (66 %) [3107];

*in tetrachloroethane at 80° for 1.5 h (61 %) [1603].

-Also obtained by reaction of glutaric anhydride with p-cresol in the presence of aluminium chloride in tetrachloroethane/nitrobenzene mixture (1:1), first at 50–60° for 2 h, then at 100° for 30 min [588].

-Also obtained by reaction of glutaryl chloride with p-methylanisole in the presence of aluminium chloride in refluxing methylene chloride for 1 h (86 %) [889].

-Also refer to: [889, 890, 941 (64 %), 1575, 2250].

m.p. 143° [1603], 141° [941], 140–141° [3107], 140° [588], 139–141° [889], 69° [1575].

N.B.: One of the reported melting point is obviously wrong.

^{1}H NMR [889], IR [588, 3107].

BIOLOGICAL ACTIVITY: Inhibition against HIV-1 integrase [2250].

Dioxime [4649-04-1] $C_{19}H_{22}N_2O_4$ mol. wt. 342.39

m.p. 175° [588].

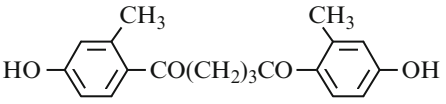
Dimethyl ether [10400-49-4] $C_{21}H_{24}O_4$ mol. wt. 340.42

-Obtained by reaction of glutaryl chloride with p-cresol methyl ether in the presence of aluminium chloride (50–70 %) [1576], in methylene chloride [2329].
-Also obtained by reaction of glutaric anhydride with p-cresol methyl ether [3064].
-Also obtained by treatment of 1,5-bis(2-hydroxy-5-methylphenyl)-1,5-pentanedione with dimethyl sulfate in the presence of sodium hydroxide in dilute ethanol (93 %) [1603].

m.p. 71–72° [1603], 69° [1576], 68.5–69.5° [3064], 68–70° [2329];
^{1}H NMR [3064], IR [3064].

1,5-Bis(4-hydroxy-2-methylphenyl)-1,5-pentanedione

[4642-34-6] $C_{19}H_{20}O_4$ mol. wt. 312.36



Synthesis
-Obtained by reaction of glutaryl chloride with m-cresol in the presence of aluminium chloride in nitrobenzene [588].

m.p. 178° [588]; IR [588].

Dioxime [4592-84-1] $C_{19}H_{22}N_2O_4$ mol. wt. 342.39

m.p. 225° [588].

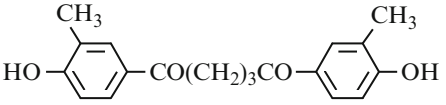
Dimethyl ether [4642-38-0] $C_{21}H_{24}O_4$ mol. wt. 340.42

-Obtained by reaction of glutaryl chloride with m-cresol methyl ether in the presence of aluminium chloride in tetrachloroethane [588].

b.p.$_{0.2}$ 150° [588]; IR [588].

1,5-Bis(4-hydroxy-3-methylphenyl)-1,5-pentanedione

[4592-83-0] $C_{19}H_{20}O_4$ mol. wt. 312.36



Synthesis
-Obtained by reaction of glutaryl chloride with o-cresol in the presence of aluminium chloride in nitrobenzene [588].

m.p. 175° [588]; IR [588].

Dioxime [4642-26-6] $C_{19}H_{22}N_2O_4$ mol. wt. 342.39

m.p. 220° [588].

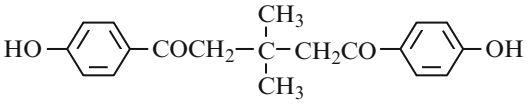
Dimethyl ether [4642-31-3] $C_{21}H_{24}O_4$ mol. wt. 340.42

-Obtained by reaction of glutaryl chloride with o-cresol methyl ether in the presence of aluminium chloride,
*in tetrachloroethane [588];
*in methylene chloride [2329].

m.p. 135–137° [2329], 130° [588]; IR [588].

1,5-Bis(4-hydroxyphenyl)-3,3-dimethyl-1,5-pentanedione

$C_{19}H_{20}O_4$ mol. wt. 312.36



Synthesis
-Refer to: [1890].

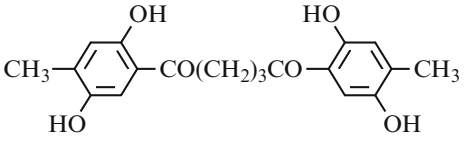
Dimethyl ether [102447-83-6] $C_{21}H_{24}O_4$ mol. wt. 340.42

-Refer to: [1328, 1890].

^{1}H NMR [1328], IR [1328].

1,5-Bis(2,5-dihydroxy-4-methylphenyl)-1,5-pentanedione

[91453-25-7] $C_{19}H_{20}O_6$ mol. wt. 344.36



Synthesis
-Obtained by treatment of 1,5-bis (2-hydroxy-5-methoxy-4-methylphenyl)-1,5-pentane-dione with boron tribromide in methylene chloride (80 %) [2103].

yellow solid [2103]; m.p. 202–203° [2103].

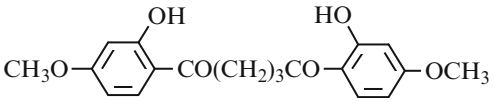
Tetramethyl ether [180578-81-8] $C_{23}H_{28}O_6$ mol. wt. 400.47

-Obtained by reaction of glutaric acid dichloride with 2,5-dimethoxytoluene in the presence of aluminium chloride,
*in methylene chloride first at 0° under an argon atmosphere, then at r.t. for 16 h (67 %) [2570];
*in carbon disulfide first at 0°, then at r.t. for 16 h (50 %) [1402].

colourless needles [1402];
m.p. 156° [1402], 152–153° [2570];
^{1}H NMR [2570], ^{13}C NMR [2570], IR [2570].

1,5-Bis(2-hydroxy-4-methoxyphenyl)-1,5-pentanedione

[4642-40-4] $C_{19}H_{20}O_6$ mol. wt. 344.36



Syntheses

-Obtained by reaction of glutaryl chloride with resorcinol monomethyl ether in the presence of aluminium chloride in nitrobenzene [588].

-Also obtained by reaction of glutaric anhydride with resorcinol monomethyl ether in the presence of aluminium chloride in nitrobenzene, first at 10–15° for 2 h, then at 30° for 1 h [588].

-Also obtained by reaction of resorcinol dimethyl ether with glutaryl chloride in the presence of aluminium chloride in nitrobenzene [592].

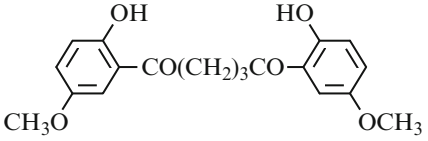
m.p. 130° [588, 592]; IR [588].

Dioxime [4714-77-6] $C_{19}H_{22}N_2O_6$ mol. wt. 374.39

m.p. 190° [588, 592].

1,5-Bis(2-hydroxy-5-methoxyphenyl)-1,5-pentanedione

[10365-74-9] $C_{19}H_{20}O_6$ mol. wt. 344.36



Syntheses

-Obtained by reaction of glutaryl dichloride with p-dimethoxybenzene in the presence of aluminium chloride [1575] in refluxing 1,2-ethylene chloride for 8 h [2103].

m.p. 122° [1575].

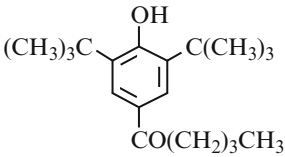
Diacetate [10365-32-9] $C_{23}H_{24}O_8$ mol. wt. 428.44

-Obtained by reaction of acetic anhydride (4 vol) with the title ketone in the presence of 1-2 drops concentrated sulfuric acid, the mixture warmed 5 min [1575].

m.p. 119° [1575].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-pentanone

[14035-37-1] $C_{19}H_{30}O_2$ mol. wt. 290.45



Syntheses

-Preparation by reaction of valeroyl chloride with 2,6-di-tert-butylphenol in the presence of aluminium chloride [2145] at −10° for 1–13 min (91 %) [2506].

-Also obtained by reaction of valeric anhydride with 2,6-di-tert-butylphenol in the presence of 5 drops 70 % perchloric acid, first at r.t. for 1 h and left overnight (91 %) [2136].

-Also refer to: [655, 951, 2139].

m.p. 89–90° [951], 85.5–87° [2139], 76–77° [2136], 75–78° [2506];
^{1}H NMR [2136], IR [2136].

BIOLOGICAL ACTIVITY: Inflammation inhibitor [2139].

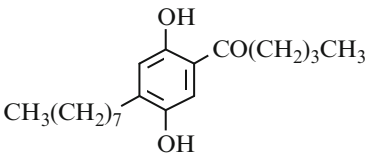
Acetate [903883-85-2] $C_{21}H_{32}O_3$ mol. wt. 332.48

-Obtained by acetylation of 3,5-di-tert-butyl-4-hydroxyvalerophenone [2145].

^{1}H NMR [2145], IR [2145].

1-(2,5-Dihydroxy-4-octylphenyl)-1-pentanone

[103798-50-1] $C_{19}H_{30}O_3$ mol. wt. 306.45



Syntheses

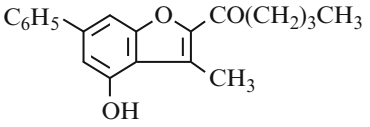
-Obtained by reaction of valeric acid with 2-octyl-hydroquinone in the presence of boron trifluoride in *sym*-tetrachloroethane at 40–50°. The mixture was allowed to stand overnight, then heated on a steam bath for 6 h (65 %) [142].

-Also refer to: [1907].

m.p. 59–60° [142].

1-(4-Hydroxy-3-methyl-6-phenyl-2-benzofuranyl)-1-pentanone

[678184-56-0] $C_{20}H_{20}O_3$ mol. wt. 308.78



Synthesis

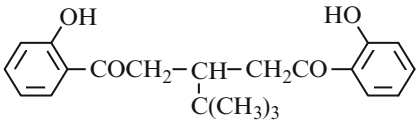
-Obtained by treatment of its methoxymethyl ether with hydrogen chloride in a tetrahydrofuran/methanol solution (1:1) [1288].

Methoxymethyl ether [678184-70-8] $C_{22}H_{24}O_4$ mol. wt. 352.43

-Refer to: [1288].

1,5-Bis(2-hydroxyphenyl)-3-tert-butyl-1,5-pentanedione

[175731-80-3] $C_{21}H_{24}O_4$ mol. wt. 340.42



Synthesis
-Obtained by treatment of its dimethyl ether with excess of trimethylsilyl iodide at 85° for 7 h (80 %) [890].

m.p. 88–89° [890]; ^{1}H NMR [890].

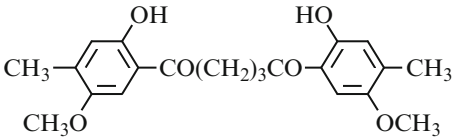
Dimethyl ether $C_{23}H_{28}O_4$ mol. wt. 368.47

-Preparation by refluxing trimethylacetaldehyde with 2-methoxyacetophenone in the presence of methanolic sodium methoxide for 18 h (38 %) [890].

m.p. 82–83° [890]; ^{1}H NMR [890].

1,5-Bis(2-hydroxy-5-methoxy-4-methylphenyl)-1,5-pentanedione

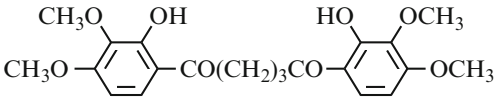
[344578-29-6] $C_{21}H_{24}O_6$ mol. wt. 372.42



Synthesis
-Obtained by reaction of glutaryl dichloride with 2,5-dimethoxy-toluene in the presence of aluminium chloride in refluxing 1,2-dichloro-ethane for 8 h [2103].

1,5-Bis(2-hydroxy-3,4-dimethoxylphenyl)-1,5-pentanedione

[10483-67-7] $C_{21}H_{24}O_8$ mol. wt. 404.41



Syntheses
-Obtained by reaction of glutaric acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride,

*in tetrachloroethane [1574];
*in nitrobenzene [592].
-Also refer to: [1575, 1890].

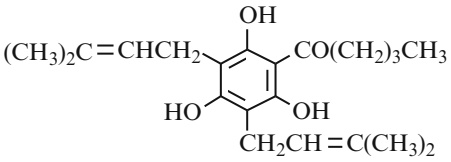
m.p. 125° [592], 123° [1574, 1575].

Dioxime [16148-67-7] $C_{21}H_{26}N_2O_8$ mol. wt. 434.45

m.p. 167–168° [592].

1-[2,4,6-Trihydroxy-3,5-bis(3-methyl-2-buten-1-yl)phenyl]-1-pentanone

[50874-43-6] $C_{21}H_{30}O_4$ mol. wt. 346.47



Syntheses

-Obtained by reaction of resvalerophenone with 1-bromo-3-methyl-2-buten (3 mol) in the presence of the weakly basic resin DeAcidite H-IP (OH^- form) in boiling benzene (13.8 %) [708].

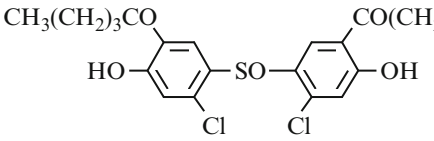
N.B.: The yield was similar at this obtained by using 2-methyl-3-buten-2-ol but the isolation was simpler [708].

-Also refer to: [707].

m.p. 86° [708].

1,1′-[Sulfonylbis(6-chloro-4-hydroxy-3,1-phenylene)]bis-1-pentanone

[50444-96-7] $C_{22}H_{24}Cl_2O_5S$ mol. wt. 471.40



Synthesis

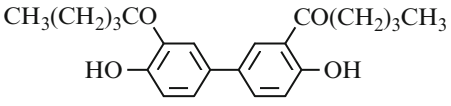
-Obtained by treatment of 4-chloro-2-hydroxyvalerophenone with thionyl chloride in the presence of aluminium chloride in carbon disulfide (58 %) [2430].

m.p. 149° [2430]; IR [2430].

USE: Antifungal [2430].

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-pentanone

[103650-06-2] $C_{22}H_{26}O_4$ mol. wt. 354.45



Syntheses

-Preparation by Fries rearrangement of 4,4′-biphenyl dipentanoate with aluminium chloride in refluxing chlorobenzene for 24 h (92 %) [2377].

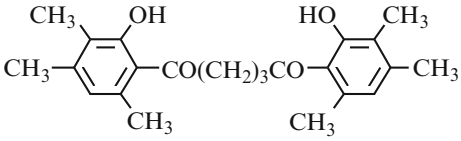
-Also refer to: [226].

m.p. 70–80.5° [2377]; IR [2377].

BIOLOGICAL ACTIVITY: Antibacterial against a cariogenic bacterium, Streptococcus mutans OMZ 176 [226].

1,5-Bis(2-hydroxy-3,4,6-trimethylphenyl)-1,5-pentanedione

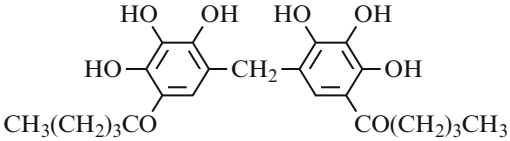
[84978-14-3] $C_{23}H_{28}O_4$ mol. wt. 368.47



Syntheses
-Refer to: [2325].
m.p. 138° [2325];
^{1}H NMR [2325], IR [2325].

1,1′-[Methylenebis(2,3,4-trihydroxy-5,1-phenylene)]bis-1-pentanone

$C_{23}H_{28}O_8$ mol. wt. 432.47

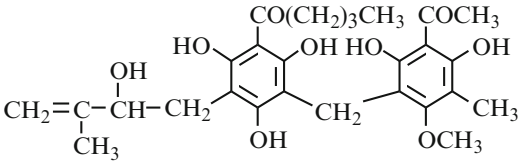


Synthesis
-Obtained by treatment of 4-valeroyl-pyrogallol with 35 % aqueous solution of formaldehyde in refluxing ethanol for 10 min [506].

m.p. 173° [506].

1-[3-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl) methyl]-2,4,6-trihydroxy-5-(2-hydroxy-3-methyl-3-butenyl) phenyl]-1-pentanone

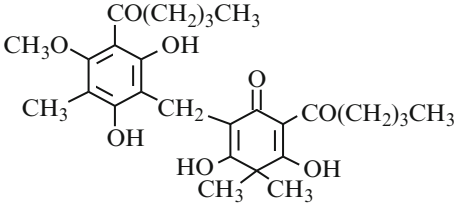
[406463-67-0] $C_{27}H_{34}O_9$ mol. wt. 502.55



Isolation from natural sources
-From the pericarps of *Mallotus japonicus* (Euphorbiaceae) [1461].

3′-[(5-Valeroyl-2,4-dihydroxy-3,3-dimethyl-6-oxo-1,4-cyclohexadien-1-yl) methyl]-2′,6′-dihydroxy-4′-methoxy-5′-methylvalerophenone
(Aspidin)

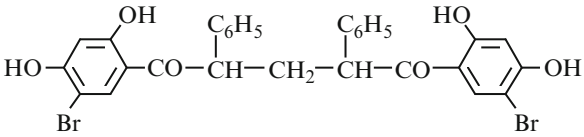
$C_{27}H_{36}O_8$ mol. wt. 488.58



Isolation from natural sources
-From *Hypericum uliginosum* HBK (**XIX**) [2408].
UV [2408].

1,5-Bis(5-bromo-2,4-dihydroxyphenyl)-2,4-diphenyl-1,5-pentanedione

[96271-43-1] $C_{29}H_{22}Br_2O_6$ mol. wt. 626.30



Synthesis
-Obtained by condensation of 5-bromo-2,4-dihydroxy-phenyl benzyl ketone with methylene iodide in the presence of sodium ethoxide [587].

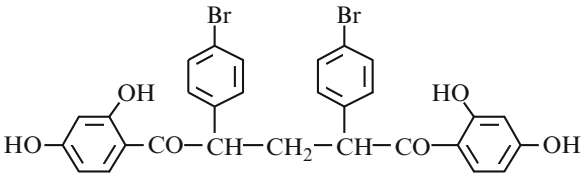
silky needles [587]; m.p. 225° [587]; IR [587].

Tetraacetate [96710-34-8] $C_{37}H_{30}Br_2O_{10}$ mol. wt. 794.45

rectangular plates [587]; m.p. 140° [587].

1,5-Bis(2,4-dihydroxyphenyl)-2,4-di(4-bromophenyl)-1,5-pentanedione

[96271-44-2] $C_{29}H_{22}Br_2O_6$ mol. wt. 626.30

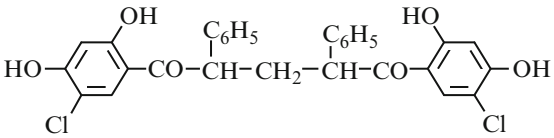


Synthesis
-Obtained by condensation of 2,4-dihydroxyphenyl 4′-bromobenzyl ketone with methylene iodide in the presence of sodium ethoxide [587].

prismatic rods [587]; m.p. 265° [587].

1,5-Bis(5-chloro-2,4-dihydroxyphenyl)-2,4-diphenyl-1,5-pentanedione

[96271-50-0] $C_{29}H_{22}Cl_2O_6$ mol. wt. 537.40



Synthesis
-Obtained by condensation of 5-chloro-2,4-dihydroxy-phenyl benzyl ketone with methylene iodide in the presence of sodium ethoxide [587].

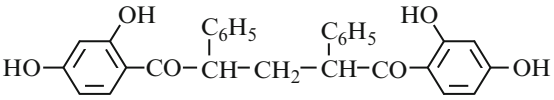
silky needles [587]; m.p. 229–230° [587];
IR [587], UV [587].

Tetraacetate [96710-35-9] $C_{37}H_{30}Cl_2O_{10}$ mol. wt. 705.54

rectangular plates [587]; m.p. 125° [587].

1,5-Bis(2,4-dihydroxyphenyl)-2,4-diphenyl-1,5-pentanedione

[96273-22-2] $C_{29}H_{24}O_6$ mol. wt. 468.51



Synthesis
-Obtained by condensation of 2,4-dihydroxyphenyl benzyl ketone with methylene iodide in the presence of sodium ethoxide [587].

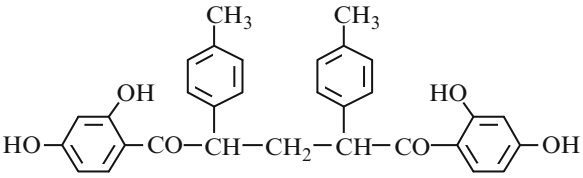
colourless rods [587]; m.p. 192° [587];
IR [587], UV [587], MS [587].

Tetramethyl ether [96676-42-5] $C_{33}H_{32}O_6$ mol. wt. 524.61

prismatic rods; m.p. 136–137° [587].

1,5-Bis(2,4-dihydroxyphenyl)-2,4-di(4-methylphenyl)-1,5-pentanedione

$C_{31}H_{28}O_6$ mol. wt. 496.56



Synthesis
-Obtained by condensation of 2,4-dihydroxyphenyl 4′-methylbenzyl ketone with methylene iodide in the presence of sodium ethoxide [587].

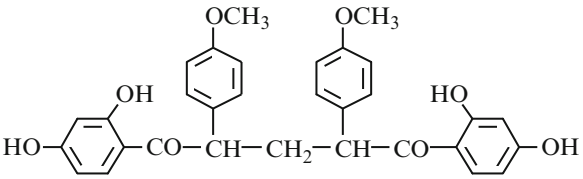
rods [587]; m.p. 218° [587]; IR [587].

Tetraacetate $C_{39}H_{36}O_{10}$ mol. wt. 664.71

rectangular plates [587]; m.p. 132° [587].

1,5-Bis(2,4-dihydroxyphenyl)-2,4-di(4-methoxyphenyl)-1,5-pentanedione

[96590-58-8] $C_{31}H_{28}O_8$ mol. wt. 528.56



Synthesis
-Obtained by condensation of 2,4-dihydroxyphenyl 4′-methoxybenzyl ketone with methylene iodide in the presence of sodium ethoxide [587].

prismatic rods [587]; m.p. 195° [587].

Tetraacetate [97924-31-7] $C_{39}H_{36}O_{12}$ mol. wt. 696.71

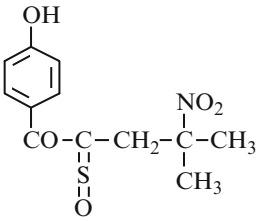
rectangular plates [587]; m.p. 130° [587].

2 Aromatic Hydroxyketones Derived from 4-Methylpentanoic Acid

2.1 Unsubstituted Hydroxyketones

1-(4-Hydroxyphenyl)-4-methyl-4-nitro-2-sulfinyl-1-pentanone

$C_{12}H_{13}NO_5S$ mol. wt. 283.30



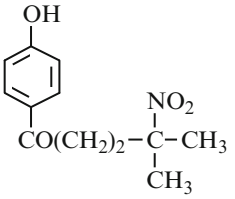
Synthesis
-Refer to: [377].

Methyl ether [92050-08-3]
$C_{13}H_{15}NO_5S$ mol. wt. 297.33
-Obtained by treatment of 1-(4-methoxyphenyl)-4-methyl-4-nitro-1-pentanone with thionyl chloride in the presence of pyridine at reflux (96°) for 6 h (7 %) [377].

yellow powder [377]; m.p. 83° [377];
^{1}H NMR [377], IR [377].

1-(4-Hydroxyphenyl)-4-methyl-4-nitro-1-pentanone

$C_{12}H_{15}NO_4$ mol. wt. 237.25



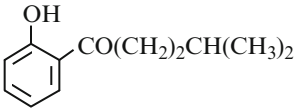
Synthesis
-Refer to: [377].

Methyl ether [92050-07-2]
$C_{13}H_{17}NO_4$ mol. wt. 251.28
-Refer to: [377 (70 %)].

colourless crystals [377]; m.p. 70° [377]; ^{1}H NMR [377].

1-(2-Hydroxyphenyl)-4-methyl-1-pentanone

[22526-26-7] $C_{12}H_{16}O_2$ mol. wt. 192.26



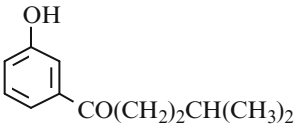
Syntheses
-Refer to: [1674, 3338].
b.p.$_{0.5}$ 115–120° [3338]; $pK_a = 4.884$ [192].

Methyl ether [22526-27-8] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Refer to: [3338].

1-(3-Hydroxyphenyl)-4-methyl-1-pentanone

$C_{12}H_{16}O_2$ mol. wt. 192.26



Synthesis

-Preparation by reaction of m-acetoxybenzoyl chloride with diisohexylcadmium in refluxing benzene for 30 min. Then, treatment of the ketoester obtained by refluxing with 10 % sodium hydroxide for 2–3 h (70 %) [2586].

b.p.$_{.2}$ 158° [2586]; m.p. 70° [2586].

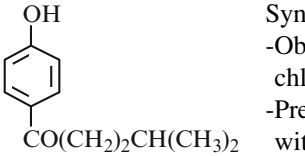
Acetate $C_{14}H_{18}O_3$ mol. wt. 234.30 b.p.$_1$ 119° [2586].

2,4-Dinitrophenylhydrazone $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 178° [2586].

1-(4-Hydroxyphenyl)-4-methyl-1-pentanone

[286439-54-1] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Obtained by treatment of its methyl ether with pyridinium chloride at 190° [627].

-Preparation by Fries rearrangement of phenyl isocaproate with aluminium chloride in nitrobenzene at 70° for 6 h (57 %) [2163].

-Also refer to: [2941, 3090].

b.p.$_{.0.5}$ 190° [2163]; m.p. 71–72° [2163].

Methyl ether [21550-01-6] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of 4-methylpentanoic acid with anisole in the presence of PPA at 80° (76–100 %) [627] or at 90–100° for 1.5 h (75 %) [2942].

-Also obtained by reaction of 4-methylpentanoyl chloride with anisole [2236] in the presence of aluminium chloride in methylene chloride at 0° (76–100 %) [627].

-Preparation by addition of the Grignard from 1-bromo-3-methylbutane to p-methoxybenzonitrile [3254].

-Also refer to: [950, 1114, 2302 (65 %), 3090, 3232, 3253].

pale yellow oil [2942];

b.p.$_{.0.5}$ 107–108° [2302]; b.p.$_1$ 131–133° [2236]; b.p.$_5$ 136–137° [950], b.p.$_3$ 138° [3254];

b.p.$_{.15}$ 169–170° [3232];

^{1}H NMR [2942, 3090], ^{13}C NMR [2942], IR [3232], UV [3254], MS [2942, 3254]; ESR spectroscopy [3254]; Phosphorescence spectroscopy [3254].

USE: Photoelimination and photocyclisation of, biradical formation in, [3253].

Semicarbazone of the methyl ether [30299-35-5] $C_{14}H_{21}N_3O_2$ m.p. wt. 263.34

m.p. 124–125° [2236], 133–133.5° [2302].

Ethyl ether [30299-36-6] $C_{14}H_{20}O_2$ mol. wt. 220.31

-Refer to: [2302 (82 %)].

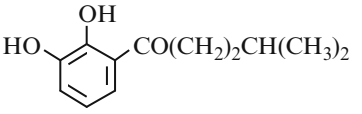
b.p.$_1$ 132–135° [2302]; m.p. 31–32° [2302].

Semicarbazone of the ethyl ether [30299-37-7] $C_{15}H_{23}N_3O_2$ mol. wt. 277.37

-Refer to: [2302]; m.p. 161.5–162° [2302].

1-(2,3-Dihydroxyphenyl)-4-methyl-1-pentanone

$C_{12}H_{16}O_3$ mol. wt. 208.26



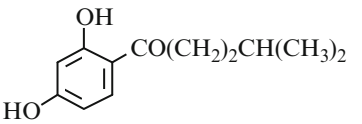
Synthesis

-Obtained (by-product) by Fries rearrangement of pyrocatechol diisocaproate with aluminium chloride in the presence of pyrocatechol for 4.5 h at 135–140° [2075].

b.p.$_5$ 195–205° [2075].

1-(2,4-Dihydroxyphenyl)-4-methyl-1-pentanone
(Resisocapronophenone)

[116529-92-1] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses

-Obtained by reaction of isocaproic acid with resorcinol in the presence of boron trifluoride for 2 h at 70° (72 %) [2312].

-Also obtained by reaction of isocaproic nitrile with resorcinol (Hoesch reaction) [1608].

-Also obtained by reaction of iso-hexylyl chloride with resorcinol at 85–90° for 20–30 min (82.7 %) [731].

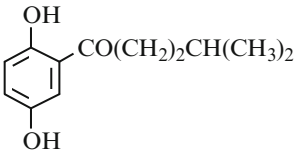
-Also refer to: [893, 1588, 2842].

b.p.$_{6\text{-}7}$ 192–194° [893, 2842];
m.p. 84.5° [1588], 83–84° [1608, 2312], 76–77.5° [893, 2842].

Hydrate $C_{12}H_{16}O_3$, x H_2O m.p. 47° [1608].

1-(2,5-Dihydroxyphenyl)-4-methyl-1-pentanone

[18787-32-1] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses

-Preparation by reaction of isocaproic acid with hydroquinone in the presence of boron trifluoride for 2 h at 125° [2063].

-Also obtained by Fries rearrangement of 4-methoxyphenyl isocaproate with aluminium chloride (5 part)/sodium chloride (2 part) mixture at 180–200° (30 %) [1796].

-Also refer to: [458, 1795].

m.p. 68° [1795, 1796], 65–66° [2063].

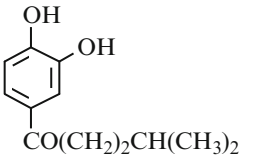
Dimethyl ether $C_{14}H_{20}O_3$ mol. wt. 236.31

-Obtained by reaction of isocaproyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in boiling carbon disulfide for 2 h (40–50 %) [458].

pale yellow oil [458]; b.p.$_7$ 172–173° [458].

1-(3,4-Dihydroxyphenyl)-4-methyl-1-pentanone

[26115-81-1] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses

-Obtained by Fries rearrangement of pyrocatechol diisocaproate with aluminium chloride in the presence of pyrocatechol for 4.5 h at 135–140° (60 %) [2075].

-Also obtained by reaction of 4-methylvaleroyl chloride with pyrocatechol in the presence of aluminium chloride in chlorobenzene at 110° for 3 h (80 %) [3226].

m.p. 127–128° [3226], 73–73.5° [2075].
One of the reported melting points is obviously wrong.

Dimethyl ether [4101-16-0] $C_{14}H_{20}O_3$ mol. wt. 236.31

b.p.$_{0.02}$ 129–133° [1525]; $n_D^{25} = 1.5337$ [1525].

1-(3,5-Dihydroxyphenyl)-4-methyl-1-pentanone

[100257-43-0] $C_{12}H_{16}O_3$ mol. wt. 208.26

Syntheses
-Obtained by treatment of its diacetate with 5 % sodium hydroxide at reflux for 4.5 h (63 %) [1406].
-Also refer to: [2781].

m.p. 102° [1406].

BIOLOGICAL ACTIVITY: Anthelmintic [2781].

2,4-Dinitrophenylhydrazone [101741-97-3] $C_{18}H_{20}N_4O_6$ mol. wt. 388.38

m.p. 245° [1406].

Diacetate [101430-33-5] $C_{16}H_{20}O_5$ mol. wt. 292.33

-Preparation by reaction of diisopentylcadmium with 3,5-diacetoxybenzoyl chloride in refluxing benzene for 1 h (77 %) [1406].

$b.p._{\cdot 0.7}$ 184–188° [1406]; m.p. 51° [1406].

2,4-Dinitrophenylhydrazone of the diacetate

[102810-70-8] $C_{22}H_{24}N_4O_8$ mol. wt. 472.45

m.p. 185° [1406].

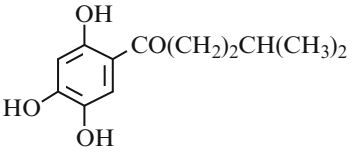
Dimethyl ether $C_{14}H_{20}O_3$ mol. wt. 236.31

-Preparation in the usual way [25 (81 %), 2990].

$b.p._{\cdot 0.5}$ 135° [25].

4-Methyl-1-(2,4,5-trihydroxyphenyl)-1-pentanone

$C_{12}H_{16}O_4$ mol. wt. 224.26

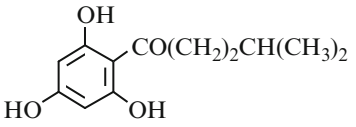


Synthesis
-Refer to: [1708].

USE: Antioxidant [1708].
Toxicity [1708].

4-Methyl-1-(2,4,6-trihydroxyphenyl)-1-pentanone
(Phloroisocaprophenone)

[2999-14-6] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Obtained by reaction of isocaproyl chloride with phloroglucinol in the presence of aluminium chloride,
*in nitrobenzene (67 %) [2618];
*in nitrobenzene and carbon disulfide mixture (67 %) [2620], (64 %) [2113], (57 %) [2624].

-Also obtained by reaction of isocapronitrile with phloroglucinol (Hoesch reaction) [1608].
-Also refer to: [1026, 1375, 1607, 2617].

m.p. 122.5° [1375], 122° [1607, 1608, 2113, 2617, 2618, 2620], 120° [2624].

Monohydrate $C_{12}H_{16}O_4, H_2O$ mol. wt. 242.28

m.p. 104° [1607, 1608], 103–104° [1375].

BIOLOGICAL ACTIVITY: Antifungal [2113].

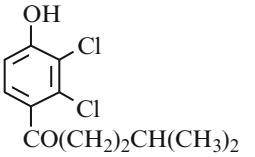
Monosodium salt [85602-44-4] $C_{12}H_{15}O_4Na$ mol. wt. 246.24

-Refer to: [1026].

2.2 Substituted Hydroxyketones

1-(2,3-Dichloro-4-hydroxyphenyl)-4-methyl-1-pentanone

[1210-21-5] $C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15



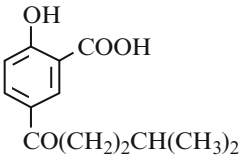
Syntheses
-To 4-methylpentanoyl chloride and 2,3-dichloroanisole in carbon disulfide was added aluminium chloride in small portions at 25°. The mixture stirred 1 h at r.t. and 45 min at 55°; pentane and aluminium chloride added, heated 3 h at 80° [2056].

-Also refer to: [2047, 2048, 2767 (84 %)].

m.p. 107.5–108.5° [2767], 86–87° [2047, 2048, 2056].
One of the reported melting points is obviously wrong.

5-Isocaproyl-2-hydroxybenzoic acid

$C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis

-Obtained by hydrolysis of methyl 5-isocaproyl-2-hydroxybenzoate with boiling 20 % solution of potassium hydroxide [730].

m.p. 132–133.5° [730].

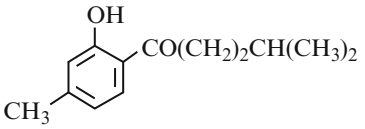
Methyl ester $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by Fries rearrangement of methyl 2-(isocaproyloxy)benzoate with aluminium chloride in boiling carbon disulfide for 2 h, then the reaction mixture heated at 90–110° for a few min after solvent elimination [730].

$b.p._{.15}$ 195–198° [730].

1-(2-Hydroxy-4-methylphenyl)-4-methyl-1-pentanone

$C_{13}H_{18}O_2$ mol. wt. 206.28



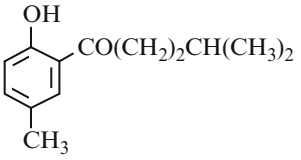
Synthesis

-Preparation by Fries rearrangement of 3-methylphenyl isocaproate with aluminium chloride without solvent at 140–150° [906].

$b.p._{.1}$ 106–107° [906].

1-(2-Hydroxy-5-methylphenyl)-4-methyl-1-pentanone

[93429-81-3] $C_{13}H_{18}O_2$ mol. wt. 206.28



Synthesis

-Preparation by Fries rearrangement of 4-methylphenyl isocaproate with aluminium chloride [423].

IR [423].

1-(4-Hydroxy-3-methylphenyl)-4-methyl-1-pentanone

[101267-59-8] $C_{13}H_{18}O_2$ mol. wt. 206.28

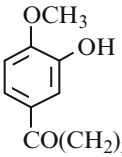
Synthesis

-Preparation by Fries rearrangement of 2-methylphenyl isocaproate with aluminium chloride [2164].

$b.p._{.0.5}$ 190° [2164].

1-(3-Hydroxy-4-methoxyphenyl)-4-methyl-1-pentanone

$C_{13}H_{18}O_3$ mol. wt. 222.28

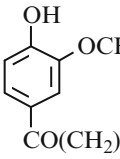


Synthesis
-Refer to: [1803].

Benzyl ether [159211-07-1]
$C_{20}H_{24}O_3$ mol. wt. 312.40
-Refer to: [1803].

1-(4-Hydroxy-3-methoxyphenyl)-4-methyl-1-pentanone

$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Obtained by Fries rearrangement of o-methoxyphenyl isocaproate with aluminium chloride in nitrobenzene, first at 80° for 45 min, then at r.t. for 24 h [319].

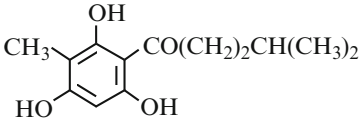
b.p.$_{21}$ 205° [319]; m.p. 35–36° [319].

Benzyl ether [159211-02-6] $C_{20}H_{24}O_3$ mol. wt. 312.40

-Refer to: [1803].

4-Methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-pentanone

[131868-27-4] $C_{13}H_{18}O_4$ mol. wt. 238.28

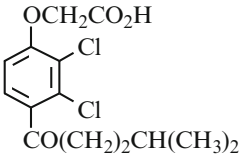


Syntheses
-Obtained by reaction of isocaproic nitrile with 3-methylphloroglucinol (Hoesch reaction) [1608].
-Also refer to: [1441].

m.p. 156° [1608], 155–156° [1441].

2-[2,3-Dichloro-4-(4-methylvaleryl)phenoxy]acetic acid

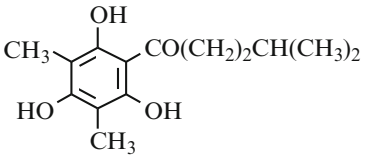
[1154-71-8] $C_{14}H_{16}Cl_2O_4$ mol. wt. 319.19



Syntheses
-Refer to: [2047, 2048, 2056, 2766].
m.p. 108.5–109.5° [2047, 2048, 2766], 106–108.5° [2056].

4-Methyl-1-(2,4,6-trihydroxy-3,5-dimethylphenyl)-1-pentanone

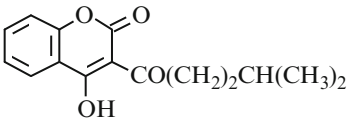
$C_{14}H_{20}O_4$ mol. wt. 252.31



Synthesis
-Refer to: [2781].
m.p. 76° [2781].

4-Hydroxy-3-(4-methyl-1-oxopentyl)-2*H*-1-benzopyran-2-one

$C_{15}H_{16}O_4$ mol. wt. 260.29

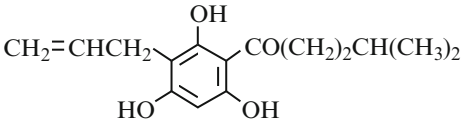


Synthesis
-Obtained by reaction of isocaproyl chloride with 4-hydroxycoumarin in pyridine containing one drop of piperidine for 3 h on a water bath [3174].

m.p. 79–80° [3174].

4-Methyl-1-[2,4,6-trihydroxy-3-(2-propenyl)phenyl]-1-pentanone
2-isocaproyl-4-(propen-2-yl)phloroglucinol (**15**) [1026].

[85602-25-1] $C_{15}H_{20}O_4$ mol. wt. 264.32



Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and allyl chloride to a solution of phloroisocaprophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

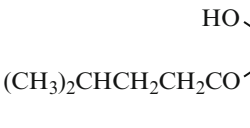
-Also obtained by reaction of allyl chloride with phloroisocaprophenone in an alkaline two-phase (aqueous-ether) system and catalyzed by CuCl [838, 3193].

m.p. 140–143° [3193];
^{1}H NMR [1026], ^{13}C NMR [1026, 3193], IR [1026].

BIOLOGICAL ACTIVITY: Bactericidal and fungicidal [1026, 3193].

1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-4-methyl-1-pentanone

$C_{17}H_{24}O_4$ mol. wt. 292.37



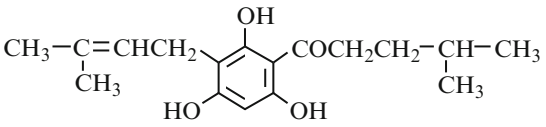
Synthesis
-Refer to: [3193].

Dimethyl ether [105334-08-5]
$C_{19}H_{28}O_4$ mol. wt. 320.43

-Refer to: [3193].

4-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-buten-1-yl)phenyl]-1-pentanone *(Caespitin)*
2-isocaproyl-4-(3-methylbuten-2-yl)phloroglucinol (**7**) [1026].

[74478-09-4] $C_{17}H_{24}O_4$ mol. wt. 292.37



Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and prenyl bromide to a solution of phloroisocaprophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

-Also prepared by adding prenyl bromide to a suspension of the sodium salt of phloroisocaprophenone in benzene, then the mixture obtained was refluxed for 3 h [1026].
-Also prepared by adding at 5° a solution of sodium methoxide in methanol, followed by isopentenyl bromide in ethyl ether to a solution of 3-methyl-1-(2,4,6-trihydroxyphenyl)-1-pentanone in benzene and ethyl ether; then the mixture was stirred at r.t. for 6 h (14 %) [2113].
-Also obtained by adding prenyl chloride to a two-phase mixture consisting of 2-(4-methyl-pentanoyl)phloroglucinol in diethyl ether and saturated aqueous sodium carbonate. A catalytic amount of CuCl was added and the mixture was stirred or shaken vigorously for 3 h at r.t. (41 %) [838].
-Also refer to: [839, 3193].

Isolation from natural sources

-Obtained from the entire plant material of *Helichrysum caespititium* [337, 1026, 2066].

straw coloured crystals [1026]; light yellow crystals [838];
m.p. 147° [2113], 132–133° [1026], 131–134° [838];
^{1}H NMR [1026], ^{13}C NMR [838, 1026], IR [838, 1026], MS [838].

BIOLOGICAL ACTIVITY: Antiprotozoal and antimicrobial [337]; Antimycobacterial [2066]; Antifungal [2113]; Bactericidal and fungicidal [1026].

4,6-Dimethyl ether [85602-35-3] $C_{19}H_{28}O_4$ mol. wt. 320.43

-Obtained by reaction of dimethyl sulfate with 2-isocaproyl-4-(3-methylbuten-2-yl) phloroglucinol (**7**) in the presence of potassium carbonate in refluxing acetone for 4 h [1026].

^{1}H NMR [1026], IR [1026].

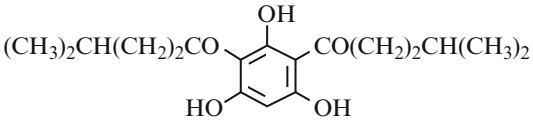
4,6-Dibenzoate (**28**), [1026] $C_{31}H_{30}O_6$ mol. wt. 498.58

-Obtained by reaction of p-bromobenzoyl chloride with 2-isocaproyl-4-(3-methylbuten-2-yl)phloroglucinol (**7**) in refluxing benzene for 2 h [1026].

^{1}H NMR [1026], IR [1026]; X-ray crystallographic data [1026].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-4-methyl-1-pentanone

[3118-37-4] $C_{18}H_{26}O_5$ mol. wt. 322.40

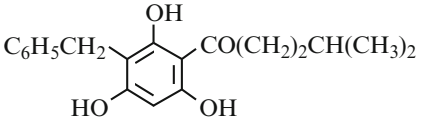


Synthesis
-Refer to: [600].

BIOLOGICAL ACTIVITY: For treatment of immune dysfunction associated with human immunodeficiency virus infection [600].

4-Methyl-1-[2,4,6-trihydroxy-3-(phenylmethyl)phenyl]-1-pentanone
2-isocaproyl-4-benzylphloroglucinol (**23**) [1026].

[85602-31-9] $C_{19}H_{22}O_4$ mol. wt. 314.38



Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and benzyl chloride to a solution of phloroiso-caprophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

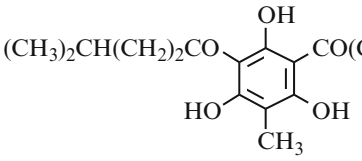
-Also obtained by reaction of benzyl chloride with phloroheptanophenone in an alkaline two-phase (aqueous-ether) system and catalyzed by CuCl [838, 3193].

m.p. 121–122° [3193];
^{1}H NMR [1026], ^{13}C NMR [1026, 3193], IR [1026].

BIOLOGICAL ACTIVITY: Bactericidal and fungicidal [1026, 3193].

1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-4-methyl-1-pentanone

[2999-17-9] $C_{19}H_{28}O_5$ mol. wt. 336.43

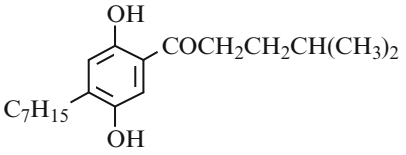


Synthesis
-Refer to: [600].

BIOLOGICAL ACTIVITY: For treatment of immune dysfunction associated with human immunodeficiency virus infection [600].

1-(4-Heptyl-2,5-dihydroxyphenyl)-4-methyl-1-pentanone

$C_{19}H_{30}O_3$ mol. wt. 306.45



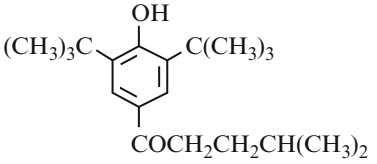
Synthesis
-Obtained by treatment of 4-heptyl-2-hydroxy-5-methoxyisocaprophenone with aluminium bromide [161].
m.p. 74–75° [161].

2,4-Dinitrophenylhydrazone $C_{25}H_{34}N_4O_6$ mol. wt. 486.57

m.p. 142–143° [161].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-4-methyl-1-pentanone

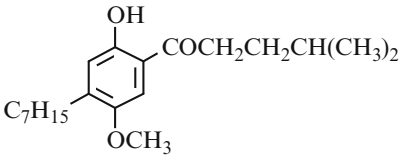
$C_{20}H_{32}O_2$ mol. wt. 304.47



Synthesis
-Obtained by reaction of isocaproyl chloride with 2,6-di-tert-butylphenol in the presence of titanium tetrachloride [1468].

1-(4-Heptyl-2-hydroxy-5-methoxyphenyl)-4-methyl-1-pentanone

[857973-71-8] $C_{20}H_{32}O_3$ mol. wt. 320.47



Synthesis
-Obtained by reaction of isocaproyl chloride with 2-heptylhydroquinone dimethyl ether in the presence of aluminium chloride in carbon disulfide [161].

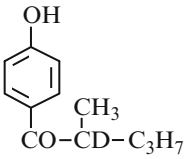
$b.p._{\cdot 0.5}$ 171° [161].

3 Aromatic Hydroxyketones Derived from Various Alkylpentanoic Acids

3.1 Unsubstituted Hydroxyketones

1-(4-Hydroxyphenyl)-2-methyl-1-pentanone-*2-d*

$C_{12}H_{15}DO_2$ mol. wt. 192.26



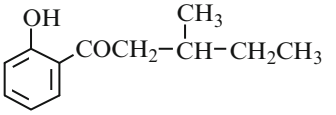
Synthesis
-Refer to: [2106].
Methyl ether [733016-52-9]
$C_{13}H_{17}DO_2$ mol. wt. 193.12

-Preparation (complex synthesis) **28a** (80 %, D = 95 %) [2106].

colourless oil [2106]; ^{1}H NMR [2106], IR [2106], MS [2106].

1-(2-Hydroxyphenyl)-3-methyl-1-pentanone

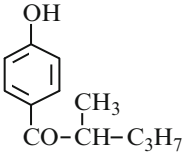
[39575-43-4] $C_{12}H_{16}O_2$ mol. wt. 192.26



Synthesis
-Refer to: [2093].
b.p.$_{15}$ 160–165° [2093]; $n_D^{30} = 1.473$ [2093].

1-(4-Hydroxyphenyl)-2-methyl-1-pentanone

$C_{12}H_{16}O_2$ mol. wt. 192.26



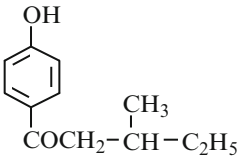
Synthesis
-Refer to: [2106].
Methyl ether [115975-32-1]
$C_{13}H_{18}O_2$ mol. wt. 206.28

-Preparation by treatment of adduct **26a** with methyl iodide (99 %) (complex synthesis) [2106].

colourless oil [2106]; ^{1}H NMR [2106], IR [2106], MS [2106].

1-(4-Hydroxyphenyl)-3-methyl-1-pentanone (+)

[62439-32-1] $C_{12}H_{16}O_2$ mol. wt. 192.26



Synthesis
-Obtained by Fries rearrangement of (+) phenyl 3-methylvalerate (58.6 %) [2093].
b.p.$_{15}$ 160–165° [2093];
$(\alpha)_D^{30} = +2.61$ [2093].

Methyl ether [66333-82-2] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by reaction of β-methylvaleroyl chloride with anisole in the presence of stannic chloride in benzene for 24 h at 50° (20 %) [2906].

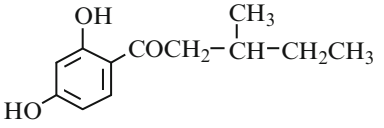
b.p.$_{14}$ 155–160° [2906]; UV [2906]; $n_D^{25} = 1.5263$ [2906].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{19}H_{22}N_4O_5$ mol. wt. 386.41

m.p. 138.6–139.4° [2906].

1-(2,4-Dihydroxyphenyl)-3-methyl-1-pentanone

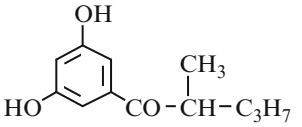
$C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis
-Refer to: [2605].
m.p. 64–66° [2605].

1-(3,5-Dihydroxyphenyl)-2-methyl-1-pentanone

$C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis
-Refer to: [25].

Dimethyl ether

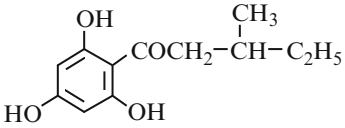
$C_{14}H_{20}O_3$ mol. wt. 236.31

-Preparation in the usual way [25 (61 %), 2990].

b.p.$_1$ 150° [25].

3-Methyl-1-(2,4,6-trihydroxyphenyl)-1-pentanone (S)

[108991-24-8] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses

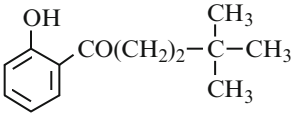
-Obtained by reaction of S-3-methylvaleryl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene for 60 h at r.t. (65 %) [3405].

-Also refer to: [2003].

m.p. 145° [3405], 129–130° [2003];
^{1}H NMR [3405], IR [3405], MS [3405].

1-(2-Hydroxyphenyl)-4,4-dimethyl-1-pentanone

[935277-48-8] $C_{13}H_{18}O_2$ mol. wt. 206.28



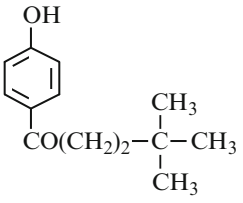
Synthesis

-Obtained by stirring a solution of salicylaldehyde, 3,3-dimethyl-1-butene, $RhCl(PPh_3)_3$, acetonitrile and sodium acetate in methylene chloride at r.t. for 7 h under an argon atmosphere (82 %) [1434].

^{1}H NMR [1434], ^{13}C NMR [1434], IR [1434].

1-(4-Hydroxyphenyl)-4,4-dimethyl-1-pentanone

$C_{13}H_{18}O_2$ mol. wt. 206.28



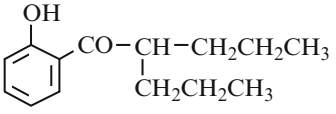
Synthesis

-Refer to: [2404].

Methyl ether [152269-19-7]
$C_{14}H_{20}O_2$ mol. wt. 220.31
-Refer to: [1557, 2404].

1-(2-Hydroxyphenyl)-2-propyl-1-pentanone

$C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses

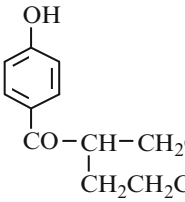
-Preparation by Fries rearrangement of phenyl valproate in the presence of aluminium chloride in chlorobenzene for 4 h at 140° (74 %) [2003].

-Also refer to: [2002].

b.p.$_{0.2}$ 89–91° (Sadtler standard N° 84927K) [2002, 2003];
^{1}H NMR (Sadtler standard N° 57879M) [2002, 2003];
IR (Sadtler standard N° 84927K) [2002, 2003], UV [2002, 2003], MS [2002, 2003].

1-(4-Hydroxyphenyl)-2-propyl-1-pentanone

[137937-44-1] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses
-Preparation by Fries rearrangement of phenyl valproate in the presence of aluminium chloride in nitromethane for 170 h at 20° (76 %) [2003].
-Also refer to: [2002].
m.p. 43° (Sadtler standard N° 84928K) [2003];
^{1}H NMR (Sadtler standard N° 57880M), [2003],

IR (Sadtler standard N° 84928K) [2003], UV [2003], MS [2003].

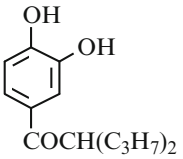
Methyl ether [119748-12-8] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Obtained by reaction of dipropylacetyl chloride with anisole in the presence of aluminium chloride in methylene chloride first at 0°, then at r.t. for 4 h [1290].

b.p.$_{13}$ 183–186° [3178].

1-(3,4-Dihydroxyphenyl)-2-propyl-1-pentanone

$C_{14}H_{20}O_3$ mol. wt. 236.31



Synthesis
-Refer to: [2183].
Dimethyl ether [180698-61-7]
$C_{16}H_{24}O_3$ mol. wt. 264.36

-Refer to: [2183].

Oxime of the dimethyl ether [180698-62-8] $C_{16}H_{25}NO_3$ mol. wt. 279.38

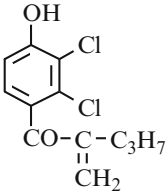
-Refer to: [2183].

^{1}H NMR [2182], ^{13}C NMR [2182].

3.2 Substituted Hydroxyketones

1-(2,3-Dichloro-4-hydroxyphenyl)-2-methylene-1-pentanone

$C_{12}H_{12}Cl_2O_2$ mol. wt. 259.13



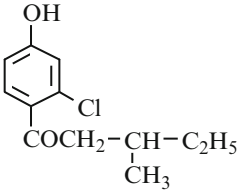
Synthesis
-Refer to: [742].
Methyl ether [101375-33-1]
$C_{13}H_{14}Cl_2O_2$ mol. wt. 273.16

-Obtained by treatment of 2,3-dichloro-4-methoxy-valeophenone with N,N,N′, N′-tetramethyl-methanediamine (92 %) [742].
-Also obtained from 2-bromo-1-(2,3-dichloro-4-methoxyphenyl)-2-methyl-1-propanone [742].

m.p. 58–60° [742]; ^{1}H NMR [742].

1-(2-Chloro-4-hydroxyphenyl)-3-methyl-1-pentanone

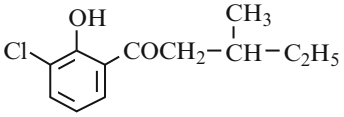
[165538-94-3] $C_{12}H_{15}ClO_2$ mol. wt. 226.70



Synthesis
-Refer to: [1717].

1-(3-Chloro-2-hydroxyphenyl)-3-methyl-1-pentanone (+)

[39575-47-8] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

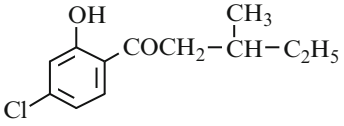


Synthesis
-Obtained by Fries rearrangement of (+) o-chlorophenyl 3-methylvalerate (53.2 %) [2093].

b.p.$_{15}$ 200–205° [2093]; $(\alpha)_D^{30} = +1.95$ [2093].

1-(4-Chloro-2-hydroxyphenyl)-3-methyl-1-pentanone (+)

[39575-48-9] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

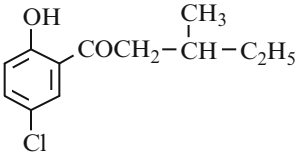


Synthesis
-Obtained by Fries rearrangement of (+) m-chlorophenyl 3-methylvalerate (58.6 %) [2093].

b.p.$_{15}$ 208–212° [2093]; $(\alpha)_D^{30} = +2.66$ [2093].

1-(5-Chloro-2-hydroxyphenyl)-3-methyl-1-pentanone (+)

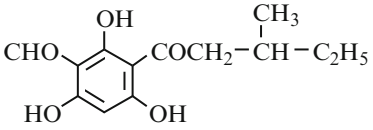
[39575-49-0] $C_{12}H_{15}ClO_2$ mol. wt. 226.70



Synthesis
-Obtained by Fries rearrangement of (+) p-chlorophenyl 3-methylvalerate (64 %) [2093].
b.p.$_{15}$ 215–220° [2093];
$(\alpha)_D^{30} = +2.91$ [2093].

2,4,6-Trihydroxy-3-(3-methyl-1-oxopentyl)benzaldehyde (S)

[120716-97-4] $C_{13}H_{16}O_5$ mol. wt. 252.27



Syntheses
-Obtained by reaction of ethyl orthoformate with 3-methyl-1-(2,4,6-trihydroxyphenyl)-1-pentanone (S) in the presence of aluminium chloride for 30 min (53 %) [3405].

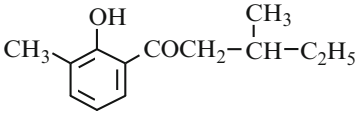
-Also refer to: [3415].

m.p. 74° [3405]; ^{1}H NMR [3405], IR [3405], MS [3405];
M+, 238 (compound **6**, p. 473).

BIOLOGICAL ACTIVITY: As photosynthetic electron transport (PET) [3405].

1-(2-Hydroxy-3-methylphenyl)-3-methyl-1-pentanone (+)

[39575-44-5] $C_{13}H_{18}O_2$ mol. wt. 206.28

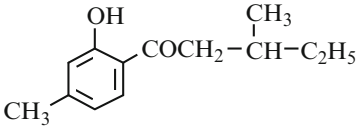


Synthesis
-Obtained by Fries rearrangement of (+) o-cresyl 3-methylvalerate (45.8 %) [2093].

b.p.$_{15}$ 195–200° [2093]; $(\alpha)_D^{30} = +2.03$ [2093].

1-(2-Hydroxy-4-methylphenyl)-3-methyl-1-pentanone (+)

[39575-45-6] $C_{13}H_{18}O_2$ mol. wt. 206.28

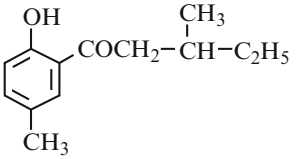


Synthesis
-Obtained by Fries rearrangement of (+) m-cresyl 3-methylvalerate (72.8 %) [2093].

b.p.$_{15}$ 208–210° [2093]; $(\alpha)_D^{30} = +2.46$ [2093].

1-(2-Hydroxy-5-methylphenyl)-3-methyl-1-pentanone (+)

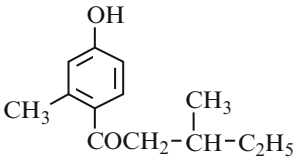
[39575-46-7] $C_{13}H_{18}O_2$ mol. wt. 206.28



Synthesis
-Obtained by Fries rearrangement of (+) p-cresyl 3-methylvalerate (61.1 %) [2093].
b.p.$_{15}$ 220–225° [2093];
$(\alpha)_D^{30} = +2.78$ [2093].

1-(4-Hydroxy-2-methylphenyl)-3-methyl-1-pentanone

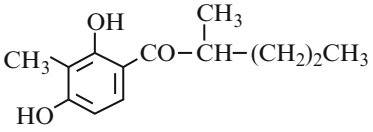
[165538-95-4] $C_{13}H_{18}O_2$ mol. wt. 206.28



Synthesis
-Refer to: [1717].

1-(2,4-Dihydroxy-3-methylphenyl)-2-methyl-1-pentanone

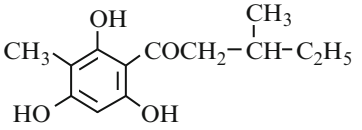
$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Refer to: [3147].
^{1}H NMR [3147], ^{13}C NMR [3147].

3-Methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-pentanone (S)

[120716-96-3] $C_{13}H_{18}O_4$ mol. wt. 238.28

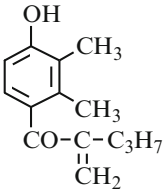


Synthesis
-Refer to: [3405].
m.p. 145° [3405];
^{1}H NMR [3405], IR [3405], MS [3405];
M+, 210 (compound **4**, p. 473).

BIOLOGICAL ACTIVITY: As photosynthetic electron transport (PET) [3405].

1-(4-Hydroxy-2,3-dimethylphenyl)-2-methylene-1-pentanone

$C_{14}H_{18}O_2$ mol. wt. 218.30



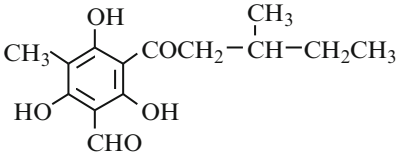
Synthesis
-Refer to: [742].
Methyl ether [101375-35-3] $C_{15}H_{20}O_2$ mol. wt. 232.32
-Obtained by treatment of 2,3-dimethyl-4-methoxyvalero-phenone with N,N,N′,N′-tetramethylmethanediamine (95 %) [742].

-Also obtained from 2-bromo-1-(2,3-dimethyl-4-methoxyphenyl)-2-methyl-1-propanone [742].

liquid [742]; ^{1}H NMR [742].

2,4,6-Trihydroxy-3-methyl-5-(3-methyl-1-oxopentyl)benzaldehyde
(Homograndinol)

[132341-31-2] racemic $C_{14}H_{18}O_5$ mol. wt. 266.29



Synthesis
-Refer to: [3033].
Isolation from natural sources
-From fresh leaves of *Eucalyptus grandis*.

(Myrtaceae) [1106, 1346, 3114, 3405, 3406, 3413].

amorphous solid [3413]; m.p. 145–146° [3405];
^{1}H NMR [3413], IR [3413], UV [3413], MS [3413]; HPLC [3413].

USE: G-inhibitor (plant growth regulator) [3413].

BIOLOGICAL ACTIVITY: Inhibitory effects of treatment with this acylphenol on TPA Induced EBV-EA Activation [3033]; Strongly inhibit photosynthesis as well as germination of cress seeds [1346]; As photosynthetic electron transport (PET) [3405].

S-isomer *(S-Homograndinol)* [116425-03-7] $C_{14}H_{18}O_5$ mol. wt. 266.29

-Obtained by reaction of methyl iodide with 3′-formyl-3-methylvalerophenone in the presence of potassium carbonate in 30 % aqueous acetone at 50° for 3 h (45 %) [3405].
-Also refer to: [3033, 3413].

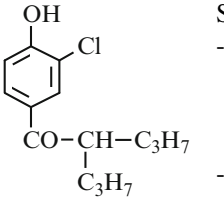
m.p. 153–155° [3405, 3413]; $(\alpha)_D^{20} = +14.1°$ [3413];
^{1}H NMR [3405, 3413], IR [3405, 3413], UV [3413], MS [3405].

BIOLOGICAL ACTIVITY: As photosynthetic electron transport (PET) [3405].

-Also refer to: [3033, 3413].

1-(3-Chloro-4-hydroxyphenyl)-2-propyl-1-pentanone

[4798-12-3] $C_{14}H_{19}ClO_2$ mol. wt. 254.76

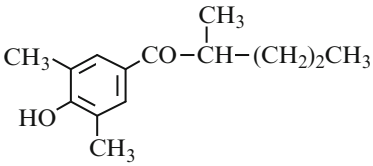


Syntheses
-To dipropylacetyl chloride, 2-chloroanisole and carbon disulfide was added aluminium chloride in small portions at 25°. The mixture stirred 1 h at r.t. and 45 min at 55° then pentane and aluminium chloride were added and heated 3 h at 80° [2056].
-Also refer to: [2767].

$b.p._{\cdot 0.5}$ 140° [2056, 2767].

1-(3,5-Dimethyl-4-hydroxyphenyl)-2-methyl-1-pentanone

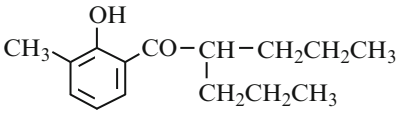
[92301-09-2] $C_{14}H_{20}O_2$ mol. wt. 220.31



Synthesis
-Refer to: [2268].
m.p. 83–83.5° [2268]; IR [2268].

1-(2-Hydroxy-3-methylphenyl)-2-propyl-1-pentanone

[137937-40-7] $C_{15}H_{22}O_2$ mol. wt. 234.34

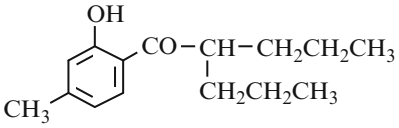


Syntheses
-Preparation by Fries rearrangement of o-cresyl valproate in the presence of aluminium chloride in chlorobenzene for 4 h at 140° (55 %) [2003].
-Also refer to: [2002].

b.p.$_{0.6}$ 124° (Sadtler standard N° 84999K) [2003];
^{1}H NMR (Sadtler standard N° 57945M) [2003],
IR (Sadtler standard N° 84999K) [2003], UV [2003], MS [2003].

1-(2-Hydroxy-4-methylphenyl)-2-propyl-1-pentanone

[137937-41-8] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Preparation by Fries rearrangement of 3-methyl-phenyl valproate in the presence of aluminium chloride in nitromethane for 170 h at 20° (63 %) [2003].
-Also refer to: [2002].

b.p.$_{1.4}$ 129° (Sadtler standard N° 85000K) [2003];
^{1}H NMR (Sadtler standard N° 57946M) [2003];
IR (Sadtler standard N° 85000K) [2003], UV [2003], MS [2003].

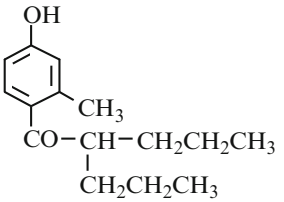
Methyl ether [137937-53-2] $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by treatment of 3-methylanisole with valproyl chloride in the presence of aluminium chloride in carbon disulfide at +5° for 6 h (46 %) [2003].
-Also obtained by direct methylation of its above ketone (95 %) [2003].

b.p.$_{0.7}$ 128–130° (Sadtler standard N° 57883M) [2003];
^{1}H NMR (Sadtler standard N° 57883M) [2003];
IR (Sadtler standard N° 84931K), [2003], UV [2003], MS [2003].

1-(4-Hydroxy-2-methylphenyl)-2-propyl-1-pentanone

[137937-46-3] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Obtained by treatment of its methyl ether below with aluminium bromide in refluxing benzene for 4 h (40 %) [2003].
-Also refer to: [2002].
m.p. 80° (Sadtler standard N° 84930K) [2003];
^{1}H NMR (Sadtler standard N° 57882M) [2003];

IR (Sadtler standard N° 84930K) [2003], UV [2003], MS [2003].

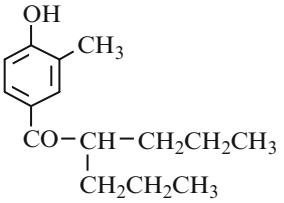
Methyl ether [137937-54-3] $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by direct methylation of its above ketone (80 %) [2003].

b.p.$_{0.7}$ 128–130° (Sadtler standard N° 57884M) [2002, 2003];
^{1}H NMR (Sadtler standard N° 57884M) [2002, 2003],
IR (Sadtler standard N° 84932K) [2002, 2003], UV [2002, 2003], MS [2002, 2003].

1-(4-Hydroxy-3-methylphenyl)-2-propyl-1-pentanone

$C_{15}H_{22}O_2$ mol. wt. 234.34

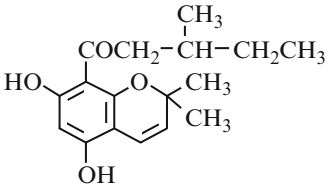


Syntheses
-Preparation by Fries rearrangement of 2-methylphenyl valproate in the presence of aluminium chloride in nitromethane for 170 h at 20° (78 %) [2003].
-Also refer to: [2002].
m.p. 86° (Sadtler standard N° 84929K) [2003];

^{1}H NMR (Sadtler standard N° 57881M) [2003];
IR (Sadtler standard N° 84929K) [2003], UV [2003], MS [2003].

5,7-Dihydroxy-2,2-dimethyl-2*H*-1-(benzopyran-8-yl)-3-methyl-1-pentanone

$C_{17}H_{22}O_4$ mol. wt. 290.36



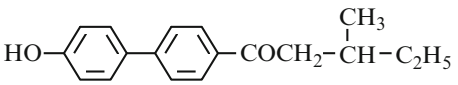
Synthesis
-Refer to: [3203].

Dimethyl ether [924889-50-9]
$C_{19}H_{26}O_4$ mol. wt. 318.41
-Obtained by adding a solution of malloapelta B in diethyl ether to the solution of the ethylmagnesium bromide in diethyl ether under a nitrogen atmosphere at −10° for 30 min (85 %) [3203].

white solid [3203]; m.p. 62.2° [3203];
^{1}H NMR [3203], IR [3203]; TLC [3203].

1-(4′-Hydroxy[1,1-biphenyl]-4-yl)-3-methyl-1-pentanone

$C_{18}H_{20}O_2$ mol. wt. 268.36



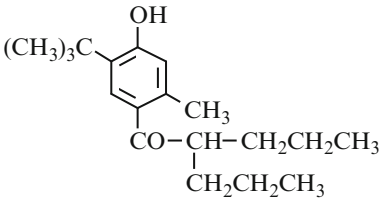
Synthesis
-Refer to: [1445].

Octyl ether [96123-20-5] $C_{26}H_{36}O_2$ mol. wt. 380.57

-Refer to: [1445].

1-[5-(1,1-Dimethylethyl)-4-hydroxy-2-methylphenyl]-2-propyl-1-pentanone

$C_{19}H_{30}O_2$ mol. wt. 290.45



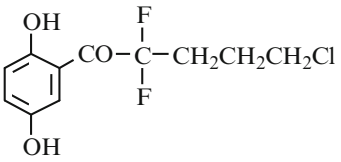
Synthesis
-Refer to: [2002].
m.p. 93° (Sadtler standard N° 84934K);
^{1}H NMR (Sadtler standard N° 57886M);
IR (Sadtler standard N° 84934K).

4 Aromatic Hydroxyketones Derived from Various Halogenopentanoic Acids

4.1 Unsubstituted Hydroxyketones

5-Chloro-1-(2,5-dihydroxyphenyl)-2,2-difluoro-1-pentanone

$C_{11}H_{11}ClF_2O_3$ mol. wt. 264.66

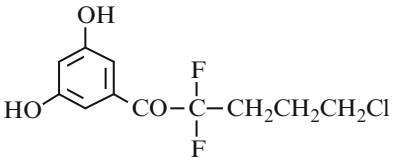


Synthesis
-Refer to: [3218].
Dimethyl ether [1039364-65-2]
$C_{13}H_{15}ClF_2O_3$ mol. wt. 292.71
-Refer to: [3218].

^{1}H NMR [3218], ^{13}C NMR [3218], ^{19}F NMR [3218], IR [3218], MS [3218].

5-Chloro-1-(3,5-dihydroxyphenyl)-2,2-difluoro-1-pentanone

$C_{11}H_{11}ClF_2O_3$ mol. wt. 264.66



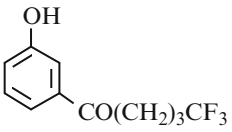
Synthesis
-Refer to: [3218].

Dimethyl ether [1039364-66-3]
$C_{13}H_{15}ClF_2O_3$ mol. wt. 292.71
-Refer to: [3218].

^{1}H NMR [3218], ^{13}C NMR [3218], ^{19}F NMR [3218], IR [3218].

5,5,5-Trifluoro-1-(3-hydroxyphenyl)-1-pentanone

[104325-67-9] $C_{11}H_{11}F_3O_2$ mol. wt. 232.20

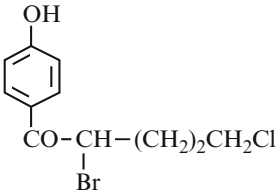


Synthesis
-Refer to: [2198].

USE: In preparation of antiinflammatory and antiallergic agents [2198].

2-Bromo-5-chloro-1-(4-hydroxyphenyl)-1-pentanone

$C_{11}H_{12}BrClO_2$ mol. wt. 291.57



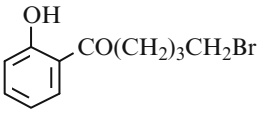
Synthesis
-Refer to: [122].

Methyl ether [1104634-92-5]
$C_{12}H_{14}BrClO_2$ mol. wt. 305.60
-Refer to: [122].

BIOLOGICAL ACTIVITY: Preparation of phenyl pentalen-1-ones as therapeutic and diagnostic estrogen receptor ligands [122].

5-Bromo-1-(2-hydroxyphenyl)-1-pentanone

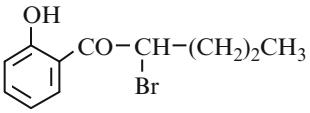
[173055-13-5] $C_{11}H_{13}BrO_2$ mol. wt. 257.13



Synthesis
-Refer to: [2623].

2-Bromo-1-(2-hydroxyphenyl)-1-pentanone

$C_{11}H_{13}BrO_2$ mol. wt. 257.13

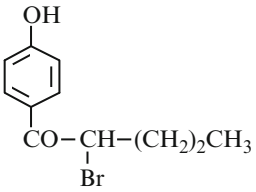


Synthesis
-Refer to: [2848].

Methyl ether [934637-35-1]
$C_{12}H_{15}BrO_2$ mol. wt. 271.15
-Refer to: [2848]; ^{1}H NMR [2848].

2-Bromo-1-(4-hydroxyphenyl)-1-pentanone

[750646-76-5] $C_{11}H_{13}BrO_2$ mol. wt. 257.13



Syntheses
-Refer to: [1379, 1381, 1383 (Chinese papers), 3471],
^{1}H NMR [1383], MS [1383];
X-ray data [1383].

USE: Preparation of 4-acetamido-3-(4-aryl-2-thiazolylamino)benzoate as fungicide and insecticide [1379]; Preparation of 2-methyl-1-(2-thiazolyl)-1*H*-benzimidazole-6-carboxylic acid ethyl ester derivatives and determination of their activity as agrochemical fungicides [1383].

Methyl ether [36412-64-3] $C_{12}H_{15}BrO_2$ mol. wt. 271.15

-Obtained by bromination of 4-methoxyvalerophenone in ethyl ether or methylene chloride with bromine in an ice bath at 0° for 10 min; then the mixture was warmed to r.t. [2043].
-Also obtained by treatment of 1-(4-methoxyphenyl)-1-pentanone with bromine in ethyl ether and glacial acetic acid at r.t. (74 %) [1114].
-Also obtained by treatment of 1-(4-methoxyphenyl)-1-pentanone with bromine in the presence of a catalytic amount of aluminium chloride (nearly quantitative yield) [2157].
-Also refer to: [1114, 1630, 1947, 2157, 2158, 3231 (60 %), 3383, 3472].

oil [3231]; b.p.$_{15}$ 150–165° [3231];
m.p. 48–49° [1114], 39–41° [2157];
^{1}H NMR [1114, 1947, 2043, 2157, 3231],
^{13}C NMR [2157], IR [3231], MS [1114].

USE: Preparation of pyrovalerone analogs as monoamine uptake inhibitors [2043].

Benzyl ether [35081-50-6] $C_{18}H_{19}BrO_2$ mol. wt. 347.25

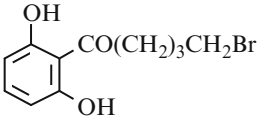
-Preparation by bromination of 4-benzyloxyvalerophenone with cupric bromide,
*in an ethyl acetate/chloroform mixture (82.6-97.5 %) [1384];
*in refluxing ethanol [546] according to the process [1382].

-Also obtained by irradiation with UV lamp of a solution of 4-benzyloxyvalerophenone and bromine in methylene chloride for 15 h between 15–18° (67 %) [556].

m.p. 84° [556].

5-Bromo-1-(2,6-dihydroxyphenyl)-1-pentanone

[1111652-02-8] $C_{11}H_{13}BrO_3$ mol. wt. 273.13

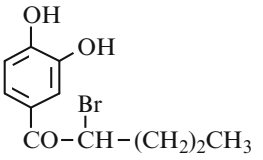


Synthesis
-Refer to: [1219 (Chinese patent)].

USE: Preparation of low swelling sulfonated polyimide proton exchange membrane for fuel cell [1219].

2-Bromo-1-(3,4-dihydroxyphenyl)-1-pentanone

$C_{11}H_{13}BrO_3$ mol. wt. 273.13



Syntheses
-Preparation [1948] using the general procedure [1738].
-Also refer to: [1947, 2043].

Dimethyl ether [850352-39-5]
$C_{13}H_{17}BrO_3$ mol. wt. 301.18

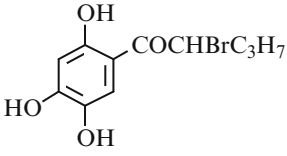
-Obtained by bromination of 3,4-dimethoxyvalerophenone in ethyl ether or methylene chloride with bromine in an ice bath at 0° for 10 min; then the mixture was warmed to r.t. [2043].

^{1}H NMR [2043].

USE: Preparation of pyrovalerone analogs as monoamine uptake inhibitors [2043]; Preparation of pyrovalerone analogs as selective dopamine transporter inhibitors [1947].

2-Bromo-1-(2,4,5-trihydroxyphenyl)-1-pentanone

$C_{11}H_{13}BrO_4$ mol. wt. 289.13



Synthesis
-Refer to: [2696].

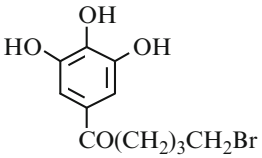
Trimethyl ether [90834-08-5]
$C_{14}H_{19}BrO_4$ mol. wt. 331.20

-Obtained by reaction of bromine with 2,4,5-trimethoxyvalerophenone in acetic acid at 35–40°, then at 25° for 40 min [2695].
-Also refer to: [2696].

m.p. 67–68° [2695, 2696];
^{1}H NMR [2695, 2696], IR [2695, 2696], MS [2695, 2696].

1-(5-Bromo-3,4,5-trihydroxyphenyl)-1-pentanone

$C_{11}H_{13}BrO_4$ mol. wt. 289.13

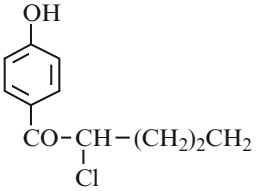


Synthesis
-Refer to: [1130].

Trimethyl ether [484676-16-6]
$C_{14}H_{19}BrO_4$ mol. wt. 331.20
-Refer to: [1130].

2-Chloro-1-(4-hydroxyphenyl)-1-pentanone

[1108128-60-4] $C_{11}H_{13}ClO_2$ mol. wt. 212.68

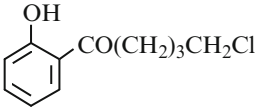


Synthesis
-Refer to: [1379 (Chinese patent)].

USE: Preparation of 4-acetamido-3-(4-aryl-2-thiazolyl-amino)benzoate as fungicide and insecticide [1379].

5-Chloro-1-(2-hydroxyphenyl)-1-pentanone

[501083-61-0] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



Synthesis
-Refer to: [2459].
^{1}H NMR [2459], MS [2459].

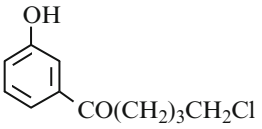
Methyl ether [43228-96-2] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

-Obtained by treatment of δ-lactone of 2-(o-methoxybenzoyl)-5-hydroxyvaleric acid with concentrated HCl (90 %) [371].
-Also refer to: [2459].

colourless oil [371]; b.p.$_{0.5}$ 100° [371];
^{1}H NMR [2459], MS [2459].

5-Chloro-1-(3-hydroxyphenyl)-1-pentanone

[501083-63-2] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



Synthesis
-Refer to: [2459].
^{1}H NMR [2459], MS [2459].

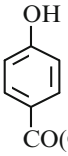
Methyl ether [258882-49-4] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

-Preparation by treatment of 5-chloro-1-(3-methoxyphenyl)-1-pentanol with chromium trioxide in dilute sulfuric acid (Jones' Reagent) in acetone first at 0°, then at r.t. for 6 h (89 %) [2460].
-Also refer to: [2459].

colourless oil [2460]; ^{1}H NMR [2460], MS [2460].

5-Chloro-1-(4-hydroxyphenyl)-1-pentanone

[83882-87-5] $C_{11}H_{13}ClO_2$ mol. wt. 212.68



Syntheses
-Obtained by reaction of 5-chlorovaleroyl chloride with phenol in the presence of aluminium chloride [2459] in nitrobenzene at 40° for 3 h (60 %) [1581].
-Also refer to: [1580, 2371, 2372].
m.p. 116–117° [1581].

Methyl ether [949-06-4] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

-Preparation: To an ethereal solution of p-methoxyphenylmagnesium bromide was added 5-chlorovaleronitrile in ether. The reaction mixture was stirred at r.t. for 10 h and hydrolyzed by 15 % hydrochloric acid (17.7 %) [2413].
-Also obtained [1589] from the method [555].
-Also refer to: [122, 1125, 1126, 1171, 1367, 1459, 1460, 1956, 3076, 3286, 3287].

m.p. 82–84° [2413], 67–68° [1460];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [1171, 1367, 1460], IR [1171].

USE: Preparation of phenyl pentalen-1-ones as therapeutic and diagnostic estrogen receptor ligands [122]; Preparation of imidazolyl inhibitors of 15-lipoxygenase [3287].

Phenyl ether [820968-19-2] $C_{17}H_{17}ClO_2$ mol. wt. 288.77

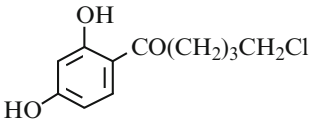
-Refer to: [2905].

Difluoromethyl ether [83882-88-6] $C_{12}H_{13}ClF_2O_2$ mol. wt. 262.68

-Refer to: [2371].

5-Chloro-1-(2,4-dihydroxyphenyl)-1-pentanone

$C_{11}H_{13}ClO_3$ mol. wt. 228.68



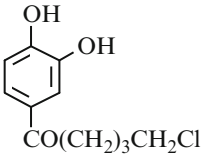
Synthesis
-Refer to: [3284].
Dimethyl ether [33245-78-2]
$C_{13}H_{17}ClO_3$ mol. wt. 256.73

-Refer to: [677, 3284].

m.p. 56–57° [677].

5-Chloro-1-(3,4-dihydroxyphenyl)-1-pentanone

$C_{11}H_{13}ClO_3$ mol. wt. 228.68



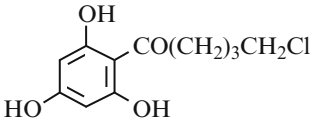
Synthesis
-Refer to: [677, 1171].
Dimethyl ether [33245-77-1]
$C_{13}H_{17}ClO_3$ mol. wt. 256.73

-Refer to: [677, 1171, 2561].

m.p. 46–47° [677], 42–45° [1171]; IR [1171].

5-Chloro-1-(2,4,6-trihydroxyphenyl)-1-pentanone

$C_{11}H_{13}ClO_4$ mol. wt. 244.67



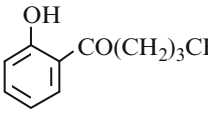
Synthesis
-Refer to: [3284].
Trimethyl ether [187396-81-2]
$C_{14}H_{19}ClO_4$ mol. wt. 286.76

-Refer to: [308, 926, 927, 3284].

m.p. 53–55° [3284], 50° [926]; ^{1}H NMR [926].

1-(2-Hydroxyphenyl)-5-iodo-1-pentanone

$C_{11}H_{13}IO_2$ mol. wt. 304.12



Synthesis
-Refer to: [371].
Methyl ether [43228-97-3]
$C_{12}H_{15}IO_2$ mol. wt. 318.15

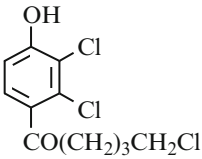
-Obtained by treatment of 5-chloro-1-(2-hydroxyphenyl)-1-pentanone with sodium iodide in boiling acetone for 30 h under nitrogen atmosphere (86 %) [371].

b.p.$_{0.005}$ 95° [371].

4.2 Substituted Hydroxyketones

5-Chloro-1-(2,3-dichloro-4-hydroxyphenyl)-1-pentanone

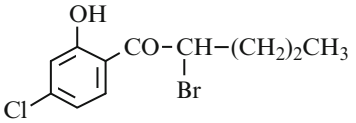
$C_{11}H_{11}Cl_3O_2$ mol. wt. 281.57



Synthesis
-Refer to: [741].
Methyl ether [115595-92-1]
$C_{12}H_{13}Cl_3O_2$ mol. wt. 295.59
-Refer to: [741].

2-Bromo-1-(4-chloro-2-hydroxyphenyl)-1-pentanone

$C_{11}H_{12}BrClO_2$ mol. wt. 291.57



Synthesis
-Refer to: [1199].
Methyl ether [1001441-59-3]
$C_{12}H_{14}BrClO_2$ mol. wt. 305.60

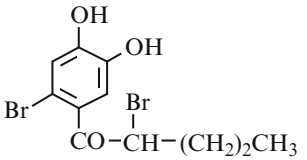
-Refer to: [1199].

^{1}H NMR [1199], IR [1199], MS [1199].

USE: For preparation of triphenyl-substituted 5-membered heterocycles as anticancer and antiinflammatory agents [1199].

2-Bromo-1-(2-bromo-4,5-dihydroxyphenyl)-1-pentanone

$C_{11}H_{12}Br_2O_3$ mol. wt. 352.03



Syntheses
-Refer to: [1947, 2043].
Dimethyl ether [850352-40-8]
$C_{13}H_{16}Br_2O_3$ mol. wt. 380.08
-Obtained by bromination of 3,4-dimethoxyvalerophenone in ethyl ether or methylene chloride with bromine in an ice bath at 0° for 10 min; then the mixture was warmed to r.t. [2043].

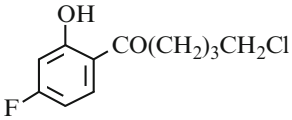
-Also refer to: [1947].

^{1}H NMR [1947, 2043].

USE: Preparation of pyrovalerone analogs as selective dopamine transporter inhibitors [1947].

5-Chloro-1-(4-fluoro-2-hydroxyphenyl)-1-pentanone

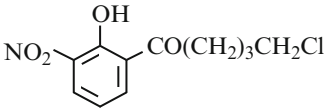
[149412-46-4] $C_{11}H_{12}ClFO_2$ mol. wt. 230.67



Synthesis
-Refer to: [2065].
m.p. 45–47° [2065]; ^{1}H NMR [2065], ^{13}C NMR [2065], IR [2065].

5-Chloro-1-(2-hydroxy-3-nitrophenyl)-1-pentanone

$C_{11}H_{12}ClNO_4$ mol. wt. 257.67

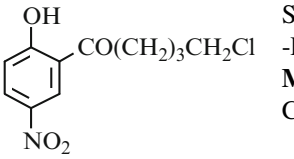


Synthesis
-Refer to: [308].
Methyl ether [187396-94-7]
$C_{12}H_{14}ClNO_4$ mol. wt. 271.70

-Refer to: [308].

5-Chloro-1-(2-hydroxy-5-nitrophenyl)-1-pentanone

$C_{11}H_{12}ClNO_4$ mol. wt. 257.67



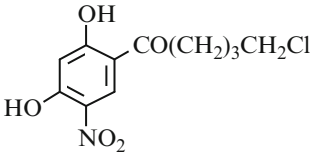
Synthesis
-Refer to: [3284].
Methyl ether [187396-95-8]
$C_{12}H_{14}ClNO_4$ mol. wt. 271.70

-Refer to: [308, 3284].

m.p. 57–58° [3284].

5-Chloro-1-(2,4-dihydroxy-5-nitrophenyl)-1-pentanone

$C_{11}H_{12}ClNO_5$ mol. wt. 273.67

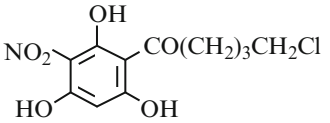


Synthesis
-Refer to: [308].
Dimethyl ether [187396-92-5]
$C_{13}H_{16}ClNO_5$ mol. wt. 301.73

-Refer to: [308].

5-Chloro-1-(2,4,6-trihydroxy-3-nitrophenyl)-1-pentanone

$C_{11}H_{12}ClNO_6$ mol. wt. 289.67

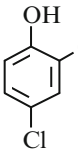


Synthesis
-Refer to: [3284].
Trimethyl ether [187396-96-9]
$C_{14}H_{18}ClNO_6$ mol. wt. 331.75

-Refer to: [308, 3284].

5-Chloro-1-(5-chloro-2-hydroxyphenyl)-1-pentanone

$C_{11}H_{12}Cl_2O_2$ mol. wt. 247.12



Synthesis
-Refer to: [3284].

Methyl ether [187396-80-1]
$C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15

-Refer to: [3284].

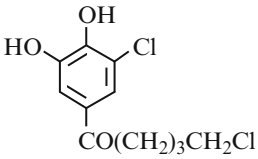
m.p. 52–54° [3284].

Benzyl ether [1146443-98-2] $C_{18}H_{18}Cl_2O_2$ mol. wt. 337.25

-Refer to: [3284].

5-Chloro-1-(3-chloro-4,5-dihydroxyphenyl)-1-pentanone

$C_{11}H_{12}Cl_2O_3$ mol. wt. 263.12



Synthesis
-Refer to: [3087].

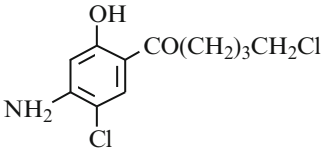
Dimethyl ether [817630-32-3]
$C_{13}H_{16}Cl_2O_3$ mol. wt. 291.17

-Refer to: [3087].

USE: Preparation of N-substituted phenylpiperazines as dual function compounds [3087].

1-(4-Amino-5-chloro-2-hydroxyphenyl)-5-chloro-1-pentanone

$C_{11}H_{13}Cl_2NO_2$ mol. wt. 262.14

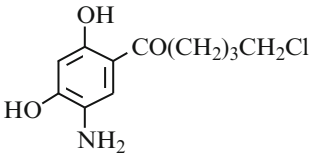


Synthesis
-Refer to: [680].

Methyl ether [166816-20-2]
$C_{12}H_{15}Cl_2NO_2$ mol. wt. 276.16
-Refer to: [680].

1-(5-Amino-2,4-dihydroxyphenyl)-5-chloro-1-pentanone

$C_{11}H_{14}ClNO_3$ mol. wt. 243.69



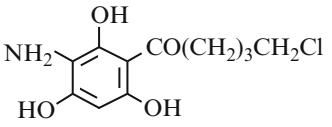
Synthesis
-Refer to: [3284].

Dimethyl ether [187396-97-0]
$C_{13}H_{18}ClNO_3$ mol. wt. 271.74
-Refer to: [308, 3284].

m.p. 87–88° [3284].

1-(3-Amino-2,4,6-trihydroxyphenyl)-5-chloro-1-pentanone

$C_{11}H_{14}ClNO_4$ mol. wt. 259.69



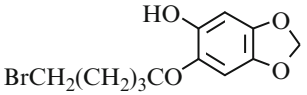
Synthesis
-Refer to: [3284].

Trimethyl ether [187396-99-2]
$C_{14}H_{20}ClNO_4$ mol. wt. 301.77

-Refer to: [308, 3284].

5-Bromo-1-(6-hydroxy-1,3-benzodioxol-5-yl)-1-pentanone

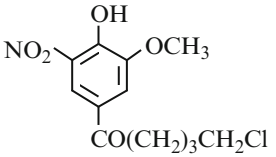
[173055-10-2] $C_{12}H_{13}BrO_4$ mol. wt. 301.14



Synthesis
-Refer to: [2623].

5-Chloro-1-(4-hydroxy-3-methoxy-5-nitrophenyl)-1-pentanone

[817630-35-6] $C_{12}H_{14}ClNO_5$ mol. wt. 287.70

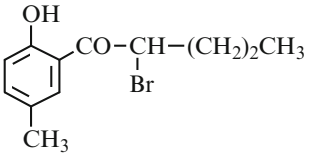


Synthesis
-Refer to: [3087].

USE: Preparation of N-substituted phenylpiperazines as dual function compounds [3087].

2-Bromo-1-(2-hydroxy-5-methylphenyl)-1-pentanone

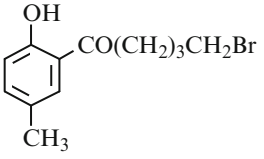
$C_{12}H_{15}BrO_2$ mol. wt. 271.15



Synthesis
-Refer to: [181].
m.p. 51–52° [181].

5-Bromo-1-(2-hydroxy-5-methylphenyl)-1-pentanone

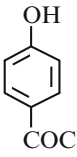
[173055-00-0] $C_{12}H_{15}BrO_2$ mol. wt. 271.15



Synthesis
-Refer to: [2623].

2-Bromo-1-(4-hydroxyphenyl)-4-methyl-1-pentanone

$C_{12}H_{15}BrO_2$ mol. wt. 271.15



Synthesis
-Refer to: [3232].

Methyl ether [33720-04-6]
$C_{13}H_{17}BrO_2$ mol. wt. 285.18

-Obtained by treatment of 1-(4-methoxyphenyl)-4-methyl-1-pentanone with bromine in a mixture of ethyl ether/dioxane at r.t. (90 %) [3232].
-Also refer to: [1114].

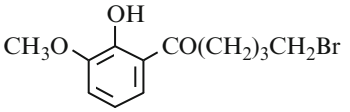
b.p.$_{0.1}$ 124–125° [3232];
^{1}H NMR [1114, 3232], IR [3232], MS [1114].

Trimethylsilyl ether [719311-19-0] $C_{21}H_{35}BrO_2Si$ mol. wt. 427.50

-Refer to: [627].

5-Bromo-1-(2-hydroxy-3-methoxyphenyl)-1-pentanone

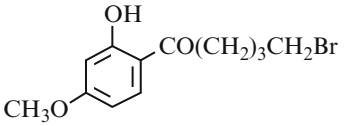
[173055-16-8] $C_{12}H_{15}BrO_3$ mol. wt. 287.15



Synthesis
-Refer to: [2623].

5-Bromo-1-(2-hydroxy-4-methoxyphenyl)-1-pentanone

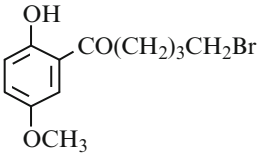
[173054-96-1] $C_{12}H_{15}BrO_3$ mol. wt. 287.15



Synthesis
-Refer to: [2623].

5-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-pentanone

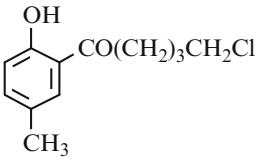
[173054-85-8] $C_{12}H_{15}BrO_3$ mol. wt. 287.15



Synthesis
-Refer to: [2623].

5-Chloro-1-(2-hydroxy-5-methylphenyl)-1-pentanone

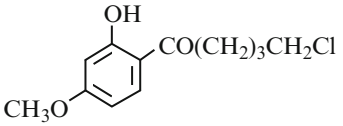
$C_{12}H_{15}ClO_2$ mol. wt. 226.70



Synthesis
-Refer to: [1127].
b.p.1 150–154° [1127]; $n_D^{17.5} = 1.5565$ [1127].

5-Chloro-1-(2-hydroxy-4-methoxyphenyl)-1-pentanone

[66832-66-4] $C_{12}H_{15}ClO_3$ mol. wt. 242.70

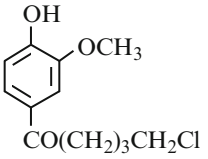


Synthesis
-Obtained by reaction of 5-chloropentanoic acid with m-methoxyphenol in the presence of boron trifluoride etherate at 90° for 1 h (62 %) [820].

yellow needles [820]; m.p. 25.5–26.5° [820];
^{1}H NMR [820], IR [820].

5-Chloro-1-(4-hydroxy-3-methoxyphenyl)-1-pentanone

[817630-37-8] $C_{12}H_{15}ClO_3$ mol. wt. 242.70



Synthesis
-Refer to: [3087].

USE: Preparation of N-substituted phenylpiperazines as dual function compounds [3087].

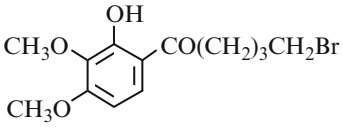
Benzyl ether [817630-36-7] $C_{19}H_{21}ClO_3$ mol. wt. 332.82

-Refer to: [3087].

USE: Preparation of N-substituted phenylpiperazines as dual function compounds [3087].

5-Bromo-1-(2-hydroxy-3,4-dimethoxyphenyl)-1-pentanone

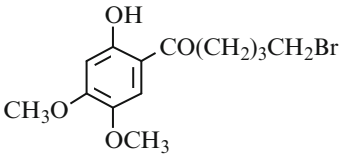
[173055-06-6] $C_{13}H_{17}BrO_4$ mol. wt. 317.18



Synthesis
-Refer to: [2623].

5-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-pentanone

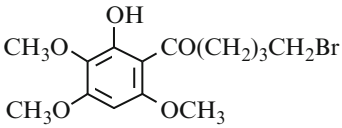
[173054-91-6] $C_{13}H_{17}BrO_4$ mol. wt. 317.18



Synthesis
-Refer to: [2623].

5-Bromo-1-(2-hydroxy-3,4,6-trimethoxyphenyl)-1-pentanone

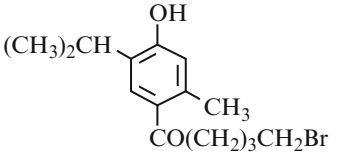
[173055-08-8] $C_{14}H_{19}BrO_5$ mol. wt. 347.20



Synthesis
-Refer to: [2623].

5-Bromo-1-[4-hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-pentanone

$C_{15}H_{21}BrO_2$ mol. wt. 313.23



Synthesis
-Refer to: [220].

Methyl ether [72236-93-2]
$C_{16}H_{23}BrO_2$ mol. wt. 327.26

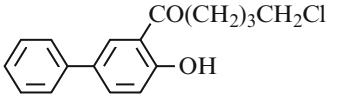
-Obtained by reaction of 5-bromopentanoyl chloride with thymol methyl ether in the presence of aluminium chloride in methylene chloride at r.t. (90 %) [220].

m. p. 40° [220].

BIOLOGICAL ACTIVITY: Amebicidal and bactericidal and molluscicidal [220].

5-Chloro-1-(4-hydroxy[1,1′-biphenyl]-3-yl)-1-pentanone

$C_{17}H_{17}ClO_2$ mol. wt. 288.77



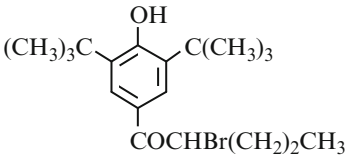
Synthesis
-Refer to: [308].

Methyl ether [187396-84-5]
$C_{18}H_{19}ClO_2$ mol. wt. 302.80

-Refer to: [308].

2-Bromo-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-pentanone

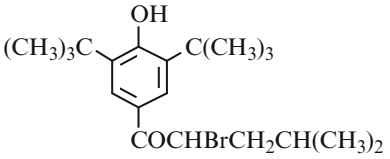
[17055-15-1] $C_{19}H_{29}BrO_2$ mol. wt. 369.34



Syntheses
-Obtained by reaction of bromine with 4-hydroxy-3,5-di-tert-butylvalerophenone in octane for 30 min at 70° (84 %) [3238, 3239].
m.p. 78–80° [3238, 3239].

2-Bromo-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-4-methyl-1-pentanone

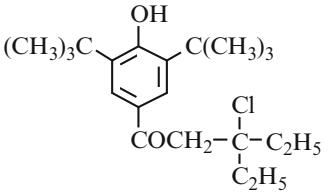
$C_{20}H_{31}BrO_2$ mol. wt. 383.37



Synthesis
-Obtained by reaction of 2-bromoisocaproyl chloride with 2,6-di-tert-butylphenol in the presence of titanium tetrachloride [1468].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-chloro-3-ethyl-1-pentanone

[174635-33-7] $C_{21}H_{33}ClO_2$ mol. wt. 352.94



Synthesis
-Refer to: [2482].
m.p. 72° [1499].

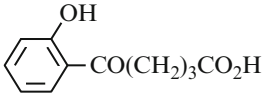
BIOLOGICAL ACTIVITY: Antiinflammatory and analgesic agent [2482].

5 Aromatic Hydroxyketones Derived from 5-Oxopentanoic Acid

5.1 Unsubstituted Hydroxyketones

5-(2-Hydroxyphenyl)-5-oxo-1-pentanoic acid

[4648-97-9] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Obtained by Fries rearrangement of phenyl glutarate with aluminium chloride,
-in the presence of solvents,

*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];

*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].
-Also obtained by reaction of glutaric anhydride with phenol in the presence of aluminium chloride in tetrachloroethane/nitrobenzene mixture (1:1) at 130–140° for 3 h (50 %) [588].
-Also obtained by dehydrogenation of 2-(4-carbomethoxybutyroyl)cyclohexanone in the presence of 10 % Pt/C in refluxing p-cymene for 24 h [331], (37 %) [332].
-Refer to: [588].

pale yellow heavy prisms [332];
m.p. 112° [902], 110° [331, 332], 100° [588];
IR [331, 332], UV [331, 332].

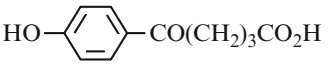
2,4-Dinitrophenylhydrazone [4648-98-0] $C_{17}H_{16}N_4O_7$ mol. wt. 388.34

-Refer to: [588].

m.p. 185° [588].

5-(4-Hydroxyphenyl)-5-oxo-1-pentanoic acid

[4648-94-6] $C_{11}H_{12}O_4$ mol. wt. 208.21



Syntheses
-Obtained by Fries rearrangement of phenyl glutarate with aluminium chloride,

-in the presence of solvents:
*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];
*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].
-Also obtained by reaction of glutaryl chloride with phenol in the presence of aluminium chloride in nitrobenzene, first at 0–5°, then at r.t. for 18 h (38 %) [588].
-Also obtained by reaction of glutaric anhydride with phenol in the presence of aluminium chloride in tetrachloroethane/nitrobenzene mixture (1:1) at 130–140° for 3 h (50 %) [588].
-Also obtained by treatment of methylphenyl glutarate ($C_{12}H_{14}O_4$; b.p.$_{12}$ 178–179°) with aluminium chloride in nitrobenzene at 50° for 20 min (60–80 %) [3135].
-Refer to: [3099].

colourless needles [588];
m.p. 202–203° [3135], 200–202° [902], 199–200° [588], 190–195° [3099];
IR [588].

2,4-Dinitrophenylhydrazone [4648-95-7] $C_{17}H_{16}N_4O_7$ mol. wt. 388.34

m.p. 175° [588].

Acetate [4648-96-8] $C_{13}H_{14}O_5$ mol. wt. 250.25

-Obtained by reaction of acetic anhydride with the title ketone in refluxing pyridine for 6 h [588].

m.p. 120° [588].

Methyl ether [4609-10-3] $C_{12}H_{14}O_4$ mol. wt. 222.24

-Obtained by reaction of glutaryl chloride with anisole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:4) [588].
-Also obtained by reaction of glutaric anhydride with anisole in the presence of aluminium chloride [2359, 3401], (90 %) [2132] in tetrachloroethane/nitrobenzene (1:2) at 0–5° [588].
-Also obtained by hydrolysis of 2-anisoylglutarimide ([19450-23-8], m.p. 169.5–170.5°) with refluxing 6 N HCl for 24 h (87 %) [3327].
-Also obtained by treatment of its ethyl ester with boiling 10 % aqueous potassium hydroxide for 6 h (87.5 %) [1422].
-Also refer to: [435, 878 (32 %), 989 (85 %), 1131, 1370, 1394, 1529 (90 %), 1567 (61 %), 2025, 2358, 2392 (93.5 %), 2519 (82 %), 2843, 3152, 3288, 3367].

m.p. 141–142° [939, 1131], 140–141° [1422], 140° [2820], 139.5–141° [3327], 139.5–140.5° [989], 138.5–141° [1529, 2358, 2359], 138–140° [1688, 2519], 138–139° [2392], 138° [588, 1567], 137–138° [3401], 137° [3288], 136–138° [1370], 133° [435], 132–135° [878], 126–128° [2132], 115–125° [874];
^{1}H NMR [435, 939, 1131, 1370, 3152], ^{13}C NMR [435], IR [588, 939, 1370], MS [435, 1567]; pK_a [2358].

BIOLOGICAL ACTIVITY: Human zinc insulin, delivery of [1131]; Anorexigen [2358].

2,4-Dinitrophenylhydrazone of the methyl ether

[4626-83-9] $C_{18}H_{18}N_4O_7$ mol. wt. 402.36

m.p. 145° [588].

Methyl ester of the methyl ether [1847-68-3] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Refer to: [219, 939, 1274, 1512, 1528, 1567, 1693, 1734, 2843, 3157, 3254];

$b.p._{\cdot 0.6}$ 152–153° [1274];
m.p. 54–55° [3254], 52–54° [1512, 1528], 52–53° [1274], 52° [939], 49–51° [3157];
^{1}H NMR [939, 1512, 1734], ^{13}C NMR [1512], IR [939, 1512], UV [3254], MS [1512, 1567, 3254]; ESR spectroscopy [3254];
Phosphorescence Spectroscopy [3254].

Ethyl ester of the methyl ether [25305-58-2] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Preparation by reaction of ethanol with γ-anisoylbutyric acid in the presence of concentrated sulfuric acid in refluxing benzene for 7 h (93 %) [1529].
-Preparation by refluxing a mixture of ethanol and γ-anisoylbutyric acid in the presence of concentrated sulfuric acid for 6 h [247].
-Also obtained (90 %) [2241] according to the procedure [3121].
-Also refer to: [2241, 2426, 2689, 2805 (24 %), 3254].

pale yellow crystalline solid [1529]; white needles [247];
colourless crystals [2241];
$b.p._{.0.15–0.20}$ 170–185° [1529]; $b.p._{.5–6}$ 193–195° [391];
m.p. 60° [2820], 59–60° [247], 58.5–59.5° [1529], 58.5–59° [2689], 56.5–56.6° [2241],
56–58° [2805], 54° [3254].
^{1}H NMR [2241], ^{13}C NMR [2241], IR [2241], MS [3254].

Ethyl ether [34670-10-5] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by reaction of glutaric anhydride with phenetole in the presence of aluminium chloride in refluxing carbon disulfide for 2 h (64 %) [3288].
-Also obtained by treatment of its ethyl ester with boiling 10 % aqueous potassium hydroxide for 6 h (70.1 %) [1422].
-Also obtained by oxidation of 5-ethoxyphenylvaleric acid (m.p. 105°) with chromic acid in dilute acetic acid (25 %) [3194].

m.p. 118° [3194], 116.5–117° [3194], 114–116° [1422], 114° [3288].

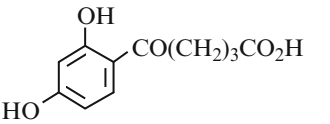
Ethyl ester [66123-78-2] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by treatment of ethyl 5-(4-methoxyphenyl)-5-oxo-1-pentanoate with pyridinium chloride at 185° for 20 h (37 %) [878].
-Also refer to: [3099].

m.p. 75–78° [3099], 74–75° [878].

5-(2,4-Dihydroxyphenyl)-5-oxo-1-pentanoic acid

[4642-43-7] $C_{11}H_{12}O_5$ mol. wt. 224.21



Syntheses
-Obtained by reaction of glutaric anhydride with resorcinol in the presence of aluminium chloride in nitrobenzene, first at 10–15° for 2 h, then at 30–32° for 2 h (78 %) [588].

-Also refer to: [346 (30 %), 3370].

m.p. 181° [445], 180° [588], 175–178° [3374]; IR [588].

2,4-Dinitrophenylhydrazone [4642-44-8] $C_{17}H_{16}N_4O_8$ mol. wt. 404.34

m.p. 285° [588].

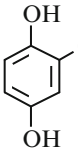
Dimethyl ether [4654-07-3] $C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained by reaction of glutaric anhydride with resorcinol dimethyl ether in the presence of aluminium chloride in nitrobenzene between −5 and 0° for 2 h (80 %) [588].
-Also refer to: [878, 1293, 1567, 1971, 2820].

m.p. 110–118° [878], 110° [588], 106–107° [1293], 98–100° [2820];
^{1}H NMR [1971], IR [588, 1971], MS [1567].

5-(2,5-Dihydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{11}H_{12}O_5$ mol. wt. 224.21



Synthesis
-Refer to: [1567].

Dimethyl ether [63467-20-9]
$C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained by reaction of glutaric anhydride with hydroquinone dimethyl ether in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture first at 0–5°, then at r.t. for 24 h [1567], (75 %) [2998].
-Also obtained by acylation of 1,4-dimethoxybenzene with γ-carbethoxybutyryl chloride as described [1365], (80 %) [112]. The acylation in polyphosphoric acid at 71° for 2.5 h gave only 28 % [112].
-Also refer to: [1210].

m.p. 98–100° [2820], 98–99° [2998], 78–98.5 (?) [112], 96–99° [1210];
N.B.: Probably 98–98.5° [112].
MS [1567].

Semicarbazone of the dimethyl ether $C_{14}H_{19}N_3O_5$ mol. wt. 309.32

m.p. 123° [2820], 122–123° [2998].

Methyl ester of the dimethyl ether [855153-59-2] $C_{14}H_{18}O_5$ mol. wt. 266.29

-Refer to: [112, 1734].

m.p. 50.5° [1734], 48–50° [112];
^{1}H NMR [1734], ^{13}C NMR [1734], IR [1734].

Ethyl ester of the dimethyl ether $C_{15}H_{20}O_5$ mol. wt. 280.32

b.p.$_{.75}$ 260–263° [2820].

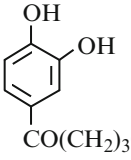
Diethyl ether [94119-33-2] $C_{15}H_{20}O_5$ mol. wt. 280.32

-Refer to: [768].

m.p. 105–106° [768]; ^{1}H NMR [768].

5-(3,4-Dihydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{11}H_{12}O_5$ mol. wt. 224.21



Syntheses
-Refer to: [477, 1293].
m.p. 210–215° [477].
Dimethyl ether [4378-55-6]
$C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained by reaction of glutaric anhydride with veratrole in the presence of aluminium chloride,
*in a nitrobenzene/tetrachloroethane mixture first at 0–5°, then at r.t. for 24 h (41 %) [1567];
*in nitrobenzene at 0° for 12 h (45 %) [1278], (68 %) [2892].
-Also refer to: [569, 1293, 2071].

Yellowish solid [2071]; colourless prisms [2892];
m.p. 152° [2820], 145.7–146° [2071], 142° [1567], 140–142° [569, 1278, 2892];
^{1}H NMR [2071, 2892], ^{13}C NMR [2071], IR [2071, 2892], MS [1567, 2071].

Methyl ester of the dimethyl ether [131699-22-4] $C_{14}H_{18}O_5$ mol. wt. 266.29

-Refer to: [569, 1567, 1734].

m.p. 58–59° [569]; ^{1}H NMR [1734], MS [1567].

Ethyl ester of the dimethyl ether [101499-71-2] $C_{15}H_{20}O_5$ mol. wt. 280.32

b.p.$_{0.05}$ 179–180° [1358]; m.p. 63° [1358], 58.5–60.5° [1363].

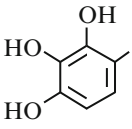
Methylenedioxy [87961-41-9] $C_{12}H_{12}O_5$ mol. wt. 236.22

-Refer to: [1132 (71 %), 2497].

^{1}H NMR [1132], IR [1132], MS [2497].

5-(2,3,4-Trihydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{11}H_{12}O_6$ mol. wt. 240.21



Synthesis
-Refer to: [592].
Trimethyl ether [16093-16-6]
$C_{14}H_{18}O_6$ mol. wt. 282.29

-Obtained by reaction of glutaryl chloride with pyrogallol trimethyl ether or in the presence of aluminium chloride in nitrobenzene [592].
-Also refer to: [1285, 1358, 1902, 2487, 2933].

m.p. 76–77° [1358], 74–76° [1902], 73–75° [1285], 72–73° [592].
^{1}H NMR [2487, 2933], IR [2933].

BIOLOGICAL ACTIVITY: Antibacterial [2933].

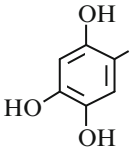
2,4-Dinitrophenylhydrazone of the trimethyl ether

[16093-17-7] $C_{20}H_{22}N_4O_9$ mol. wt. 462.42

m.p. 155° [592].

5-(2,4,5-Trihydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{11}H_{12}O_6$ mol. wt. 240.21



Synthesis
-Refer to: [2196].

Trimethyl ether [92865-60-6]
$C_{14}H_{18}O_6$ mol. wt. 282.29

-Obtained by reaction of glutaric anhydride with 1,2,4-trimethoxybenzene in the presence of boron trifluoride at 0° for 3 days (95 %) [2274].
-Also refer to: [112].

m.p. 164–165° [2274], 162–164° [112].

Methyl ester of trimethyl ether $C_{15}H_{20}O_6$ mol. wt. 296.32

m.p. 90.5–92.5° [112].

Ethyl ester of trimethyl ether $C_{16}H_{22}O_6$ mol. wt. 310.35

-Obtained by acylation of 1,2,4-trimethoxybenzene with γ-carbethoxybutyric acid in the presence of polyphosphoric acid for 2.5 h at 45° (62.6 %) [112].

colourless broad prismatic plates [112]; m.p. 80–82° [112].

Triethyl ether [63213-33-2] $C_{17}H_{24}O_6$ mol. wt. 324.37

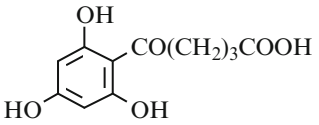
-Obtained by reaction of glutaric anhydride with 1,2,4-triethoxybenzene in the presence of aluminium chloride in carbon tetrachloride first at r.t., then at 70° for 2 h (90 %) [2196].

m.p. 121° [2196].

BIOLOGICAL ACTIVITY: Spasmolytic action [2196]; Choleretic action [2196].

5-(2,4,6-Trihydroxyphenyl)-5-oxo-1-pentanoic acid

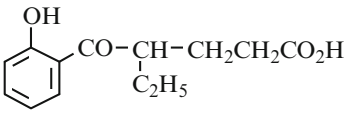
$C_{11}H_{12}O_6$ mol. wt. 240.21



Synthesis
-Refer to: [3374].
m.p. 247–249° [3374].

4-Ethyl-5-(2-hydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Refer to: [2300].

Methyl ether

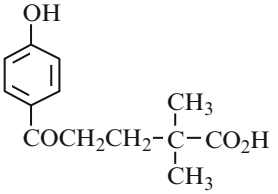
$C_{14}H_{18}O_4$ mol. wt. 250.29

-Refer to: [2299, 2300 (72 %)].

b.p.$_1$ 190° [2299, 2300].

5-(4-Hydroxyphenyl)-2,2-dimethyl-5-oxo-1-pentanoic acid

$C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Refer to: [2358].

Methyl ether [61468-98-2]

$C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of 2,2-dimethylglutaric anhydride with anisole in the presence of aluminium chloride [2359],

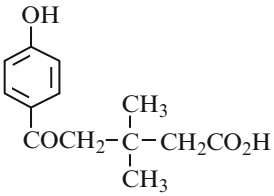
*first at 0°, then at r.t. (10 %) [2358];
*at 0–5° (80–85 %) [1097].
-Also refer to: [2479].

m.p. 102° [2358, 2359], 92–94° [2479], 90° [1097];
^{1}H NMR [1097, 2358, 2479], ^{13}C NMR [2479],
IR [2479], UV [1097], MS [2479]; pK_a [2358].

BIOLOGICAL ACTIVITY: Anorexigen [2358].

5-(4-Hydroxyphenyl)-3,3-dimethyl-5-oxo-1-pentanoic acid

[135312-40-2] $C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Obtained by treatment of 5-(4-methoxyphenyl)-3,3-dimethyl-5-oxo-1-pentanoic acid with pyridinium chloride at 185° for 20 h (76 %) [878].
m.p. 112–114° [878].

Methyl ether [31526-44-0] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of 3,3-dimethylglutaric anhydride with anisole in the presence of aluminium chloride,
*in methylene chloride with ice-ethanol bath cooling and stirring for 3 h (96 %) [878];
*in nitrobenzene for 3 weeks at 0° (95 %) [172].

oil [172, 878]; ^{1}H NMR [172], IR [172].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{20}H_{22}N_4O_7$ mol. wt. 430.42

m.p. 177.5–180° [172].

Ethyl ester of the methyl ether [31526-46-2] $C_{16}H_{22}O_4$ mol. wt. 278.35

-Obtained by treatment of 5-(4-methoxyphenyl)-3,3-dimethyl-5-oxo-1-pentanoic acid with ethanol in the presence of hydrogen chloride gas (quantitative yield) [172].

^{1}H NMR [172].

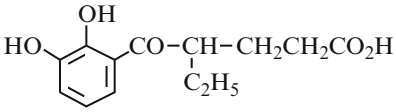
Ethyl ester [119348-66-2] $C_{15}H_{20}O_4$ mol. wt. 264.32

-Obtained by treatment of 5-(4-hydroxyphenyl)-3,3-dimethyl-5-oxo-1-pentanoic acid in ethanol with methanesulfonic acid at 25° for 25 h (79 %) [878].

m.p. 98–100° [878].

4-Ethyl-5-(2,3-dihydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{13}H_{16}O_5$ mol. wt. 252.27



Synthesis
-Refer to: [2300].

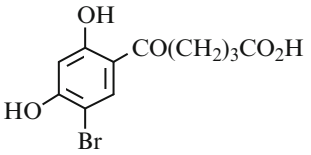
Dimethyl ether $C_{15}H_{20}O_5$ mol. wt. 280.32

-Refer to: [2300 (67 %)]; $b.p._{\cdot 0.4}$ 190° [2300].

5.2 Substituted Hydroxyketones

5-(5-Bromo-2,4-dihydroxyphenyl)-5-oxo-1-pentanoic acid

[16093-14-4] $C_{11}H_{11}BrO_5$ mol. wt. 303.11



Synthesis

-Obtained by reaction of glutaryl chloride with 4-bromo-resorcinol in the presence of aluminium chloride in nitrobenzene [592].

m.p. 123° [592].

2,4-Dinitrophenylhydrazone [16093-59-7] $C_{17}H_{15}BrN_4O_8$ mol. wt. 483.23

m.p. 225° [592].

Dimethyl ether [16093-36-0] $C_{13}H_{15}BrO_5$ mol. wt. 331.16

-Obtained by reaction of glutaryl chloride with 4-bromoresorcinol dimethyl ether in the presence of aluminium chloride in nitrobenzene at 0° for 13 h (35 %) [592].

m.p. 134–135° [592].

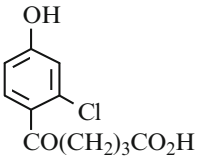
2,4-Dinitrophenylhydrazone of the dimethyl ether

[16093-37-1] $C_{19}H_{19}BrN_4O_8$ mol. wt. 511.29

m.p. 181° [592].

5-(2-Chloro-4-hydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{11}H_{11}ClO_4$ mol. wt. 242.66



Synthesis

-Refer to: [1567].

Methyl ether [71354-35-3]

$C_{12}H_{13}ClO_4$ mol. wt. 256.69

-Obtained by reaction of glutaric anhydride with 3-chloroanisole in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture first at 0–5°, then at r.t. for 24 h (48 %) [1567].

m.p. 114–116° [1567]; IR [1567], MS [1567].

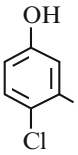
Methyl ester of the methyl ether [71354-36-4] $C_{13}H_{15}ClO_4$ mol. wt. 270.71

-Refer to: [1567].

$b.p._{.1}$ 200° [1567]; MS [1567].

5-(2-Chloro-5-hydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{11}H_{11}ClO_4$ mol. wt. 242.66



Synthesis
-Refer to: [1567].

Methyl ether [71354-33-1]
$C_{12}H_{13}ClO_4$ mol. wt. 256.69

-Obtained by reaction of glutaric anhydride with 4-chloroanisole in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture first at 0–5°, then at r.t. for 24 h (61 %) [1567].

m.p. 105° [1567]; IR [1567], MS [1567].

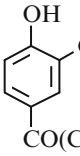
Methyl ester of the methyl ether [71354-34-2] $C_{13}H_{15}ClO_4$ mol. wt. 270.71

-Refer to: [1567].

b.p.$_1$ 190° [1567]; MS [1567].

5-(3-Chloro-4-hydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{11}H_{11}ClO_4$ mol. wt. 242.66



Synthesis
-Refer to: [1567].

Methyl ether [71354-31-9]
$C_{12}H_{13}ClO_4$ mol. wt. 256.69

-Obtained by reaction of glutaric anhydride with anisole in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture first at 0–5°, then at r.t. for 24 h (80.3 %) [1567].
-Also refer to: [1779, 3228].

m.p. 160–162° [1779], 156° [1567]; IR [1567], MS [1567].

BIOLOGICAL ACTIVITY: Refer to: [1779, 3228].

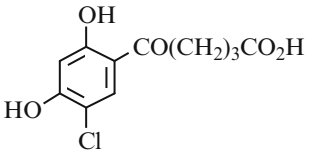
Methyl ester of the methyl ether [71354-32-0] $C_{13}H_{15}ClO_4$ mol. wt. 270.71

-Refer to: [1567].

m.p. 76° [1567]; MS [1567].

5-(5-Chloro-2,4-dihydroxyphenyl)-5-oxo-1-pentanoic acid

[16093-18-8] $C_{11}H_{11}ClO_5$ mol. wt. 258.66



Synthesis
-Obtained by reaction of glutaryl chloride with 4-chloro-resorcinol in the presence of aluminium chloride in nitrobenzene [592].
m.p. 140° [592].

2,4-Dinitrophenylhydrazone [16093-19-9] $C_{17}H_{15}ClN_4O_8$ mol. wt. 438.78

m.p. 171° [592].

Dimethyl ether [16093-30-4] $C_{13}H_{15}ClO_5$ mol. wt. 286.71

-Obtained by reaction of glutaryl chloride with 4-chlororesorcinol dimethyl ether in the presence of aluminium chloride in nitrobenzene [592].

m.p. 160° [592].

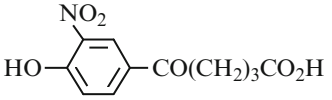
2,4-Dinitrophenylhydrazone of the dimethyl ether

[16093-31-5] $C_{19}H_{19}ClN_4O_8$ mol. wt. 466.84

m.p. 171° [592].

5-(4-Hydroxy-3-nitrophenyl)-5-oxo-1-pentanoic acid

$C_{11}H_{11}NO_6$ mol. wt. 253.21



Synthesis
-Refer to: [2494].

Methyl ether $C_{12}H_{13}NO_6$ mol. wt. 267.24

-Preparation from γ-anisoylbutyric acid [2494].

colourless prisms [2494]; m.p. 145° [2494].

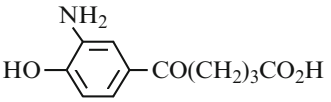
Ethyl ether $C_{13}H_{15}NO_6$ mol. wt. 281.26

-Preparation from γ-phenetoylbutyric acid [2494].

colourless plates [2494]; m.p. 127° [2494].

5-(3-Amino-4-hydroxyphenyl)-5-oxo-1-pentanoic acid

$C_{11}H_{13}NO_4$ mol. wt. 223.23



Synthesis
-Refer to: [2494].

Methyl ether $C_{12}H_{15}NO_4$ mol. wt. 237.26

-Refer to: [2494].

pale brown needles [2494]; m.p. 162–164° [2494].

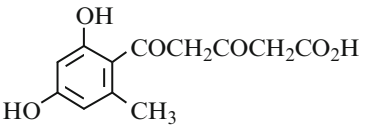
Ethyl ether $C_{13}H_{17}NO_4$ mol. wt. 251.28

-Refer to: [2494].

almost colourless plates [2494]; m.p. 176–178° [2494].

5-(2,4-Dihydroxy-6-methylphenyl)-3,5-dioxo-1-pentanoic acid

$C_{12}H_{12}O_6$ mol. wt. 252.22



Syntheses
-Refer to: [454, 1330].

Dimethyl ether [66757-68-4]
$C_{14}H_{16}O_6$ mol. wt. 280.28

-Obtained by treatment of 2,4-dimethoxy-6-methylacetophenone with sodium amide in liquid ammonia, followed by carbon dioxide [2974].
-Also refer to: [1168, 1330 (54 %)].

liquid [1330]; ^{1}H NMR [1168, 1330], IR [1168, 1330].

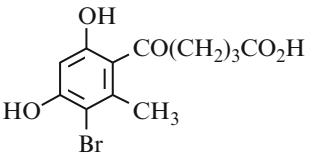
Dibenzyl ether [97271-30-2] $C_{26}H_{24}O_6$ mol. wt. 432.47

-Obtained from 5-(2,4-dibenzyloxy-6-methylphenyl)-1,3-butanedione (78 %) [454].
-Also refer to: [455].

colourless oil [454].

5-(5-Bromo-2,4-dihydroxy-6-methylphenyl)-5-oxo-1-pentanoic acid

[16093-45-1] $C_{12}H_{13}BrO_5$ mol. wt. 317.14



Synthesis
-Obtained by reaction of glutaryl chloride with 4-bromo-orcinol in the presence of aluminium chloride in nitrobenzene [592].
m.p. 176° [592].

2,4-Dinitrophenylhydrazone [16093-46-2] $C_{18}H_{17}BrN_4O_8$ mol. wt. 497.26

m.p. 179° [592].

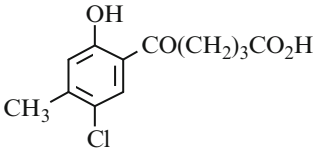
Dimethyl ether [16093-47-3] $C_{14}H_{17}BrO_5$ mol. wt. 345.19

-Obtained by reaction of glutaryl chloride with 4-bromoorcinol dimethyl ether in the presence of aluminium chloride in nitrobenzene [592].

m.p. 117° [592].

5-(5-Chloro-2-hydroxy-4-methylphenyl)-5-oxo-1-pentanoic acid

[4609-06-7] $C_{12}H_{13}ClO_4$ mol. wt. 256.69



Synthesis
-Obtained by reaction of glutaric anhydride with 4-chloro-3-methylphenol in the presence of aluminium chloride in tetrachloroethane/nitrobenzene mixture (1:1) [588].

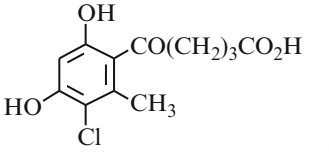
m.p. 140° [588]; IR [588].

2,4-Dinitrophenylhydrazone $C_{18}H_{17}Cl_2N_4O_7$ mol. wt. 436.81

m.p. 210° [588].

5-(5-Chloro-2,4-dihydroxy-6-methylphenyl)-5-oxo-1-pentanoic acid

[16093-43-9] $C_{12}H_{13}ClO_5$ mol. wt. 272.68



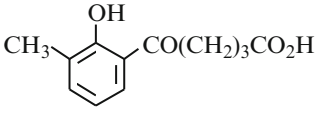
Synthesis
-Obtained by reaction of glutaryl chloride with 4-chloro-orcinol in the presence of aluminium chloride in nitrobenzene [592].
m.p. 172° [592].

2,4-Dinitrophenylhydrazone [16093-44-0] $C_{18}H_{17}ClN_4O_8$ mol. wt. 452.81

m.p. 191° [592].

5-(2-Hydroxy-3-methylphenyl)-5-oxo-1-pentanoic acid

[4642-27-7] $C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Obtained by reaction of glutaric anhydride with o-cresol in the presence of aluminium chloride in tetrachloro-ethane/nitrobenzene mixture (1:1) at 120–130° for 3 h (60 %) [588].

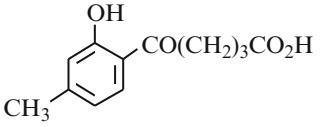
m.p. 125° [588]; IR [588].

2,4-Dinitrophenylhydrazone [4642-28-8] $C_{18}H_{18}N_4O_7$ mol. wt. 402.36

m.p. 180° [588].

5-(2-Hydroxy-4-methylphenyl)-5-oxo-1-pentanoic acid

[4642-35-7] $C_{12}H_{14}O_4$ mol. wt. 222.24



Syntheses

-Obtained by reaction of glutaric anhydride with m-cresol in the presence of aluminium chloride in tetrachloroethane (80 %) [588], (36 %) [2724].

-Also refer to: [3224, 3366, 3398, 3399].

m.p. 140–141.5° [3398], 140° [588], 135° [3224], 134–135° [2724];
IR [588, 2724], UV [3398, 3399].

2,4-Dinitrophenylhydrazone [4642-36-8] $C_{18}H_{18}N_4O_7$ mol. wt. 402.36

m.p. 200° [588].

Methyl ester [63023-50-7] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by refluxing for 10 h a mixture of the title ketone, methanol and concentrated sulfuric acid (90 %) [2724].

-Also refer to: [3224].

$b.p._{10}$ 169–170° [2724]; m.p. 50° [3224];
^{1}H NMR [2724, 3224], IR [2724, 3224].

Methyl ester of the methyl ether [29207-19-0] $C_{14}H_{18}O_4$ mol. wt. 250.29

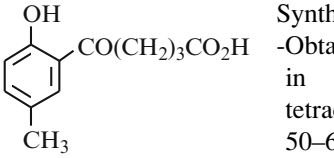
-Obtained by reaction of dimethyl sulfate with the methyl ester above in the presence of aqueous sodium hydroxide at r.t. for 1 h and then heated on a water bath for 3 h (70 %) [2724].

-Also refer to: [3398, 3399].

m.p. 38.5–39.2° [3399], 38.5–39° [3398];
^{1}H NMR [2724], IR [2724, 3398], UV [3398, 3399];
TLC [2724].

5-(2-Hydroxy-5-methylphenyl)-5-oxo-1-pentanoic acid

[4649-01-8] $C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis

-Obtained by reaction of glutaric anhydride with p-cresol in the presence of aluminium chloride in tetrachloroethane/nitrobenzene mixture (1:1), first at 50–60° for 2 h, then at 100° for 30 min [588].

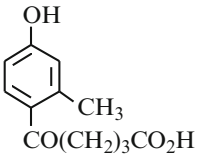
m.p. 95° [588]; IR [588].

2,4-Dinitrophenylhydrazone [4649-02-9] $C_{18}H_{18}N_4O_7$ mol. wt. 402.36

m.p. 150° [588].

5-(4-Hydroxy-2-methylphenyl)-5-oxo-1-pentanoic acid

[4642-32-4] $C_{12}H_{14}O_4$ mol. wt. 222.24



Synthesis
-Obtained by reaction of glutaryl chloride with m-cresol in the presence of aluminium chloride in nitrobenzene [588].
m.p. 200° [588]; IR [588].

2,4-Dinitrophenylhydrazone [4642-33-5] $C_{18}H_{18}N_4O_7$ mol. wt. 402.36

m.p. 190° [588].

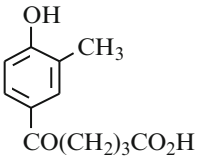
Methyl ether [4642-37-9] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by reaction of glutaryl chloride with m-cresol methyl ether in the presence of aluminium chloride in tetrachloroethane [588].
-Also obtained by reaction of glutaric anhydride with m-cresol methyl ether in the presence of aluminium chloride in tetrachloroethane/nitrobenzene mixture (1:1) at 0–5° (70 %) [588, 1567].
-Also refer to: [2820, 3366].

m.p. 138° [2820], 121° [1567], 120° [588];
IR [588], MS [1567].

5-(4-Hydroxy-3-methylphenyl)-5-oxo-1-pentanoic acid

[4592-82-9] $C_{12}H_{14}O_4$ mol. wt. 222.24



Syntheses
-Obtained by reaction of glutaryl chloride with o-cresol in the presence of aluminium chloride, in nitrobenzene [588].
-Also obtained by reaction of glutaric anhydride with o-cresol in the presence of aluminium chloride in tetrachloroethane/nitrobenzene mixture (1:1) at 120–130° for 3 h (40 %) [588].

m.p. 184° [588]; IR [588].

2,4-Dinitrophenylhydrazone [4680-89-1] $C_{18}H_{18}N_4O_7$ mol. wt. 402.36

m.p. 180° [588].

Methyl ether [4642-30-2] $C_{13}H_{16}O_4$ mol. wt. 236.27

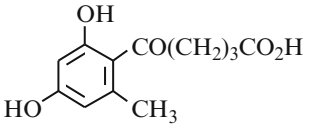
-Obtained by reaction of glutaryl chloride with o-cresol methyl ether in the presence of aluminium chloride in tetrachloroethane [588].

-Also obtained by reaction of glutaric anhydride with o-cresol methyl ether in the presence of aluminium chloride in tetrachloroethane/nitrobenzene mixture (1:1) at 0–5° (75 %) [588].
-Also refer to: [1567, 2820, 2838].

m.p. 141° [2820], 140° [588], 139° [1567], 126° [2838];
IR [588].

5-(2,4-Dihydroxy-6-methylphenyl)-5-oxo-1-pentanoic acid

[16093-39-3] $C_{12}H_{14}O_5$ mol. wt. 238.24



Synthesis
-Obtained by reaction of glutaryl chloride with orcinol in the presence of aluminium chloride in nitrobenzene [592].

m.p. 218° [592].

Oxime [16093-40-6] $C_{12}H_{15}NO_5$ mol. wt. 253.25

m.p. 140° [592].

Dimethyl ether [16093-41-7] $C_{14}H_{18}O_5$ mol. wt. 266.29

-Obtained by reaction of glutaryl chloride with orcinol dimethyl ether in the presence of aluminium chloride in nitrobenzene [592].

m.p. 130° [592].

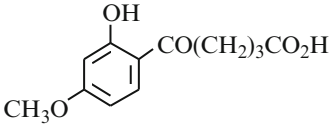
2,4-Dinitrophenylhydrazone of the dimethyl ether

[16093-42-8] $C_{20}H_{22}N_4O_8$ mol. wt. 446.42

m.p. 155° [592].

5-(2-Hydroxy-4-methoxyphenyl)-5-oxo-1-pentanoic acid

[4642-41-5] $C_{12}H_{14}O_5$ mol. wt. 238.24



Syntheses
-Obtained by reaction of glutaric anhydride with resorcinol monomethyl ether in the presence of aluminium chloride in nitrobenzene, first at 10–15° for 2 h, then at 30–32° for 1 h (75 %) [588].

-Also refer to: [1971, 2820].

m.p. 159° [588], 157° [2820];
^{1}H NMR [1971], IR [588, 1971].

2,4-Dinitrophenylhydrazone [4642-42-6] $C_{18}H_{18}N_4O_8$ mol. wt. 418.36

m.p. 138° [588].

Methyl ester [66832-64-2] $C_{13}H_{16}O_5$ mol. wt. 252.27

-Obtained by reaction of dimethyl sulfate with γ-(2,4-dihydroxybenzoyl)butyric acid in the presence of potassium carbonate in refluxing acetone for 6 h (74 %) [346].
-Preparation from 5-(2-hydroxy-4-methoxyphenyl)-5-oxopentanoic acid by esterification with boron trifluoride/methanol [820].

m.p. 60–60.5° [820], 58° [346];
^{1}H NMR [820], MS [820].

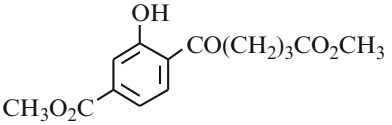
Ethyl ester $C_{14}H_{18}O_5$ mol. wt. 266.29

-Preparation from 5-(2-hydroxy-4-methoxyphenyl)-5-oxopentanoic acid by esterification with boron trifluoride/ethanol [820].

$b.p._{0.07}$ 160–164° [820]; ^{1}H NMR [820], MS [820].

Methyl 5-(2-hydroxy-4-carbomethoxyphenyl)-5-oxo-1-pentanoate

$C_{14}H_{16}O_6$ mol. wt. 280.28



Synthesis
-Refer to: [3398].

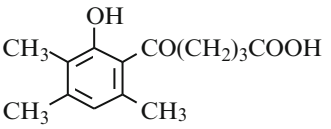
Methyl ether [29207-22-5]
$C_{15}H_{18}O_6$ mol. wt. 294.30

-Preparation: Methyl 4-(2-methoxy-p-toluoyl)-butyrate (m.p. 38.5–39°) was converted without purification of intermediates by the following sequence of reagents: N-bromosuccinimide in CCl_4 with ABIN, silver nitrate in aqueous acetonitrile, chromic acid in acetic acid, methanolic HCl [3398].
-Also refer to: [3399].

m.p. 78–79° [3398, 3399];
IR [3398], UV [3398, 3399].

5-(2-Hydroxy-3,4,6-trimethylphenyl)-5-oxo-1-pentanoic acid

[84978-13-2] $C_{14}H_{18}O_4$ mol. wt. 250.30



Synthesis
-Refer to: [2325].
m.p. 155–157° [2325]; ^{1}H NMR [2325], IR [2325].

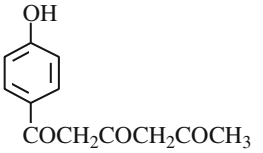
Chapter 4
Hexanones

1 Aromatic Hydroxyketones Derived from Hexanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(4-Hydroxyphenyl)-1,3,5-hexanetrione

$C_{12}H_{12}O_4$ mol. wt. 220.22



Synthesis
-Refer to: [1168].

Methyl ether [4808-89-3]

$C_{13}H_{14}O_4$ mol. wt. 234.25

-Preparation: Trityl-lithium in THF was injected into pentane-2,4-dione under nitrogen at −15°. When the red colour persisted methyl p-methoxybenzoate in THF was injected. The solution was stirred at −15° and trityl-lithium solution added to just maintain the red colour [1168].
-Also obtained by reaction of acetylacetone with methyl p-methoxybenzoate in the presence of sodium hydride in 1,2-dimethoxyethane (72 %) [1218, 2944].

pale yellow crystals [1168];
m.p. 85–86° [1218], 81° [2944], 80–81° [1168];
^{1}H NMR [1168], IR [1168], UV [1168], MS [1168].
N.B.: Several tautomers [1168].

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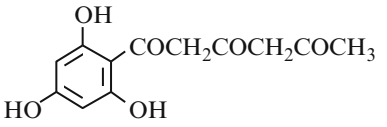
1-(2,4,6-Trihydroxyphenyl)-1,3,5-hexanetrione

$C_{12}H_{12}O_6$ mol. wt. 252.22



Synthesis
-Refer to: [2699].

Trimethyl ether [76631-01-1]
$C_{15}H_{18}O_6$ mol. wt. 294.30

-Preparation by acylation of dianion of 2,4-pentanedione with methyl 2,4,6-trimethoxybenzoate (61 %) [2699].

yellow crystals [2699]; m.p. 68.5–71.5° [2699];
^{1}H NMR [2699], IR [2699], MS [2699].

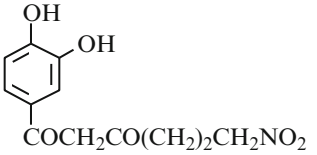
Tribenzyl ether [76631-02-2] $C_{33}H_{30}O_6$ mol. wt. 522.60

-Preparation by acylation of dianion of 2,4-pentanedione with methyl 2,4,6-tribenzyloxybenzoate (100 %) [2699].

yellow oil [2699]; ^{1}H NMR [2699], MS [2699].

1-(3,4-Dihydroxyphenyl)-6-nitro-1,3-hexanedione

$C_{12}H_{13}NO_6$ mol. wt. 267.24



Synthesis
-Refer to: [2780].

Dimethyl ether
$C_{14}H_{17}NO_6$ mol. wt. 295.29

-Obtained by reaction of 1-(3,4-dimethoxyphenyl)-1-trimethylsilyloxyethene with 4-nitrobutyryl chloride in tetrahydrofuran in the presence of methyllithium in ethyl ether at −100° (55 %) [2780].

m.p. 95–96° [2780]; ^{1}H NMR [2780], IR [2780], MS [2780].

1-(2-Hydroxyphenyl)-1,3-hexanedione

[80856-35-5] $C_{12}H_{14}O_3$ mol. wt. 206.24

Syntheses
-Obtained by reaction of 2-hydroxyacetophenone with methyl butyrate in the presence of sodium hydride (51 %) [2807].
-Also refer to: [3400].

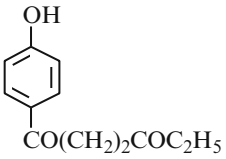
pale yellow oil [2807]; b.p.$_2$ 135° [2807];
^{1}H NMR [2807], IR [2807], UV [2807].

Methyl ether [1001024-93-6] $C_{13}H_{16}O_3$ mol. wt. 220.27

-Obtained by reaction of 2-methoxybenzoyl chloride with 2-pentanone in the presence of LDA (lithium diisopropylamide; 1.5 equiv.) in tetrahydrofuran (72 %) [3400].

1-(4-Hydroxyphenyl)-1,4-hexanedione

$C_{12}H_{14}O_3$ mol. wt. 206.24



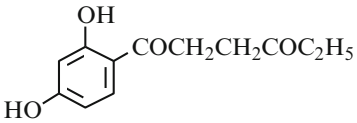
Synthesis
-Refer to: [2953].
Methyl ether [62596-41-2]
$C_{13}H_{16}O_3$ mol. wt. 220.27

-Obtained from propanal and 1-(4-methoxyphenyl)-2-propen-1-one (64 %) [2953].
-Also refer to: [162, 2856].

$b.p._{.0.65}$ 168° [2953]; m.p. 77° [162], 75° [2953];
^{1}H NMR [2856, 2953], ^{13}C NMR [2856], IR [2856, 2953], MS [2856].

1-(2,4-Dihydroxyphenyl)-1,4-hexanedione

$C_{12}H_{14}O_4$ mol. wt. 222.24



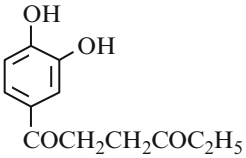
Synthesis
-Refer to: [2953].
Dimethyl ether [67756-20-1]
$C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained from propanal and 1-(2,4-dimethoxyphenyl)-2-propen-1-one (60 %) [2953].

$b.p._{.0.1}$ 155° [2953]; m.p. 55–57° [2953],
^{1}H NMR [2953], IR [2953].

1-(3,4-Dihydroxyphenyl)-1,4-hexanedione

$C_{12}H_{14}O_4$ mol. wt. 222.24



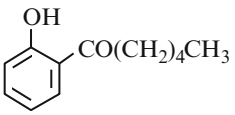
Synthesis
-Refer to: [2953].
Dimethyl ether [67756-23-4]
$C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained from propanal and 1-(3,4-dimethoxyphenyl)-2-propen-1-one (60 %) [2953].

$b.p._{.0.2}$ 155° [2953]; m.p. 79° [2953],
^{1}H NMR [2953], IR [2953].

1-(2-Hydroxyphenyl)-1-hexanone

[3226-15-1] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Phenol was energetically mixed with finely divided aluminium chloride (1 mol) and heated to 100° (1 mol of hydrochloric acid is evolved); 1 mol of n-caproyl chloride was then added and heated to 125–130° for 1 h (56 %) [2700].

-Also obtained by Fries rearrangement of phenyl caproate with aluminium chloride for 2 h at 160–180° (50 %) [726] or in tetrachloroethane [3169].

-Also obtained [2478] by the method [2074].

-Also obtained by adding TMSOTf (0.96 mmol) to a solution of 2-(1-hexynyl) phenol (0.48 mmol) and isobutyraldehyde (0.57 mmol) in ethyl ether under nitrogen at −78°. After the reaction mixture had been stirred at −78° for 3 h, it was warmed slowly to r.t. and stirred for 14 h until the reaction was complete (**4a**) (20 %) (Table 2, entry 2 in [2403]).

-Also obtained by treatment of 2-(1-hexynyl)phenol with TMSOTf (2 equiv.) in ethyl ether at r.t. for 22 h (**4**) (94 %) (Table 6, entry 5 in [2403]).

-Also obtained by treatment of 1-(2-hydroxyphenyl)-1-hexanol with manganese dioxide in methylene chloride for 7 h at r.t. (46 %) [77].

-Also obtained by Fries rearrangement of phenyl caproate with aluminium chloride at 140° for 45 min (45 %) [932].

-Also obtained by zeolite-catalyzed Friedel-Crafts reaction of anisole with caproic acid [3266].

-Also obtained by treatment of 2-(1-hexynyl)phenol with TMSOTf in ether for 22 h at r.t. (94 %) [2403].

-Also obtained by reaction of 2-(1-hexynyl)phenol with isopropyl aldehyde in the presence of TMSOTf in ether at −78°, then at r.t. for 14 h (20 %) [2403].

-Also obtained by reaction of 2-(1-hexynyl)phenol with 4-nitrophenylbenzaldehyde in the presence of TMSOTf in ether at −78°, then at r.t. for 14 h (37 %) [2403].

-Also refer to: [260, 2134, 2946].

colourless oil [77]; light-yellow oil [2403];
b.p.$_{0.1}$ 83° [932], b.p.$_{0.6}$ 96–98° [3169], b.p.$_{1.2}$ 106–107° [2478],
b.p.$_{10}$ 142–143°, b.p.$_{15}$ 145–147° [726];
m.p. 22° [726], 17.2–17.4° [2700];
^{1}H NMR [77, 2403], ^{13}C NMR [77, 2403], IR [77], UV [1996], MS [77];
TLC [1994]; pKa [2590]; dipole moment [2590]; $n_D^{25} = 1.5262$ [932].

USE: Preparation of chromanones and related chalcones *via* trimethylsilyl triflate-promoted electrophilic addition of (o-hydroxyphenyl)alkynes to aldehydes [2403]; Preparation and reduction of, [260].

2,4-Dinitrophenylhydrazone [18405-71-5] $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 153° [932, 3169], 84–85° [524].
N.B.: One of the reported melting point is obviously wrong.

Methyl ether [35031-70-0] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by treatment of 2-(1-hexynyl)anisole with TMSOTf (2 equiv.) in ethyl ether at r.t. for 90 h (**4**) (51 %) (Table 6, entry 6 in [2403]).
-Also obtained by direct acylation of 2-bromoanisole with caproaldehyde by palladium catalysis (60 %) [2668].
-Also obtained treatment of 1-(2-methoxyphenyl)-1-hexyne with p-toluenesulfonic acid (PTSA) in ethanol at 78° for 144 h (80 %) [2337].
-Also obtained by treatment of 2-(1-hexynyl)anisole with TMSOTf in ether for 90 h at r.t. (51 %) [2403].
-Also obtained by action of hexanoyl chloride with anisole,
*in the presence of ferric chloride at reflux for 5 h (4 %) [3435];
*in the presence of aluminium chloride at reflux for 5 h (6 %) [3435].
-Also refer to: [1485, 1840, 1999, 3227 (67 %)].

light-yellow oil [2403]; m.p. 111–112° [3227];
^{1}H NMR [1485, 1840, 2337, 2403, 2668, 3227],
^{13}C NMR [1485, 1840, 2337, 2403, 2668],
IR [1485, 1840, 2668], MS [1485, 2668].

USE: Preparation of chromanones and related chalcones *via* trimethylsilyl triflate-promoted electrophilic addition of (o-hydroxyphenyl)alkynes to aldehydes [2403].

Ethyl ether $C_{14}H_{20}O_2$ mol. wt. 220.31

-Obtained by action of hexanoyl chloride with phenetole,
*in the presence of ferric chloride at reflux for 5 h (1 %) [3435];
*in the presence of aluminium chloride at reflux for 5 h (6 %) [3435].

Phenylhydrazone $C_{18}H_{22}N_2O$ mol. wt. 282.38

m.p. 102–103° [726].

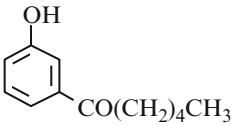
Oxime [204859-45-0] $C_{12}H_{17}NO_2$ mol. wt. 207.27

m.p. 112° [2555]; ^{1}H NMR [2555], IR [2555].

USE: For preparation of copper/lead/zinc salicylaldoxime complexes [2555].

1-(3-Hydroxyphenyl)-1-hexanone

[103119-13-7] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses

-Preparation by reaction of m-acetoxybenzoyl chloride with dipentylcadmium in refluxing benzene for 30 min. Then, treatment of keto-ester obtained by refluxing with 10 % sodium hydroxide for 2–3 h (77 %) [2586].

-Also obtained (**13**) by treatment of *trans*-3-(3-hex-2-enoyl)phenol (**11**) with hydrogen over Pd/C in ethyl acetate (58 %) [3292].
-Also obtained by treatment of its methyl ether with aluminium chloride in benzene by heating on a water bath for 2 h (80 %) [966].
-Also refer to: [583].

$b.p._{.1}$ 147–150° [2586]; m.p. 69° [2586], 63° [966].

Acetate $C_{14}H_{18}O_3$ mol. wt. 234.30

$b.p._{.0.5}$ 127–128° [2586].

2,4-Dinitrophenylhydrazone of the acetate $C_{20}H_{22}N_4O_6$ mol. wt. 414.42

m.p. 158° [2586].

Methyl ether [342423-70-5] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by condensation of pentylmagnesium bromide with m-methoxybenzamide in ethyl ether. The reaction was carried out at 60° for 48 h under hydrogen atmosphere (60–70 %) [966].
-Also obtained by direct acylation of 3-bromoanisole with caproaldehyde by palladium catalysis (88 %) [2668].
-Also refer to: [967, 1485, 1840, 2868, 3440].

$b.p._{.20}$ 220° [966, 967];
^{1}H NMR [1485, 1840, 2668, 2868], ^{13}C NMR [1485, 1840, 2668, 2868], IR [1485, 1840, 2668, 2868], MS [2668]; $n_D^{35} = 1.5189$ [967].

USE: Structures and catalytic activity in C-C coupling reactions of dinuclear and trinuclear triazolyldiylidene palladium complexes [3440]; Aquapalladium complex catalyst for intermolecular hydroamination of alkynes [2868].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{19}H_{22}N_4O_5$ mol. wt. 386.41

m.p. 148° [967].

Benzyl ether [92532-18-8] $C_{19}H_{22}O_2$ mol. wt. 282.38

-Obtained by treatment of 3-(benzyloxy)phenyl-1-hexanol with pyridinium chlorochromate in methylene chloride at r.t. for 1.5 h (98 %) [2199].
-Also refer to: [583, 2197].

oil [2199].

BIOLOGICAL ACTIVITY: Antiallergic and inflammation inhibitor [2197, 2199].

2,4-Dinitrophenylhydrazone $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

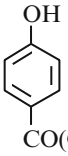
m.p. 196° [2586].

4-Nitrophenylhydrazone $C_{18}H_{21}N_3O_3$ mol. wt. 327.38

m.p. 158° [967].

1-(4-Hydroxyphenyl)-1-hexanone

[2589-72-2] $C_{12}H_{16}O_2$ mol. wt. 192.26



Syntheses
-Phenol was energetically mixed with finely divided aluminium chloride (1 mol) and heated to 100° (1 mol of hydrochloric acid is evolved); 1 mol of caproyl chloride was then added and heated to 125–130° for 1 h (34 %) [2700].

-Also obtained by reaction of caproyl chloride with phenol in the presence of aluminium chloride,
*in methylene chloride for 1 h at 0°, then at r.t. overnight (74 %) [114] or for 14 h at r.t. (45 %) [1910];
*in nitrobenzene first at 5–10°, then at r.t. for some hours (81 %) [2970].
-Also obtained by reaction of caproic acid with phenol,
*in the presence of boron trifluoride for 3 h at 65–70° (72.9 %) [1938] or for 2 h at 70° (66 %) [1685];
*in the presence of polyphosphoric acid for 20 min on a boiling water bath (41 %) [2240] or for 10 min at 100° (40 %) [2238];
*in the presence of fused zinc chloride for few min (8 %) [726].
-Also obtained by Fries rearrangement of phenyl caproate,
*in the presence of polyphosphoric acid for 10 min at 100° (36 %) [2238];
*in the presence of aluminium chloride at 140° for 45 min (30 %) [932], in tetrachloroethane [3169] or in nitrobenzene [1116], (43 %) [2947];
*in the presence of aluminium chloride in refluxing carbon disulfide for 5 h. Then, the mixture was kept at 80–90° for 2 h and at 140–150° for 1 h after solvent elimination [1222].
-Also obtained [2478] by the method [2074].
-Also obtained by anaerobic co-metabolic oxidation of 4-hexylphenol by *Thauera* sp. strain R5 [2861].

-Also obtained by reaction of caproic acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3277].
-Also refer to: [113, 414, 1415, 1536 (96 %), 2690, 2692, 2772, 2937, 2977, 3454].

b.p.$_{0.01}$ 160° [2970], b.p.$_{1}$ 167° [932, 1536], b.p.$_{1}$ 174–176° [2947], b.p.$_{2.9}$ 198° [1938], b.p.$_{10}$ 207–208° [2700], b.p.$_{15}$ 211–212° [1685], b.p.$_{15}$ 220–230° [2478];
white solid [1910];
m.p. 64.2–64.6° [1910], 64–65° [3277], 63–64° [726], 62° [2240], 61° [1536, 1685, 1938, 2700, 3169], 60° [932] (Sadtler standard N° 65673K), 59–60° [2478];
^{1}H NMR [114, 1910] (Sadtler standard N° 38624M), ^{13}C NMR [114, 1910], IR [1910] (Sadtler standard N° 65673K), UV [1995], MS [1910, 2861]; TLC [1910].

BIOLOGICAL ACTIVITY: Inhibition of 17-β hydroxysteroid dehydrogenase 3 [1910]; Non-steroidal inhibitors of 17-β-HSD in treatment of hormone-dependent cancers [1909]; Estrogenic activity [2692].

2,4-Dinitrophenylhydrazone $C_{18}H_{20}N_4O_5$ mol. wt. 372.38

m.p. 187° [3169], 184° [932].

isoNicotinylhydrazone [101720-12-1] $C_{18}H_{21}N_3O_2$ mol. wt. 311.38

m.p. 205° [520, 521].

USE: Chemotherapy of leprosy [520, 521].

Semicarbazone $C_{13}H_{19}N_3O_2$ mol. wt. 249.31

m.p. 149° [2240].

Benzoate $C_{19}H_{20}O_3$ mol. wt. 296.37

m.p. 105.5° [2700].

Caproate $C_{18}H_{26}O_3$ mol. wt. 290.40

-Obtained by reaction of caproic acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3277].

m.p. 67–68° [3277].

Sulfate Refer to: [114] (73 %); ^{1}H NMR [114], ^{13}C NMR [114].

Methyl ether [6397-82-6] $C_{13}H_{18}O_2$ mol. wt. 206.28

-Obtained by Friedel-Crafts acylation of anisole with caproic anhydride,
*in the presence of large molecular sizes on mesoporous silica catalyst at 453K for 4 h (73 %) [1466], [1480];
*in the presence of microcrystalline beta zeolite-II for 6 h at 130° under argon (75 %) [1594];
*in the presence of lithium perchlorate at 60° for 1.5 h (92 %) [267];
*in the presence of $SbCl_5$-$LiClO_4$ mixture in refluxing methylene chloride for 30 min (92 %) [2176];
*in the presence of $(C_6H_5CN)_2PtCl_2$ (2.5 ml%) and $AgSbF_6$ (5 mol%) (77 %) [1046].
-Also obtained by direct acylation of 4-bromoanisole with caproaldehyde by palladium catalysis (90 %) [2668].
-Preparation: potassium carbonate and $PdCl_2$ were added to a mixture of SDS and water and heated to 60° with stirring. Then 4-methoxyphenylboronic acid and caproic anhydride (or caproyl chloride) were added to the solution and the mixture held at 60° for 6 h (23–30 %) [3346].
-Also obtained from hexanoic anhydride and (4-methoxyphenyl)boronic acid using tris(p-methoxyphenyl)phosphane as the ligand (91 %) [1139].
-Also obtained by reaction of (4-methoxyphenyl)boronic acid with hexanoic anhydride in the presence of a Pd, Ni, Pd, or Cu catalyst [1137].
-Also obtained by reaction of hexanoic acid with anisole,
*over three large pore zeolites-beta (BEA), faujasite (FAU) and mordenite (MOR) [3246];
*in the presence of montmorillonite-enwrapped titanium as a solid acid catalyst [937];
*in the presence of $Cs_{2.5}H_{0.5}PW_{12}O_{40}$ at 110° for 5 h (63 %) [1636];
*in the presence of PPA at 90–100° for 1.5 h [2942] or for 1.5 h at 80° (80 %) [869];
*over HZSM-5 catalyst for 48 h at 423° K (20 %) [3265].
-Obtained by reaction of dimethyl sulfate with 4-hexanoylphenol in the presence of aqueous sodium hydroxide for 4 h at reflux [2478].
-Also obtained by direct β-alkylation of secondary alcohols with primary alcohols catalyzed by a CpIr complex (69 %) [1009, 1060].
-Also obtained treatment of 1-(4-methoxyphenyl)-1-hexyne,
*with p-toluenesulfonic acid (PTSA) in ethanol at 78° for 60 h (81 %) [2337];
*with 2-aminophenol in the presence of palladium nitrate in dioxane at 120° for 3 h (71 %) [2867].
-Also obtained by reaction of hexanoyl chloride with anisole in the presence of graphite in refluxing 1,2-dichloroethane for 8 h (66 %) [1723].
-Also obtained by reaction of 4-methoxybenzyl alcohol with 1-pentene in the presence of $RhCl_3.H_2O$ and 2-amino-4-methylpyridine at 130° for 12 h (77 %) [1556].
-Also obtained by reaction of 1-pentene with 4-methoxybenzaldehyde in toluene at 150° for 24 h under a mixture of chlorotris(triphenylphosphine)rhodium (5 mol%) and 20 mol% of 2-amino-3-picoline (66 %) [1559].

-Also obtained by Friedel-Crafts acylation reaction of caproic anhydride with anisole, using the combined catalyst system of $TiCl(OTf)_3$ and TfOH (98 %) [1483].
-Also obtained by Friedel-Crafts acylation of anisole in the presence of a Lewis acid catalyst while using carboxylic acid or trisubstituted-silyl carboxylate as acylating agent and carrying out the reaction in the presence of p-trifluoromethylbenzoic acid anhydride and, if necessary, a silver salt [2997].
-Also obtained by zeolite-catalyzed Friedel-Crafts reaction of anisole with caproic acid [3266].
-Also obtained by action of hexanoyl chloride with anisole,
*in the presence of ferric chloride at reflux for 5 h (33 %) [3435];
*in the presence of aluminium chloride at reflux for 5 h (65 %) [3435].
-Also refer to: [698, 842, 895 (49.3 %), 913, 1114, 1138, 1200, 1202, 1415, 1425, 1765, 1829, 1840, 1871, 1980, 2016, 2173 (67 %), 2180, 2240, 2406 (82 %), 2485, 2849, 3227 (quantitatif), 3262, 3421].

b.p.$_{1.6}$ 72–74° [1265], b.p.$_{0.25}$ 104° [3227], b.p.$_{0.4}$ 113–114° [2478], b.p.$_{5}$ 140–142° [3435], b.p.$_{5}$ 141–142° [3479], b.p.$_{0.5}$ 145° [869], b.p.$_{8}$ 156° [2735], b.p.$_{10}$ 165° [2240], b.p.$_{14}$ 172–174° [3178], b.p.$_{15}$ 183° [2478];
white solid [3346];
m.p. 60° [1485], 41° [2735, 2901, 3479], 39–40° [1186, 1870], 38–39° [895], 38° [2240], 37–38° [869], 36–37° [2016], 34–35° [1978], 34° [2478];
^{1}H NMR [698, 1060, 1186, 1485, 1840, 1870, 1876, 1980, 2668, 2867, 2868, 3227, 3346], ^{13}C NMR [698, 1060, 1249, 1485, 1801, 1840, 1876, 1978, 1980, 2668, 2999],
IR [698, 929, 1249, 1485, 1840, 1978, 1980, 2668, 2867, 2868, 2999],
UV [869, 1978], MS [698, 1186, 1485, 1870, 1978, 2668, 3346].

USE: Aquapalladium complex catalyst for intermolecular hydroamination of alkynes [2868].

2,4-Dinitrophenylhydrazone of the methyl ether

[102161-19-3] $C_{19}H_{22}N_4O_5$ mol. wt. 386.41

m.p. 146–147° [869], 145–146° [2016], 141° [869, 3479].

Phenylhydrazone of the methyl ether $C_{19}H_{24}N_2O$ mol. wt. 296.41

m.p. 28° [2901].

Semicarbazone of the methyl ether [101777-85-9] $C_{14}H_{21}N_3O_2$ mol. wt. 263.34

m.p. 143° [895], 142.5° [3178], 128–129° [869].

Ethyl ether [35031-74-4] $C_{14}H_{20}O_2$ mol. wt. 220.31

-Obtained by reaction of hexanoyl chloride with phenetole,
*in the presence of ferric chloride at reflux for 5 h (28 %) [3435];
*in the presence of aluminium chloride at reflux for 5 h (61 %) [3435].
-Also refer to: [1829].

oil [3435];
b.p.$_{.2}$ 140–142° [3435], b.p.$_{.7}$ 179–182° [1235];
m.p. 45° [1235];
IR [3435]; GLC [3435].

Phenyl ether [695196-65-7] $C_{18}H_{20}O_2$ mol. wt. 268.36

-Obtained by treatment of diphenyl oxide with caproyl chloride under Friedel-Crafts conditions [516].

b.p.$_{.15}$ 236–238° [516];
m.p. 49° [244], 39° [516].

3-Chloropropyl ether $C_{15}H_{21}ClO_2$ mol. wt. 268.78

-Obtained by reaction of 1-bromo-3-chloropropane with 4-hydroxycaprophenone in the presence of potassium carbonate in refluxing 2-butanone (95 %) [969].

4-Hexanoylphenyl ether [791137-06-9] $C_{24}H_{30}O_3$ mol. wt. 366.49

-Obtained by reaction of hexanoyl chloride with diphenyl ether in the presence of aluminium chloride in refluxing carbon disulfide for 30 min (71 %) [463].

m.p. 104–105.5° [463].
^{1}H NMR [460], ^{13}C NMR [460], MS [460].

Dioxime of the hexanoylphenyl ether $C_{24}H_{32}N_2O_3$ mol. wt. 396.53

-Preparation: A suspension of the diketone, 100 % excess of hydroxylamine hydrochloride, and powdered anhydrous sodium carbonate in propanol [463].

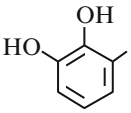
m.p. 104–105.5° [721], 103–104.5° [463], 87–88° [463].
87–88° and 103–104.5° (two forms) [463].

Dihydrazone of the hexanoylphenyl ether $C_{24}H_{34}N_4O$ mol. wt. 394.56

m.p. 103–104.5° [721].

1-(2,3-Dihydroxyphenyl)-1-hexanone

[862666-34-0] $C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis

-Obtained by deprotection of its dimethyl ether with boron tribromide in methylene chloride at 0°. Then, the mixture was stirred overnight at r.t. (87 %) [82].

brown solid [82]; m.p. 52° [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

USE: Reactant for preparation of lithium gallium/titanium ketone complexes [82].

Dimethyl ether [1854-73-5] $C_{14}H_{20}O_3$ mol. wt. 236.31

-Obtained by treatment of 1-(2,3-dimethoxyphenyl)-1-hexanol in acetone with potassium dichromate in dilute sulfuric acid (Jones reagent) at r.t. for 3 h (31 %) [82].

-Also obtained by treatment of 2,3-dimethoxyphenylpentyl-carbinol with potassium dichromate in dilute sulfuric acid at 30° (57 %) [3148].

colourless oil [82]; b.p.$_{20}$ 178–180° [3148];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

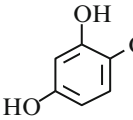
2,4-Dinitrophenylhydrazone of the dimethyl ether

[1854-72-4] $C_{20}H_{24}N_4O_6$ mol. wt. 416.43

m.p. 125° [3148].

1-(2,4-Dihydroxyphenyl)-1-hexanone

[3144-54-5] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses

-Preparation by reaction of caproic acid with resorcinol,

*in the presence of boron trifluoride at 70° for 2 h (90 %) [2312] or for 2–3 h between 65 and 85° [503];

*in the presence of zinc chloride (68–78 %) [2501];

*in the presence of polyphosphoric acid at 90° for 30 min [2907].

-Also obtained by reaction of capronitrile with resorcinol (Hoesch reaction) (27 %) [1371].

-Also obtained by reaction of ethyl caproate with resorcinol in the presence of zinc chloride, the mixture was heated for 1 h at its boiling point (60 %) [3160].

-Also obtained by reaction of hexanoyl chloride with resorcinol at 85–90° for 20–30 min (87.5 %) [731]. The same result was obtained in the presence of zinc chloride.

-Also obtained by reaction of hexanoyl chloride with resorcinol in the presence of aluminium chloride in 1,2-dichloroethane for 5 h at 65° [284].
-Identification into catalytic hydrothermal treatment of wood biomass at 280° for 15 min in the presence of alkaline solution (NaOH, Na_2CO_3, KOH, K_2CO_3) [1601].
-Also obtained by reduction of 2,4-dihydroxysorbophenone [2907].
-Also refer to: [126, 129, 229 (93 %), 893, 1079, 1239, 1562, 1598, 1599, 1657, 1673, 1798, 1892, 2114, 2498, 2637, 2640, 2692, 2769, 2787, 2841, 2842, 2910, 3010, 3051, 3077, 3099, 3168, 3208, 3449].

white crystals [3160]; colourless needles [229];
b.p.$_{0.3}$ 144–146° [229], b.p.$_3$ 170–175° [1562], b.p.$_3$ 184–185° [1448], b.p.$_{6–7}$ 196–197° [2841, 2842, 3099], b.p.$_9$ 205–208° [1448], b.p.$_{10}$ 200–210° [2907],
b.p.$_{15}$ 210–220° [731], b.p.$_{14}$ 217–218° [3160], b.p. 343–345° (d) [3160];
m.p. 58° [503], 56–57° [1562, 3160], 56° [229, 2312], 55–56° [1448], 55° [731], 54.5–56° [893, 1673, 2842];
^{1}H NMR [1239], ^{13}C NMR [1239]; GC-MS [1601].

BIOLOGICAL ACTIVITY: Nematocide: 4-Hexanoylresorcinol at 100 ppm controlled *Pratylenchus penetrans* [1798]; Responses of *Phytophthora sojae* zoospores to isoflavones and analogs [3161]; Inhibition of polyphenol oxidase (**PPO**) [2030]; Binary classification models for endocrine disrupter effects mediated through the estrogen receptor [2640]; Effect of K_2CO_3 concn. and biomass/water ratio on products distribution in hydrothermal upgrading of biomass [1597]; Effect of RbOH and CsOH on product distribution in catalytic hydrothermal treatment of pine wood biomass [1600]; Antiseptic and germicidal product [2734]; Differentiation-inducing factor 1 (DIF-1) as protease-inhibitory and antiviral compound [129]; Reproductive effects (germination) [126, 238]; Picornavirus activity inhibitor [126]; Estrogenic [2769]; Antiviral [126]; Antifungal [2114, 2769]; Fungicides for hydocarbon lubricants and hydraulic fluids [2498] and for lubricants for optical instruments [2637]; Cytotoxicity [126].

USE: In detn. of uranium by spectrophotometry [2891]; Wine preservation by, [3168].

2,4-Dinitrophenylhydrazone [109252-18-8] $C_{18}H_{20}N_4O_6$ mol. wt. 388.38

-Refer to: [2907].

m.p. 232–235° [2907].

Diacetate $C_{16}H_{20}O_5$ mol. wt. 292.33

-Obtained by boiling the 2,4-dihydroxycaprophenone with sodium acetate and acetic anhydride for several hours (poor yield) [3160].

thick yellow oil [3160]; b.p.$_{13}$ 229–232° [3160].

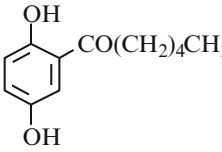
Dimethyl ether [312488-55-4] $C_{14}H_{20}O_3$ mol. wt. 236.31

-Preparation by reaction of n-caproyl chloride with 1,3-dimethoxybenzene,
*in the presence of aluminium chloride in methylene chloride at 0–5° for 2.5 h (90 %) [2188];
*in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].
-Also obtained (by-product) by reaction of dimethyl sulfate with 2,4-dihydroxycaprophenone in the presence of 20 % sodium hydroxide solution [3160].

white crystals [3160]; m.p. 36° [2188], 35–36° [3160];
^{1}H NMR [2188], IR [2188], MS [2188].

1-(2,5-Dihydroxyphenyl)-1-hexanone

[4693-18-9] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses
-Preparation by reaction of caproic acid with hydroquinone [2102] in the presence of boron trifluoride at 125° for 2 h in a sealed tube (94 %) [2312] or heated for 2 h at 125° [2063].
-Also obtained by reaction of caproyl chloride with hydroquinone in the presence of aluminium chloride in nitrobenzene heated on a water bath for 3 h [1442].

-Also obtained by Fries rearrangement of hydroquinone dicaproate with aluminium chloride for 5 h at 150–160° [1442].
-Also obtained by treatment of its dimethyl ether with hydrobromic acid in refluxing acetic acid for 6 h [1442].
-Also refer to: [1481, 2063, 2102, 3168, 3204].

m.p. 85–86° [2312], 82–83° [2102], 82° [3204], 81–83° [2063], 81–82° [1442].

USE: Wine preservation by, [3168].

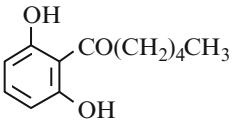
Dimethyl ether [430425-41-5] $C_{14}H_{20}O_3$ mol. wt. 236.31

-Obtained by reaction of caproyl chloride with hydroquinone dimethyl ether,
*in the presence of aluminium chloride in nitrobenzene, first at r.t. overnight, then the mixture heated on a water bath for 3 h [1442];
*in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].
-Also refer to: [1919].

b.p.$_{0.5}$ 132–134° [1919], b.p.$_{15}$ 175–180° [1442]; m.p. 15° [1919].

1-(2,6-Dihydroxyphenyl)-1-hexanone
(2-Caproylresorcinol)

$C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses
-Obtained by Fries rearrangement of 1,3-dihydroxyphenyl caproate (b.p.$_{11}$ 166–175°) with aluminium chloride in nitrobenzene at 60° for 4 h (40 %) [1877].

-Also refer to: [2629, 2672].

m.p. 74° [2672], 142–143° [1877].
N.B.: One of the reported melting point is obviously wrong.

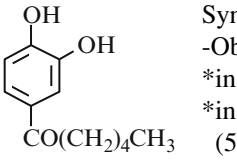
Dimethyl ether [5673-08-5] $C_{14}H_{20}O_3$ mol. wt. 236.31

-Obtained by reaction of 2,6-dimethoxybenzoyl chloride with dipentylcadmium (51 %) [2629].
-Also refer to: [2672].

oil [2629]; b.p.$_2$ 142° [2672], b.p.$_{14}$ 182–184° [2629];
^{1}H NMR [2629], IR [2629].

1-(3,4-Dihydroxyphenyl)-1-hexanone

[4009-78-3] $C_{12}H_{16}O_3$ mol. wt. 208.26



Syntheses
-Obtained by reaction of caproic acid with pyrocatechol,
*in the presence of zinc chloride at reflux [726];
*in the presence of boron trifluoride for 2.5 h at 150° (55 %) [2312].

-Also obtained by Fries rearrangement of pyrocatechol dicaproate with aluminium chloride in the presence of pyrocatechol at 135–140° for 4.5 h (72 %) [2075] or for 5 h (30 %) [283].
-Also obtained by treatment of guaiacol caproate in carbon disulfide at 90° for 50 min, then at 135–140° for 2 h after solvent elimination (30–47 %) [2075].
-Also obtained by reaction of guaiacol caproate with aluminium chloride in nitrobenzene [726].
-Also refer to: [1770, 2075, 2508].

b.p.$_4$ 212–220° [2075], b.p.$_{15}$ 240–250° [726];
m.p. 94° [2312], 93.8° [2075], 93–94° [726, 2955], 91–93° [283];
^{1}H NMR [283], UV [985]; paper chromatography [2508].

BIOLOGICAL ACTIVITY: Protective agent against the lethal effects of X-rays [1809].

Dimethyl ether [52375-87-8] $C_{14}H_{20}O_3$ mol. wt. 236.31

-Obtained by Friedel-Crafts acylation reaction of caproic anhydride with veratrole,
*in the presence of a catalyst generated from gallium trichloride and a silver salt ($AgClO_4$ or $AgSbF_6$) (high yields) [2175];
*using the combined catalyst system of $TiCl(OTf)_3$ and TfOH (94 %) [1483];
*in the presence of $SbCl_5$-$LiClO_4$ mixture in refluxing methylene chloride for 30 min (87 %) [2176].
-Also obtained by reaction of caproyl chloride with veratrole,
*in the presence of zinc chloride in refluxing carbon disulfide for 4 h (49 %) [1565];
*in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].
-Also obtained by Friedel-Crafts acylation of veratrole in the presence of a Lewis acid catalyst while using carboxylic acid or trisubstituted-silyl carboxylate as acylating agent and carrying out the reaction in the presence of p-trifluoromethylbenzoic acid anhydride and, if necessary, a silver salt [2997].
-New inhibitor of the CoQ-dependent redox reactions in mitochondria and chromatophores [1729].
-Also refer to: [1112, 1202, 1249, 2172, 2174, 2999, 3056, 3364].

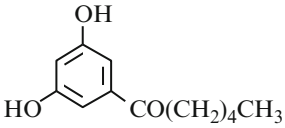
viscous liquid [1565]; $b.p._{.1}$ 150° [1565], $b.p._{.17}$ 176–178° [3056];
^1H NMR [1249, 2999], ^{13}C NMR [1249, 2999], IR [1249, 2999, 3364].

Semicarbazone of the dimethyl ether [101109-36-8] $C_{15}H_{23}N_3O_3$ mol. wt. 293.37

colourless needles [1565]; m.p. 178° [1565].

1-(3,5-Dihydroxyphenyl)-1-hexanone

[105401-56-7] $C_{12}H_{16}O_3$ mol. wt. 208.26



Synthesis
-Obtained by treatment of its diacetate with 5 % sodium hydroxide at reflux for 4.5 h (63 %) [1406].

m.p. 106° [1406].

2,4-Dinitrophenylhydrazone [109248-78-4] $C_{18}H_{20}N_4O_6$ mol. wt. 388.38

m.p. 222° (d) [1406].

Diacetate [101430-19-7] $C_{16}H_{20}O_5$ mol. wt. 292.33

-Preparation by reaction of dipentylcadmium with 3,5-diacetoxybenzoyl chloride in refluxing benzene for 1 h (77 %) [1406].

$b.p._{.0.8}$ 189–192° [1406].

2,4-Dinitrophenylhydrazone of the diacetate

[102810-66-2] $C_{22}H_{24}N_4O_8$ mol. wt. 472.45

m.p. 152° [1406].

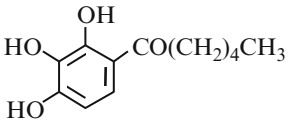
Dimethyl ether [41497-32-9] $C_{14}H_{20}O_3$ mol. wt. 236.31

-Preparation by reaction of pentylmagnesium bromide with 3,5-dimethoxybenzamide in refluxing ethyl ether for 5 h (88 %) [2990].
-Also obtained by reaction of pentylmagnesium bromide with 3,5-dimethoxybenzonitrile in refluxing THF for 3 h, followed by heating with 6 N HCl at reflux (65 %) [2209].
-Also refer to: [238, 543, 2899].

white solid [2209]; b.p.$_7$ 175–176° [2990];
m.p. 53° [2990], 49–51° [543];
^{1}H NMR [543, 2209], ^{13}C NMR [2209], IR [2209], UV [543], MS [2209].

1-(2,3,4-Trihydroxyphenyl)-1-hexanone
(4-Hexanoylpyrogallol)

[43043-26-1] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Obtained by reaction of caproic acid with pyrogallol in the presence of zinc chloride (Nencki reaction),
*at 150° for 45 min (41 %) [1643];
*at 140–145° for 4 h (70 %) [506];
*at 135–140° for 2 h (50 %) [1283];
*at 130–140° for 1.5 h (32 %) [1260].
-Also refer to: [1643, 3168].

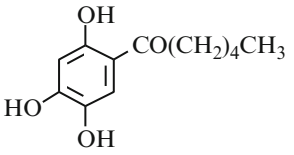
white needles [1260];
m.p. 86.5–87° [1260], 86–87° [506], 84° [1643], 72–74° [1283].

BIOLOGICAL ACTIVITY: Protection against whole-body irradiation [1810].

USE: Wine preservation by, [3168].

1-(2,4,5-Trihydroxyphenyl)-1-hexanone

[105476-10-6] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Obtained by reaction of caproyl chloride with 1,2,4-trihydroxybenzene in the presence of aluminium chloride in nitrobenzene [292].
-Also refer to: [291, 771, 1708].

m.p. 113–114° [291], 108–111° [292].

USE: Antioxidant [1708]; Antioxidant for fats, oils and paraffin waxes [292]; Toxicity [1708].

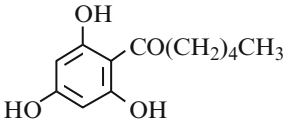
Trimethyl ether [90834-06-3] $C_{15}H_{22}O_4$ mol. wt. 266.34

-Obtained by reaction of hexanoyl chloride with 1,2,4-trimethoxybenzene in the presence of aluminium chloride (60–74 %) [771].
-Also obtained by reaction of hexanoic anhydride with 1,2,4-trimethoxybenzene in the presence of aluminium chloride in methylene chloride at 60° for 1 h (65 %) [772].
-Also obtained by reaction of caproic acid with 1,2,4-trimethoxybenzene in the presence of polyphosphoric acid for 7 h at 45–50° [2695].

white powder [772]; m.p. 82–84° [772, 2695];
^{1}H NMR [772, 2695], ^{13}C NMR [772], IR [772, 2695], MS [772, 2695].

1-(2,4,6-Trihydroxyphenyl)-1-hexanone
(Phlorocaprophenone) (THPH)

[5665-89-4] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Obtained by reaction of caproyl chloride with phloroglucinol,
*in the presence of aluminium chloride;
*in nitrobenzene (60–70 %) [421], (63 %) [2646], (51 %) [2618];

*in nitrobenzene and carbon disulfide mixture (61 %) [2113], (51 %) [2620];
*in methylene chloride at r.t. [1129];
*in the presence of boron trifluoride etherate, first at 0°, then at r.t. for 48 h under nitrogen [2786].
-Also obtained by reaction of hexanoic acid with phloroglucinol in the presence of boron trifluoride etherate [3019].
-Also obtained by reaction of caproyl nitrile with phloroglucinol (Hoesch reaction) [1376, 1699].

-Also obtained by acid hydrolysis of its 2,4-di-β-D-glucopyranoside [1089].
-Also obtained by adding phloroglucinol to a solution of phosphorous oxychloride plus aluminium chloride and stirred under nitrogen. Hexanoic acid was added and the reaction stirred under nitrogen at 0° for 8 h, then at 6° for 40 h (40–54 %) [3201].
-Also obtained by treatment of its trimethyl ether with boron tribromide in chloroform first at −18°, then at reflux for 3 h [2764].
-Also refer to: [74, 129, 153, 180, 1026, 1038, 1065, 1439, 1776, 1942, 2012, 2771, 3168, 3202].

Isolation from natural sources

-Of *Populus tritis* bud exudate [955].
-In bud exudate of *Populus koreana*, *Populus maximowiczii* and *Populus suaveolens* (Salicaceae) [1164].

yellow amorphous solid [1129]; pale beige needles [2764];
m.p. 120–121° [421, 1376, 1439], 120° [2113, 2646], 118° [1699, 2618, 2620], 108–110° [2764];
^{1}H NMR [421, 2764, 3019], ^{13}C NMR [3019],
IR [421, 2764, 3019], UV [2764, 3019], MS [421, 1129]; GC-MS [1164].

USE: Assembly and photodimerization of bis(pyridyl)ethylene with phloroglucinols [1038]; Wine preservation by, [3168].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773, 1776]; Antagonist both thromboxane A_2 and Leukotriene D_4 [3019]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129]; Antifungal [2113]; Differentiation-inducing factor 1 (DIF-1) as protease-inhibitory and antiviral compound [129]; Effect on gibberellin-inducible α-amylase synthesis in barley aleurone cells [153].

Hydrate $C_{12}H_{16}O_4$, H_2O mol. wt. 242.28

m.p. 95–96° [1376], 95° [1699].

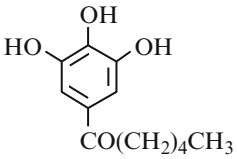
Trimethyl ether [86360-63-6] $C_{15}H_{22}O_4$ mol. wt. 266.34

-Refer to: [1065, 2764].

pale yellow oil [2764]; ^{1}H NMR [2764], IR [2764], UV [2764].

1-(3,4,5-Trihydroxyphenyl)-1-hexanone

[6345-66-0] $C_{12}H_{16}O_4$ mol. wt. 224.26



Syntheses
-Refer to: [1048, 1426].

USE: Colour photog. emulsions latent image stabilizer [1048].

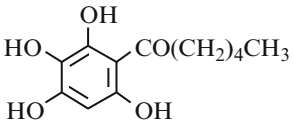
Trimethyl ether [170489-32-4] $C_{15}H_{22}O_4$ mol. wt. 266.34

-Refer to: [1425, 1426].

^{1}H NMR [1426], MS [1426].

1-(2,3,4,6-Tetrahydroxyphenyl)-1-hexanone

$C_{12}H_{16}O_5$ mol. wt. 240.26



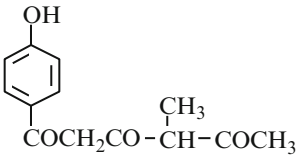
Synthesis
-Refer to: [1353].

Tetramethyl ether
$C_{16}H_{24}O_5$ mol. wt. 296.36

-Refer to: [1353].

1-(4-Hydroxyphenyl)-4-methyl-1,3,5-hexanetrione

$C_{13}H_{14}O_4$ mol. wt. 234.25



Synthesis
-Refer to: [1168].

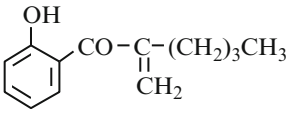
Methyl ether [92120-37-1]
$C_{14}H_{16}O_4$ mol. wt. 248.28

-Preparation: Trityl-lithium in THF was injected into 3-methylpentane-2,4-dione under nitrogen at −15°. When the red colour persisted methyl p-methoxybenzoate in THF was injected. The solution was stirred at −15° and trityl-lithium solution added to just maintain the red colour [1168].

yellow crystals [1168]; m.p. 56–57° [1168];
^{1}H NMR [1168], IR [1168], UV [1168], MS [1168].

1-(2-Hydroxyphenyl)-2-methylene-1-hexanone

[935277-51-3] $C_{13}H_{16}O_2$ mol. wt. 204.27



Synthesis
-Obtained by stirring a solution of salicylaldehyde, 1-hexyne, $RhCl(PPh_3)_3$, acetonitrile and sodium acetate in methylene chloride at r.t. for 1 h under an argon atmosphere (45 %) [1434].

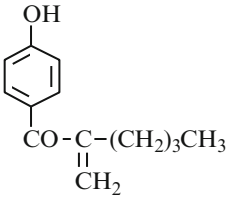
^{1}H NMR [1434], IR [1434].

Methyl ether $C_{14}H_{18}O_2$ mol. wt. 218.30

^{1}H NMR [2881], ^{13}C NMR [2881], IR [2881], MS [2881].

1-(4-Hydroxyphenyl)-2-methylene-1-hexanone

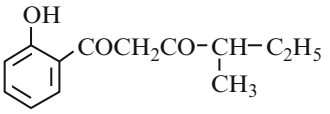
$C_{13}H_{16}O_2$ mol. wt. 204.27



Synthesis
-Refer to: [1560].
Methyl ether [473835-69-7]
$C_{14}H_{18}O_2$ mol. wt. 218.30
-Obtained by efficient and selective hydroacylation of 1-hexyne with p-methoxybenzaldehyde by a chelation-assisted catalytic system (76 %) [1560].

1-(2-Hydroxyphenyl)-4-methyl-1,3-hexanedione

[80856-36-6] $C_{13}H_{16}O_3$ mol. wt. 220.27

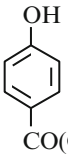


Synthesis
-Obtained by reaction of 2-hydroxyacetophenone with methyl 2-methylbutyrate in the presence of sodium hydride (61.8 %) [2807].

b.p.$_{0.7}$ 114–120° [2807];
^{1}H NMR [2807], IR [2807], UV [2807].

1-(4-Hydroxyphenyl)-5-methyl-1-hexanone

[161582-00-9] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses
-Refer to: [38, 39].

Methyl ether [92300-78-2]
$C_{14}H_{20}O_2$ mol. wt. 220.31

-Preparation by reaction of 5-methylhexanoyl chloride with anisole in the presence of aluminium chloride in carbon disulfide under cooling for 70 min, then at r.t. (91 %) [2237].
-Also refer to: [2236].

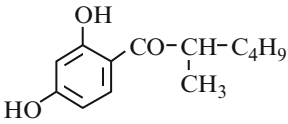
b.p.$_1$ 131–133° [2236, 2237].

Semicarbazone of the methyl ether [93762-01-7] $C_{15}H_{23}N_3O_2$ mol. wt. 277.37

m.p. 124–125° [2237].

1-(2,4-Dihydroxyphenyl)-2-methyl-1-hexanone

[406174-64-9] $C_{13}H_{18}O_3$ mol. wt. 222.28



Syntheses
-Obtained by reaction of 2-methylhexanoic acid with resorcinol in the presence of zinc chloride for 2 h at 150° (52 %) [2829].
-Also obtained by enzymatic enantioselective deacetylation of its 2,4-diacetyl ester [2829].

oil [2829];
^{1}H NMR [2829], ^{13}C NMR [2829], IR [2829], UV [2829], MS [2829]; TLC [2829].

Diacetates $C_{17}H_{22}O_5$ mol. wt. 306.36

-Refer to: [2829].
*racemic [406174-68-3].
-Obtained by reaction of acetic anhydride with 1-(2,4-dihydroxyphenyl)-2-methyl-1-hexanone in the presence of catalytic amount of N,N-dimethylaminopyridine at 22–25° (90 %) [2829].

oil [2829];
^{1}H NMR [2829], ^{13}C NMR [2829], IR [2829], UV [2829], MS [2829]; TLC [2829].

*levogyre (−) [406174-80-9].
-Obtained by chemical acetylation of monoacetate [2829].

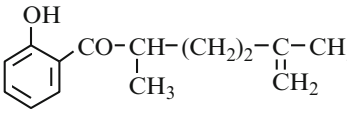
$(\alpha)_D^{25} = -41.5°$ (chloroform) [2829].

*dextrogyre (+) [406174-76-3].
-Obtained by treatment of racemic ketone with PPL pre-incubated in THF at 40–42° for 10 h in the presence of butanol (60 %) [2829].

$(\alpha)_D^{25} = +37.9°$ (chloroform) [2829].

1-(2-Hydroxyphenyl)-2-methyl-5-methylene-1-hexanone

$C_{14}H_{18}O_2$ mol. wt. 218.30

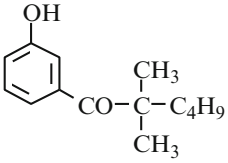


Synthesis
-Obtained by intermolecular hydroacylation between salicylaldehyde and 2-methyl-1,5-hexadiene (6 equiv.) in the presence of $RhCl(PPh_3)_3$ (0.2 equiv.) in methylene chloride for 24 h at r.t. (95 %) [1435].

^{1}H NMR [1435].

1-(3-Hydroxyphenyl)-2,2-dimethyl-1-hexanone

[104325-46-4] $C_{14}H_{20}O_2$ mol. wt. 220.31



Synthesis
-Refer to: [2197].

Phenoxymethyl ether [104341-05-1]
$C_{21}H_{26}O_3$ mol. wt. 326.44
-Refer to: [729, 2197].

BIOLOGICAL ACTIVITY: Antiallergic and inflammation inhibitor [2197].

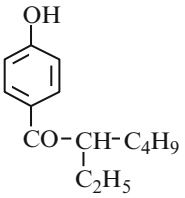
Benzyl ether [103119-42-2] $C_{21}H_{26}O_2$ mol. wt. 310.44

-Refer to: [583, 729, 2197].

BIOLOGICAL ACTIVITY: Lipoxygenase inhibition by, [583].

2-Ethyl-1-(4-hydroxyphenyl)-1-hexanone
1-(4-hydroxyphenyl)-2-ethylpentyl ketone

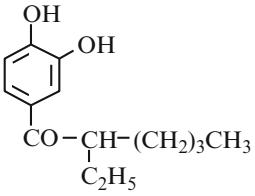
$C_{14}H_{20}O_2$ mol. wt. 220.31



Synthesis
-Obtained by Fries rearrangement of phenyl 2-ethylcaproate with aluminium chloride in nitrobenzene for 48 h at 40° under an argon atmosphere [1116].

1-(3,4-Dihydroxyphenyl)-2-ethyl-1-hexanone

$C_{14}H_{20}O_3$ mol. wt. 236.31



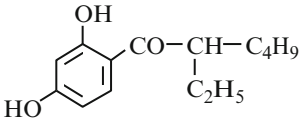
Synthesis
-Refer to: [952].

Dimethyl ether [150396-49-4]
$C_{16}H_{24}O_3$ mol. wt. 264.36
-Refer to: [952].

USE: Starting materials in synthesis of calixbisethylhexyl benzocrown [952].

1-(2,4-Dihydroxyphenyl)-2-ethyl-1-hexanone

[83671-25-4] $C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses
-Obtained by heating a mixture of 2-ethylhexanoic acid, resorcinol and fused zinc chloride [2702] at 150° [2517].
-Also refer to: [1806, 1807, 2946].

b.p.$_{.8}$ 186° [1806, 1807].

BIOLOGICAL ACTIVITY: Antifungal activity against *Dreschlera oryzae*, *Macrophomina phaseolina*, *Fusarium solani* and *Pythium aphanidermatum* [2702].

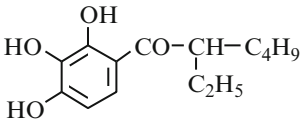
Diacetate [251463-55-5] $C_{18}H_{24}O_5$ mol. wt. 320.39

-Obtained by reaction of acetic anhydride with the title ketone in the presence of pyridine (>80 %) [2517].

viscous oil [2517];
^{1}H NMR [2517], ^{13}C NMR [2517], IR [2517], UV [2517], MS [2517].

1-(2,3,4-Trihydroxyphenyl)-2-ethyl-1-hexanone

$C_{14}H_{20}O_4$ mol. wt. 252.31



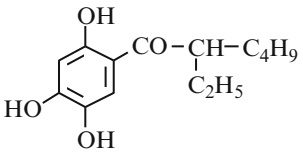
Synthesis

-Obtained by reaction of 2-ethylcaproic acid with pyrogallol in the presence of strongly acidic ion exchanger Amberlyst-15 at 120° for 24 h (56 %) [231].

^{1}H NMR [231], ^{13}C NMR [231].

1-(2,4,5-Trihydroxyphenyl)-2-ethyl-1-hexanone

[100864-42-4] $C_{14}H_{20}O_4$ mol. wt. 252.31



Synthesis

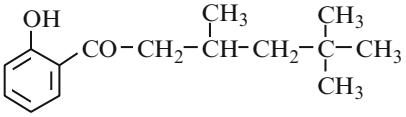
-Obtained by reaction of 2-ethylcaproyl chloride with 1,2,4-trihydroxybenzene in the presence of aluminium chloride in nitrobenzene [292] at r.t. for several hrs, and heated 0.5 h at 65° [290].

m.p. 94–97° [290, 292].

USE: Antioxidant in fats and oils [290]; Antioxidant for fats, oils and paraffin waxes [292].

1-(2-Hydroxyphenyl)-3,5,5-trimethyl-1-hexanone

[154737-33-4] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses

-Obtained by Fries rearrangement of phenyl 3,5,5-trimethylhexanoate with titanium tetrachloride in chlorobenzene at 140° for 2 h under argon (70 %) [628].

-Refer to: [110, 417].

^{1}H NMR [628]; TLC [628].

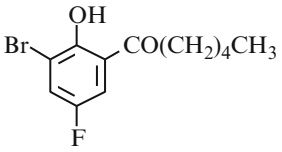
Oxime [50652-75-0] $C_{15}H_{23}NO_2$ mol. wt. 249.35

USE: In extn. of copper and nickel from sulfate solns. [110].

1.2 Substituted Hydroxyketones

1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-hexanone

[1960-58-3] $C_{12}H_{14}BrFO_2$ mol. wt. 289.14



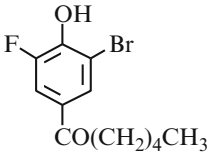
Synthesis
-Obtained by Fries rearrangement of 2-bromo-4-fluoro-phenyl caproate with aluminium chloride at 130–140° for 3 h (46 %) [1550].
b.p.$_{0.2}$ 135° [1550].

2,4-Dinitrophenylhydrazone [1841-68-5] $C_{18}H_{18}BrFN_4O_5$ mol. wt. 469.27

m.p. 147° [1550].

1-(3-Bromo-5-fluoro-4-hydroxyphenyl)-1-hexanone

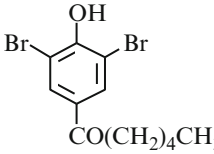
[329-44-2] $C_{12}H_{14}BrFO_2$ mol. wt. 289.14



Synthesis
-Obtained by reaction of bromine with 3-fluoro-4-hydroxy-hexanophenone in acetic acid [516].
m.p. 95° [516].

1-(3,5-Dibromo-4-hydroxyphenyl)-1-hexanone

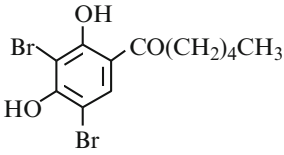
[20683-49-2] $C_{12}H_{14}Br_2O_2$ mol. wt. 350.05



Syntheses
-Obtained by reaction of bromine with 4-hydroxy-caprophenone in aqueous acetic acid [516].
-Also refer to: [433].
m.p. 68° [516].

1-(3,5-Dibromo-2,4-dihydroxyphenyl)-1-hexanone

[238074-76-5] $C_{12}H_{14}Br_2O_3$ mol. wt. 366.05

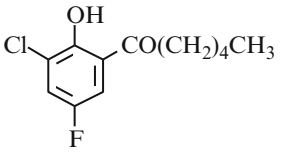


Syntheses
-Obtained by reaction of bromine with 2,4-dihydroxy-caprophenone in acetic acid first at r.t., then at 40–50° for a short time (33 %) [3160].
-Also refer to: [998].

pale yellow needles [3160]; m.p. 102–103° [3160].

1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-hexanone

[1644-57-1] $C_{12}H_{14}ClFO_2$ mol. wt. 244.69



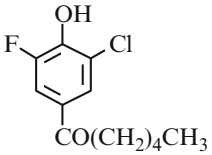
Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-fluorophenyl caproate with aluminium chloride at 130–140° for 3 h (62 %) [1550].
b.p.$_4$ 130° [1550].

2,4-Dinitrophenylhydrazone [1957-52-4] $C_{18}H_{18}ClFN_4O_5$ mol. wt. 424.82

m.p. 150° [1550].

1-(3-Chloro-5-fluoro-4-hydroxyphenyl)-1-hexanone

$C_{12}H_{14}ClFO_2$ mol. wt. 244.69



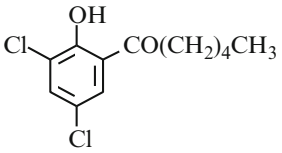
Synthesis
-Refer to: [1404].

Methyl ether [371757-70-9]
$C_{13}H_{16}ClFO_2$ mol. wt. 258.72
-Obtained by reaction of caproyl chloride with 2-chloro-6-fluoroanisole in the presence of aluminium chloride in methylene chloride [1404].

-Also refer to: [2407].

1-(3,5-Dichloro-2-hydroxyphenyl)-1-hexanone

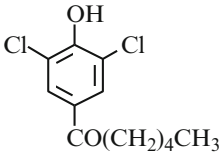
[3226-18-4] $C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15



Syntheses
-Obtained by Fries rearrangement of 2,4-dichlorophenyl caproate with aluminium chloride [3170].
-Also refer to: [433].
m.p. 59.5° [3170]; UV [3170].

1-(3,5-Dichloro-4-hydroxyphenyl)-1-hexanone

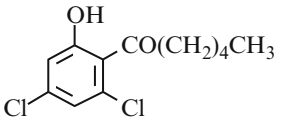
[131427-28-6] $C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15



Synthesis
-Refer to: [433].

1-(4,6-Dichloro-2-hydroxyphenyl)-1-hexanone

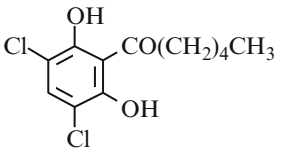
[52016-87-2] $C_{12}H_{14}Cl_2O_2$ mol. wt. 261.15



Synthesis
-Refer to: [2740].
m.p. 39–41° [2740].

1-(3,5-Dichloro-2,6-dihydroxyphenyl)-1-hexanone

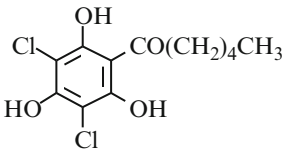
$C_{12}H_{14}Cl_2O_3$ mol. wt. 277.15



Synthesis
-Refer to: [1261].
b.p. 180–185° [1261]; m.p. 119–120° [1261].

1-(3,5-Dichloro-2,4,6-trihydroxyphenyl)-1-hexanone
(TH-DIF-1)

[118222-71-2] $C_{12}H_{14}Cl_2O_4$ mol. wt. 293.15



Syntheses
-Obtained by reaction of sulfuryl chloride (2 equiv.) with 2,4,6-trihydroxycaprophenone in a chloroform/ethanol mixture at r.t. [1129].
-Also refer to: [129, 1772, 2012].

yellow amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129]; Differentiation-inducing factor 1 (DIF-1) as protease-inhibitory and antiviral compound [129].

Trimethyl ether [861889-69-2] $C_{15}H_{20}Cl_2O_4$ mol. wt. 335.23
(TM-DIF-1)

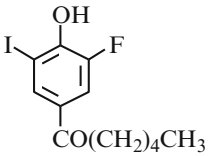
-Obtained by reaction of methyl p-toluenesulfonate with the titled ketone in the presence of potassium carbonate in acetone at r.t. for 16 h (95 %) [1129].
-Also refer to: [1772].

colourless oil [1129]; ^{1}H NMR [1129], ^{13}C NMR [1129], MS [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(3-Fluoro-4-hydroxy-5-iodophenyl)-1-hexanone

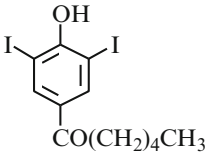
[350-16-3] $C_{12}H_{14}FIO_2$ mol. wt. 336.14



Synthesis
-Obtained by reaction of iodine with 3-fluoro-4-hydroxycaprophenone in ethanol in the presence of yellow mercuric oxide [519].
lustrous colourless leaflets [519];
m.p. 102° [519].

1-(4-Hydroxy-3,5-diiodophenyl)-1-hexanone

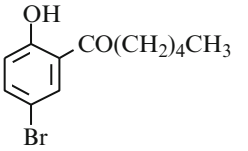
$C_{12}H_{14}I_2O_2$ mol. wt. 444.05



Synthesis
-Obtained by reaction of iodine with 4-hydroxycaprophenone in ethanol in the presence of yellow mercuric oxide [516].
colourless prisms [516]; m.p. 69° [516].

1-(5-Bromo-2-hydroxyphenyl)-1-hexanone

[103797-90-6] $C_{12}H_{15}BrO_2$ mol. wt. 271.15



Syntheses
-Preparation by Fries rearrangement of 4-bromophenyl caproate in the presence of aluminium chloride [2797], (69 %) [1640],
*in tetrachloroethane at 120° for 30 min (86 %) [2026];
*without solvent for 30 min at 150–160° [1701].

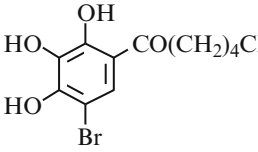
plates [2026]; $b.p._{.1}$ 145–150° [2026], $b.p._{0.5}$ 150–155° [1640];
m.p. 60.5° [1701], 58–59° [2026]; IR [1640].

2,4-Dinitrophenylhydrazone [101728-14-7] $C_{18}H_{19}BrN_4O_5$ mol. wt. 451.28

m.p. 206° [2026].

1-(5-Bromo-2,3,4-trihydroxyphenyl)-1-hexanone

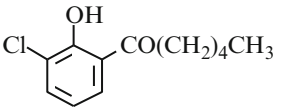
$C_{12}H_{15}BrO_4$ mol. wt. 303.15



Synthesis
-Obtained by reaction of bromine with 4-caproylpyrogallol in acetic acid [506].
m.p. 111° [506].

1-(3-Chloro-2-hydroxyphenyl)-1-hexanone

[3226-17-3] $C_{12}H_{15}ClO_2$ mol. wt. 226.70



Syntheses
-Obtained by Fries rearrangement of 2-chlorophenyl caproate with aluminium chloride [3170].
-Also refer to: [1673, 3013].

b.p.$_1$ 135–137° [3170]; m.p. 78–80° [3013], 56–57° [1673].
N.B.: One of the reported melting point is obviously wrong.
UV [3170]; GC [3012, 3013]; polarity of [3013].

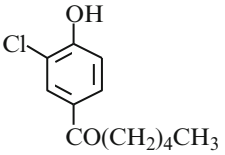
Oxime [101002-14-6] $C_{12}H_{16}ClNO_2$ mol. wt. 241.72

-Refer to: [2742, 3077].

BIOLOGICAL ACTIVITY: As lipoxygenase inhibitor [3077].

1-(3-Chloro-4-hydroxyphenyl)-1-hexanone

[3226-35-5] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

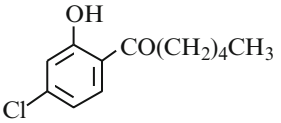


Syntheses
-Obtained by Fries rearrangement of 2-chlorophenyl caproate with aluminium chloride [3170].
-Also refer to: [381].

m.p. 79–81° [381], 77° [3170]; UV [3170].

1-(4-Chloro-2-hydroxyphenyl)-1-hexanone

[50444-92-3] $C_{12}H_{15}ClO_2$ mol. wt. 226.70



Syntheses
-Preparation by Fries rearrangement of 3-chlorophenyl caproate with aluminium chloride,
*without solvent at 130° for 2 h (74 %) [2802];
*in nitrobenzene at 25° for 6 h (92 %) [2802].

-Also refer to: [2428–2431].

b.p.$_3$ 150° [2802].

USE: Reaction of, with thionyl chloride in the presence of aluminium chloride, [2430].

Phenylhydrazone [77132-64-0] $C_{18}H_{21}ClN_2O$ mol. wt. 316.83

m.p. 81–82° [2429].

USE: Cyclization of, indole deriv. from, [2429].

2,4-Dinitrophenylhydrazone $C_{18}H_{19}ClN_4O_5$ mol. wt. 406.80

m.p. 207° [2802].

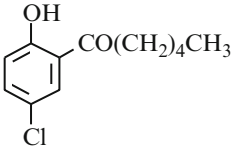
Methyl ether $C_{13}H_{17}ClO_2$ mol. wt. 240.73

-Obtained by methylation of the above ketone in the usual way (88 %) [2802].

$b.p._{.33}$ 135° [2802].

1-(5-Chloro-2-hydroxyphenyl)-1-hexanone

[3226-16-2] $C_{12}H_{15}ClO_2$ mol. wt. 226.70



Syntheses
-Obtained by Fries rearrangement of 4-chlorophenyl caproate with aluminium chloride [3170], (55.3 %) [1640].
-Also obtained by oxidation of 4-chloro-2-hexylphenol in the presence of selenium oxide in aqueous dioxane [3235].

-Also obtained by reaction of hexanoyl chloride with 4-chlorophenol in the presence of aluminium chloride (50 %) [2680].
-Also refer to: [1702, 1798, 2134].

$b.p._{.1}$ 129–132° [2680], $b.p._{.0.7}$ 135–138° [1640];
m.p. 57–58° [2680], 57° [3170], 56.5° [1702], 56° [3235];
IR [1640], UV [3170].

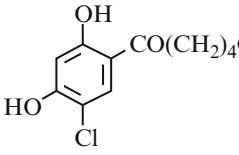
BIOLOGICAL ACTIVITY: Nematocide [1798].

Oxime [401935-06-6] $C_{12}H_{16}ClNO_2$ mol. wt. 241.72

-Topical preparations comprising at least one aryloxime and bisabolol [483].

1-(5-Chloro-2,4-dihydroxyphenyl)-1-hexanone

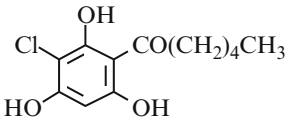
$C_{12}H_{15}ClO_3$ mol. wt. 242.70



Synthesis
-Refer to: [1808, 3126].
b.p.5 134° [1808]; m.p. 80° [3126].

1-(3-Chloro-2,4,6-trihydroxyphenyl)-1-hexanone
(TH-DIF-3), (Cl-THPH)

[200878-66-6] $C_{12}H_{15}ClO_4$ mol. wt. 258.70



Syntheses
-Obtained by reaction of sulfuryl chloride (1 equiv.) with 2,4,6-trihydroxycaprophenone in a chloroform/ethanol mixture at r.t. [1129].
-Also refer to: [126, 129, 1772, 2260].

yellow amorphous solid [1129];
^{1}H NMR [126], UV [2260], MS [1129, 2260].

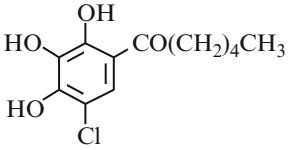
BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129]; Differentiation-inducing factor 1 (DIF-1) as protease-inhibitory and antiviral compound [129]; Antiviral [126].

Trimethyl ether [916895-75-5] $C_{15}H_{21}ClO_4$ mol. wt. 300.78

-Refer to: [1772].

1-(5-chloro-2,3,4-trihydroxyphenyl)-1-hexanone

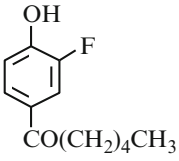
$C_{12}H_{15}ClO_4$ mol. wt. 258.70



Synthesis
-Obtained by reaction of chlorine with 4-caproylpyrogallol in acetic acid [506].
m.p. 95–96° [506].

1-(3-Fluoro-4-hydroxyphenyl)-1-hexanone

[695196-63-5] $C_{12}H_{15}FO_2$ mol. wt. 210.25



Synthesis
-Obtained by refluxing 3-fluoro-4-methoxyhexanophenone with pyridinium chloride for 15 min [516].
b.p.$_{15}$ 200° [516]; m.p. 64° [516].

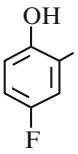
Methyl ether [371757-62-9] $C_{13}H_{17}FO_2$ mol. wt. 224.27

-Obtained by Friedel-Crafts acylation of 2-fluoroanisole with caproyl chloride in the presence of aluminium chloride in carbon disulfide (75–85 %) [516] or in methylene chloride (92 %) [1404].
-Also refer to: [2407].

m.p. 62° [516], 61–62° [1404]; ^{1}H NMR [1404], ^{13}C NMR [1404].

1-(5-Fluoro-2-hydroxyphenyl)-1-hexanone

[319-31-3] $C_{12}H_{15}FO_2$ mol. wt. 210.25



Syntheses
-Preparation by Fries rearrangement of 4-fluorophenyl caproate with aluminium chloride [1641] at 130° for 2 h (87 %) or at 150° (47 %) [2991].
-Also refer to: [1549].

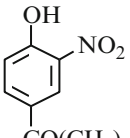
b.p.$_{12}$ 146–147° [2991]; m.p. 49–50° [2991], 31° [1549].

2,4-Dinitrophenylhydrazone [860-34-4] $C_{18}H_{19}FN_4O_5$ mol. wt. 390.37

m.p. 176° [1549].

1-(4-Hydroxy-3-nitrophenyl)-1-hexanone

[70079-25-3] $C_{12}H_{15}NO_4$ mol. wt. 237.26



Syntheses
-Obtained by reaction of caproyl chloride with 2-nitrophenol in the presence of aluminium chloride in nitrobenzene for 2.5 h at 55–60° (26 %) [465].
-Also obtained by treatment of 4-caproylphenol with concentrated nitric acid in concentrated sulfuric acid at 0° for 1 h 15 min [1222].

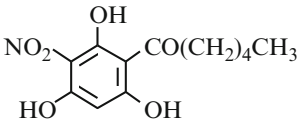
m.p. 37.2–37.6° [465], 37–38° [1222].

2,4-Dinitrophenylhydrazone $C_{18}H_{19}N_5O_7$ mol. wt. 417.38

m.p. 162.6–163.2° [465].

1-(2,4,6-Trihydroxy-3-nitrophenyl)-1-hexanone

[119691-96-2] $C_{12}H_{15}NO_6$ mol. wt. 269.25



Syntheses

-Obtained by adding hexane, then a mixture of concentrated sulfuric acid and fuming nitric acid at 0° to a solution of 1-(2,4,6-trihydroxyphenyl)-1-hexanone in concentrated sulfuric acid below 0° (70–80 %) [3414].

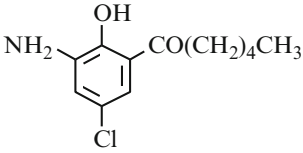
-Also refer to: [153].

bright yellow needles [3414]; m.p. 50–53° [3414];
^{1}H NMR [3414], IR [3414], MS [3414].

BIOLOGICAL ACTIVITY: Germination inhibitory activity [3414]; PET inhibitory activity [3414]. Effect on gibberellin-inducible α-amylase synthesis in barley aleurone cells [153].

1-(3-Amino-5-chloro-2-hydroxyphenyl)-1-hexanone

$C_{12}H_{16}ClNO_2$ mol. wt. 241.72

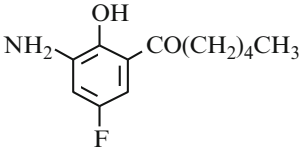


Synthesis

-Refer to: [2105].

1-(3-Amino-5-fluoro-2-hydroxyphenyl)-1-hexanone

$C_{12}H_{16}FNO_2$ mol. wt. 225.26

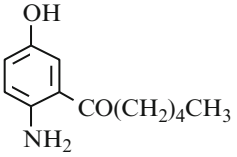


Synthesis

-Refer to: [2105].

1-(2-Amino-5-hydroxyphenyl)-1-hexanone

[404919-00-2] $C_{12}H_{17}NO_2$ mol. wt. 207.27



Syntheses

-Obtained by hydrogenation of 1-(5-benzyloxy-2-nitrophenyl)-2-hexyn-1-one (91 %) [1232].

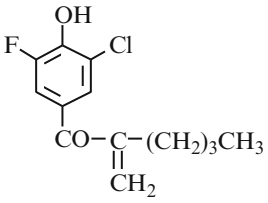
-Also refer to: [3331, 3332].

^{1}H NMR [3332].

USE: For preparation of indoles and indazoles as thyromimetics [1232, 3331].

1-(3-Chloro-5-fluoro-4-hydroxyphenyl)-2-methylene-1-hexanone

$C_{13}H_{14}ClFO_2$ mol. wt. 256.70

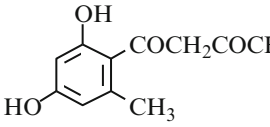


Synthesis
-Refer to: [1404].

Methyl ether $C_{14}H_{16}ClFO_2$ mol. wt. 270.73
-Obtained by reaction of aqueous 37 % formaldehyde with 3-chloro-5-fluoro-4-methoxycaprophenone in the presence of potassium carbonate in methanol at 50° for 18 h [1404].

1-(2,4-Dihydroxy-6-methylphenyl)-1,3,5-hexanetrione

$C_{13}H_{14}O_5$ mol. wt. 250.25



Synthesis
-Refer to: [1259].

Dimethyl ether [62643-36-1]
$C_{15}H_{18}O_5$ mol. wt. 278.30

-Obtained by adding methyl *O,O′*-dimethylorsellinate (m.p. 36–38°) to the dilithium salt of dilithioacetylacetone in THF under nitrogen at 0° and the mixture was stirred at 25° for 16 h (88 %) [1259].

m.p. 63–65° [1259]; ^{1}H NMR [1259], IR [1259], UV [1259].

Dibenzyl ether [38071-42-0] $C_{27}H_{26}O_5$ mol. wt. 430.50

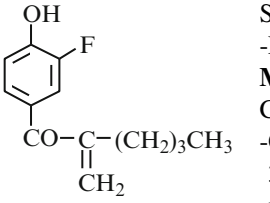
-Obtained by treatment of dilithioacetylacetone with methyl *O,O′*-dibenzylorsellinate in THF for 36 h at 25° (71 %) [1259].

m.p. 55.5–57° [1259]; ^{1}H NMR [1259], IR [1259], UV [1259].

Hemihydrate of the dibenzyl ether $C_{27}H_{26}O_5$, 0.5 H_2O mol. wt. 439.51

1-(3-Fluoro-4-hydroxyphenyl)-2-methylene-1-hexanone

$C_{13}H_{15}FO_2$ mol. wt. 222.26



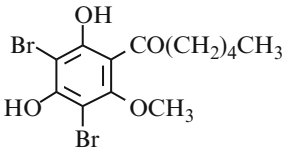
Synthesis
-Refer to: [1404].

Methyl ether [942037-66-3]
$C_{14}H_{17}FO_2$ mol. wt. 236.29
-Obtained by reaction of aqueous 37 % formaldehyde with 3-fluoro-4-methoxycaprophenone in the presence of potassium carbonate in methanol at 50° for 18 h [1404].

^{1}H NMR [1404].

1-(3,5-Dibromo-2,4-dihydroxy-6-methoxyphenyl)-1-hexanone

[118191-29-0] $C_{13}H_{16}Br_2O_4$ mol. wt. 396.08

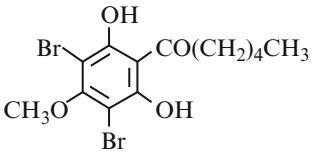


Synthesis
-Preparation by halogenation of 1-(2,4-dihydroxy-6-methoxyphenyl)-1-hexanone with bromine in water [2012].

BIOLOGICAL ACTIVITY: Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

1-(3,5-Dibromo-2,6-dihydroxy-4-methoxyphenyl)-1-hexanone
(Br-DIF-1)

[118191-30-3] $C_{13}H_{16}Br_2O_4$ mol. wt. 396.08



Syntheses
-Obtained by reaction of pyridinium tribromide with 2,6-dihydroxy-4-methoxyhexanophenone in pyridine and the mixture was stirred for 1 h (62 %) [1129].
-Preparation by halogenation of 1-(2,6-dihydroxy-4-methoxyphenyl)-1-hexanone with bromine in water [2012].

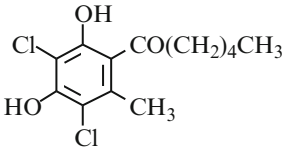
-Also refer to: [1772, 1773, 2341].

yellow amorphous solid [1129];
^{1}H NMR [1129], ^{13}C NMR [1129], MS [1129].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]. Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129]; Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

1-(3,5-Dichloro-2,4-dihydroxy-6-methylphenyl)-1-hexanone

[118191-31-4] $C_{13}H_{16}Cl_2O_3$ mol. wt. 291.17

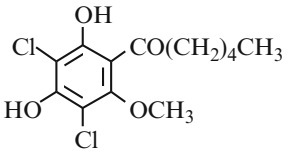


Synthesis
-Refer to: [2012].

BIOLOGICAL ACTIVITY: As differentiation inducing factor [2012].

1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-hexanone
(DIF-1), (2-MIDIF-1)

[118191-28-9] $C_{13}H_{16}Cl_2O_4$ mol. wt. 307.17



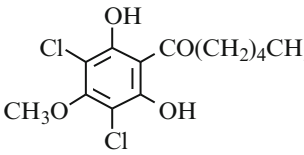
Syntheses
-Obtained by reaction of chlorine with 2,4-dihydroxy-6-methoxyhexanophenone in water [2012].
-Also refer to: [74, 128, 129, 1773, 1776, 2869].

^{1}H NMR [2012], MS [2012].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773, 1776, 2341]; Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012]; Differentiation-inducing factor 1 (DIF-1) as protease-inhibitory and antiviral compound [129]; As cysteine protease activity modulator [128].

1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-hexanone
(DIF-1)

[111050-72-7] $C_{13}H_{16}Cl_2O_4$ mol. wt. 307.17



Syntheses
-Preparation by adding a solution of sulfuryl chloride (2.16 equiv.) in ethanol to a solution of 2,6-dihydroxy-4-methoxyhexanophenone in chloroform at r.t.; then, the solution was stirred for 1 h at r.t. (93 %) [1129].

-Also obtained by reaction of chlorine with 2,6-dihydroxy-4-methoxyhexanophenone in water [2012].
-Also refer to: [74, 126–129, 207, 935, 1135, 1586, 1593, 1775, 1860, 2021, 2248, 2341, 2682, 2729, 2737, 3368, 3395, 3402].

Isolation from natural sources

-Found in *Dictyostelium discoideum* [318, 1654, 1776].
-From *Dictyostecoideum* [2869].

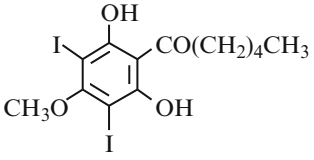
yellow amorphous solid [126, 127, 1129];
m.p. 101° [126, 127];
^{1}H NMR [1129, 2012], ^{13}C NMR [1129], UV [2012],
MS [1129, 2012], X-ray data [2012]; GC [2154].

BIOLOGICAL ACTIVITY: Structure and function of polyketide synthase in cellular slime mold for differentiation-inducing factor-1 formation [2682]; β-amyloid level redn. by treatment with differentiation-inducing factor [2207]; Antitumor activities of derivs. of DIF-1 [1677, 1775]; Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; Cell type specificity

of a diffusible inducer is detd. by a GATA family transcription factor in Dictyostelium [1659]; DIF-1: Stalk-cell differentiation; Anticancer drug [1129]; DIF-1 derivs. for treating diabetes and obesity [1773]; A UDP-glucose deriv. in required for vacuolar autophagic cell death [3136]; Antileukemic activities of Dictyostelium secondary metabolites [1678]; Antitumor substance [1776]; Inhibits progesterone-induced oocyte maturation in *Xenopus laevis* [1776]; Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012]; Cell type detn. in *Dictyostelium discoideum* by differentiation-inducing factor DIF-1 [2005]; Novel development rescuing factors secreted by Dictyostelium cells that are involved in restoration of mutant lacking MAP kinase ERK2 [3153]; Potent antiproliferative [2869]; Novel development rescuing factors secreted by Dictyostelium cells that are involved in restoration of mutant lacking MAP kinase ERK2 [3153]; Effects of differentiation-inducing factor-1 (DIF-1) of Dictyostelium discoideum on bacteria, fungi, and an influenza virus [1789]; Differentiation-inducing factor 1 (DIF-1) as protease-inhibitory and antiviral compound [129]; As cysteine protease activity modulator [128]; Differentiation-inducing factor D. discoideum raises intracellular calcium concentration and suppresses cell growth in rat pancreatic AR42J cells [1778]; Prespore-specific gene transcriptional repression by, in *Dictyostelium* [935]. -Also refer to: [1263, 1675, 1774, 1804, 1926, 2309, 2341, 3029].

1-(2,6-Dihydroxy-3,5-diiodo-4-methoxyphenyl)-1-hexanone
(I-DIF-1)

[861889-71-6] $C_{13}H_{16}I_2O_4$ mol. wt. 490.08



Syntheses
-Obtained by reaction of benzyltrimethylammonium dichloroiodate (2.09 equiv.) with 2,6-dihydroxy-4-methoxyhexanophenone in the presence of calcium carbonate in a methylene chloride/methanol mixture (2:1) at r.t. for 2 h (57 %) [1129].

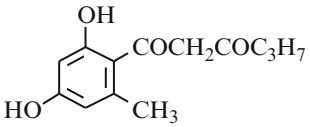
-Also refer to: [1772, 1773, 2341].

yellow amorphous solid [1129];
^{1}H NMR [1129], ^{13}C NMR [1129], MS [1129].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2,4-Dihydroxy-6-methylphenyl)-1,3-hexanedione

$C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Refer to: [3142].

Dimethyl ether [66346-51-8]
$C_{15}H_{20}O_4$ mol. wt. 264.32

-Obtained by treatment of a mixture of orcacetophenone dimethyl ether and ethyl butyrate with pulverised sodium at 115–120° for 1.5 h (48 %) [2814].
-Also obtained by treatment of a mixture of orcpropiophenone, butyric anhydride and sodium butyrate at 180–190° for 8 h [3142].

viscous brown oil [3142]; pale yellow oil [2814];
$b.p._{20–25}$ 220–225° [2814].

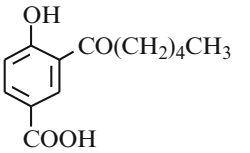
Copper salt of the dimethyl ether $(C_{15}H_{19}O_4)_2Cu$ mol. wt. 590.17

-Preparation from the above dimethyl ether and copper acetate [2814].

m.p. 175–177° [2814].

3-Hexanoyl-4-hydroxybenzoic acid

[136039-85-5] $C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Obtained by hydrolysis of its ethyl ester [967].
m.p. 188° [967].

Acetate $C_{15}H_{18}O_5$ mol. wt. 278.30

-Obtained by acetylation of 3-hexanoyl-4-hydroxybenzoic acid [967].

m.p. 100° [967].

Methyl ether $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by methylation of 4-hydroxy-3-valeroylbenzoic acid [967].

m.p. 160° [967].

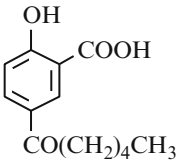
Ethyl ester $C_{15}H_{20}O_4$ mol. wt. 264.32

-Obtained by reaction of hexanoyl chloride with ethyl 4-hydroxybenzoate in the presence of aluminium chloride in tetrachloroethane, then the reaction mixture was heated at 120° for 3–4 h [967].

$b.p._{.20}$ 200° [967].

5-Hexanoyl-2-hydroxybenzoic acid

[78418-00-5] $C_{13}H_{16}O_4$ mol. wt. 236.27



Syntheses

-Obtained by hydrolysis of methyl 5-caproyl-2-hydroxy-benzoate with boiling 20 % solution of potassium hydroxide [730].

-Also refer to: [689] (82 %).

m.p. 117° [730], 116–117° [689].

Methyl ester [78417-95-5] $C_{14}H_{18}O_4$ mol. wt. 250.29

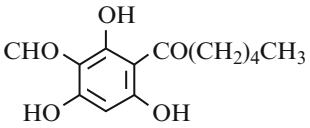
-Obtained by Fries rearrangement of methyl 2-(caproyloxy)benzoate with aluminium chloride in boiling carbon disulfide for 2 h, then the reaction mixture heated at 90–110° for a few min after solvent elimination (82 %) [1259].

-Also refer to: [689] (77 %).

b.p.$_{20}$ 202–205° [730]; m.p. 58–60° [689], 50–51° [730];
^{1}H NMR [689].

2,4,6-Trihydroxy-3-(1-oxohexyl)benzaldehyde

[96573-32-9] $C_{13}H_{16}O_5$ mol. wt. 252.27



Syntheses

-Obtained by reaction of ethyl orthoformate with 2,4,6-trihydroxycaprophenone in the presence of aluminium chloride in methylene chloride with cooling in an ice bath for 30 min (70 %) [421].

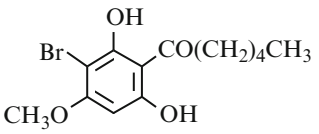
-Also refer to: [3033].

m.p. 134–136° [421]; ^{1}H NMR [421], IR [421], MS [421].

BIOLOGICAL ACTIVITY: Inhibitory effects of treatment with this acylphenol on TPA Induced EBV-EA Activation [3033]; As photosynthetic electron transport (PET) [3405].

1-(3-Bromo-2,6-dihydroxy-4-methoxyphenyl)-1-hexanone
(Br-DIF-3)

[861889-70-5] $C_{13}H_{17}BrO_4$ mol. wt. 317.18



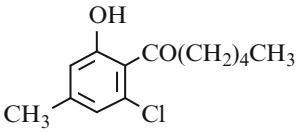
Syntheses
-Obtained by reaction of pyridinium tribromide with 2,6-dihydroxy-4-methoxyhexanophenone in pyridine and the mixture was stirred for 1 h (28 %) [1129].
-Also refer to: [1773, 2341].

colourless amorphous solid [1129];
^{1}H NMR [1129], ^{13}C NMR [1129], MS [1129].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2-Chloro-6-hydroxy-4-methylphenyl)-1-hexanone

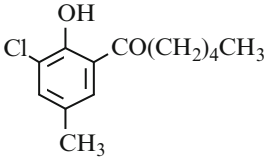
[24490-27-5] $C_{13}H_{17}ClO_2$ mol. wt. 240.73



Synthesis
-Refer to: [3138].
Fluorescence spectra [3138].

1-(3-Chloro-2-hydroxy-5-methylphenyl)-1-hexanone

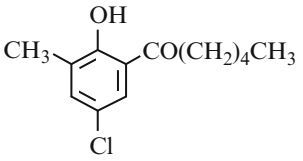
$C_{13}H_{17}ClO_2$ mol. wt. 240.73



Synthesis
-Refer to: [2679].
b.p.$_1$ 150–152° [2679]; m.p. 25–27° [2679];
$n_D^{30} = 1.5396$ [2679].

1-(5-Chloro-2-hydroxy-3-methylphenyl)-1-hexanone

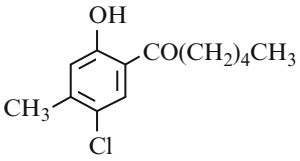
$C_{13}H_{17}ClO_2$ mol. wt. 240.73



Synthesis
-Refer to: [2679].
b.p.$_1$ 149–151° [2679]; $n_D^{25} = 1.5428$ [2679].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-hexanone

[196813-77-1] $C_{13}H_{17}ClO_2$ mol. wt. 240.73



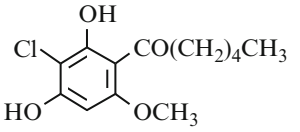
Syntheses
-Obtained by reaction of caproic acid with 4-chloro-3-methylphenol in the presence of boron trifluoride,
*for 1 h at 100° in a sealed tube (85 %) [1684];
*for 2 h at 70–80° (31 %) or 30 h at this temperature (70 %) [1684].

-Also refer to: [1686, 2679, 3138].

b.p.$_1$ 152–154° [2679]; m.p. 56–57° [1684], 42–44° [2679];
IR (Sadtler standard N° 8988) [1684]; fluorescence spectral data [3138].

1-(3-Chloro-2,4-dihydroxy-6-methoxyphenyl)-1-hexanone

[227946-80-7] $C_{13}H_{17}ClO_4$ mol. wt. 272.73

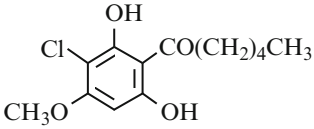


Syntheses
-Refer to: [74, 127, 128, 1771, 2869].
^{1}H NMR [127], MS [127].

BIOLOGICAL ACTIVITY: In the treatment of cancer (PDE1 inhibitor) [1771]; As cysteine protease activity modulator [128]; Inhibition of enzyme human leukemia K562 cells [74]; Inhibition growth human leukemia K562 cells [74]; Antiviral (HRV-14 and HRV-16) [127]; Cytotoxicity [127].

1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-1-hexanone
(DIF-3)

[113411-17-9] $C_{13}H_{17}ClO_4$ mol. wt. 272.73



Syntheses
-Preparation by adding a solution of sulfuryl chloride (1.1 equiv.) in ethanol to a solution of 2,6-dihydroxy-4-methoxyhexanophenone in chloroform at r.t.; then, the solution was stirred for 1 h at r.t. [1129].

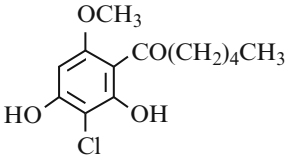
-Also refer to: [74, 318, 1653, 1677, 1772, 1773, 1777, 2011, 2869, 3031, 3153, 3256].

colourless amorphous solid [1129];
^{1}H NMR [1129], ^{13}C NMR [1129], MS [1129]; GC [2154].

BIOLOGICAL ACTIVITY: Antitumor activities of derivs. of DIF-1 [1677]; DIF-3 (3 M); Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129]; DIF-1 derivs. for treating diabetes and obesity [1773]; Involvement of GSK-3β and DYRK1B in differentiation-inducing factor-3-induced phosphorylation of cyclin D1 in HeLa cells [3030]; Novel development rescuing factors secreted by Dictyostelium cells that are involved in restoration of mutant lacking MAP kinase ERK2 [3153]; Cell differentiation regulation by, in *Dictyostelium discoideum* [1653]; Differentiation-inducing factor, from *Dictyostelium discoideum*, characterization of, [2011].

1-(5-Chloro-4,6-dihydroxy-2-methoxyphenyl)-1-hexanone

[227946-81-8] $C_{13}H_{17}ClO_4$ mol. wt. 272.73

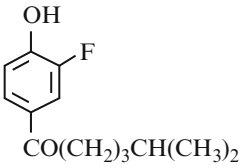


Synthesis
-Refer to: [128].
^{1}H NMR [127]; MS [127].

BIOLOGICAL ACTIVITY: As cysteine protease activity modulator [128].

1-(3-Fluoro-4-hydroxyphenyl)-5-methyl-1-hexanone

$C_{13}H_{17}FO_2$ mol. wt. 224.27

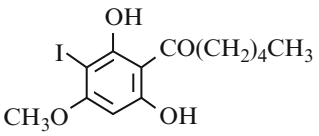


Synthesis
-Refer to: [38].

Methyl ether [161581-92-6]
$C_{14}H_{19}FO_2$ mol. wt. 238.30
-Refer to: [38].

1-(2,6-Dihydroxy-3-iodo-4-methoxyphenyl)-1-hexanone
(I-DIF-3)

[861889-72-7] $C_{13}H_{17}IO_4$ mol. wt. 364.18



Syntheses
-Obtained by reaction of benzyltrimethylammonium dichloroiodate (1.1 equiv.) with 2,6-dihydroxy-4-methoxyhexanophenone in the presence of calcium carbonate in a methylene chloride/methanol mixture (2:1) at r.t. for 2 h [1129].

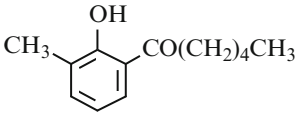
-Also refer to: [1773, 2341].

yellow amorphous solid [1129];
^{1}H NMR [1129], ^{13}C NMR [1129], MS [1129].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2-Hydroxy-3-methylphenyl)-1-hexanone

[132858-60-7] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses
-Obtained by Fries rearrangement of o-cresyl caproate with aluminium chloride for 30 min at 160–180° (60 %) [726] or (37 %) [1644].
-Also refer to: [2270, 2679].

b.p.$_1$ 131–132° [2679], b.p.$_{15–16}$ 150–154° [2270], b.p.$_{15}$ 152–154° [726, 1644]; m.p. 23° [726]; $n_D^{20} = 1.5338$ [2679].

2,4-Dinitrophenylhydrazone $C_{19}H_{22}N_4O_5$ mol. wt. 386.41

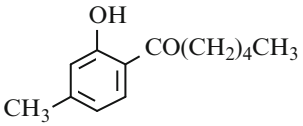
m.p. 178–179° [2270].

Phenylhydrazone $C_{19}H_{24}N_2O$ mol. wt. 296.41

m.p. 93–94° [726].

1-(2-Hydroxy-4-methylphenyl)-1-hexanone

[52122-70-0] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses

-Preparation by Fries rearrangement of 3-methylphenyl caproate with aluminium chloride,

*without solvent for 2 h at 160° (93 %) [726], at 140–150° [906], 10–20 min at 120–140° (91 %) [243] or 2 h at 120–148° (73 %) [1644];

*in nitrobenzene for 24 h at 25° (62 %) [243] or at 25–30° for 48 h (64 %) [244];

*in the presence of a mixture of graphite and methanesulfonic acid at 160° for 30 min (80 %) [2833].

-Also obtained by reaction of caproic acid with m-cresol,

*in the presence of boron trifluoride for 6 h at 80° (88 %) [1685];

*in the presence of polyphosphoric acid for 1 h at 80° (22 %) [2916];

*in the presence of a mixture of graphite and methanesulfonic acid at 120° for 2 h (88 %) [2834] or at 140° for 5 min (90 %) [2833].

-Also refer to: [108–110, 1452, 2833, 3077, 3270].

b.p.$_{0.1}$ 90–115° [109], b.p.$_{0.4}$ 101° [2916], b.p.$_1$ 115–117° [906], b.p.$_3$ 134–135° [243], b.p.$_2$ 135–137° [2679], b.p.$_{15}$ 162–164° [726, 1644], b.p.$_{18}$ 171–173° [1685];

m.p. 23–24° [726, 1644], 20–21° [1685];

^{1}H NMR [2834], ^{13}C NMR [2834], IR [2834]; $n_D^{25} = 1.5339$ [2679].

Oxime [50652-74-9] $C_{13}H_{19}NO_2$ mol. wt. 221.30

-Refer to: [108, 483, 2742, 3077].

USE: Topical preparations comprising at least one aryloxime and bisabolol [483]; In copper extraction from aqueous solutions [108]; In extn. of copper and nickel from sulfate solns. [110]; Chelation with, of metals, [109].

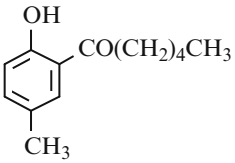
BIOLOGICAL ACTIVITY: As lipoxygenase inhibitor [3077].

Phenylhydrazone $C_{19}H_{24}N_2O$ mol. wt. 296.41

m.p. 97–97.5° [243], 94° [2916], 92–93° [726].

1-(2-Hydroxy-5-methylphenyl)-1-hexanone

[101002-28-2] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses

-Preparation by Fries rearrangement of 4-methylphenyl caproate with aluminium chloride for 2 h at 160° (80 %) [726], 10 min at 120° (89 %) [2647], 1 h at 100° (74 %) [1644] or 72 h at 25–30° (60 %) [244].

-Also refer to: [1921, 2134, 2679].

b.p.$_2$ 132–133° [2679], b.p.$_{15}$ 150–152° [726, 1644], b.p.$_{15}$ 163° [2647]; m.p. 19° [726]; $n_D^{25} = 1.5315$ [2679].

Oxime [99283-86-0] $C_{13}H_{19}NO_2$ mol. wt. 221.30

-Refer to: [2742, 3013, 3077].

GC [3013]; polarity of [3013].

BIOLOGICAL ACTIVITY: As lipoxygenase inhibitor [3077].

Oxime (*E*) $C_{13}H_{19}NO_2$ mol. wt. 221.30

MS [1921].

Phenylhydrazone $C_{19}H_{24}N_2O$ mol. wt. 296.41

m.p. 110–112° [726].

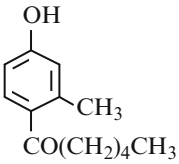
Methyl ether $C_{14}H_{20}O_2$ mol. wt. 220.31

-Preparation by reaction of caproyl chloride with 4-methylanisole in the presence of aluminium chloride in carbon disulfide (72 %) [515].

pale yellow oil [515]; b.p.$_{12}$ 176–179° [515].

1-(4-Hydroxy-2-methylphenyl)-1-hexanone

[132858-61-8] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses

-Obtained by reaction of caproic acid with m-cresol in the presence of polyphosphoric acid for 1 h at 80° (6 %) [2916].

-Also obtained by Fries rearrangement of 3-methylphenyl caproate with aluminium chloride in nitrobenzene at 25–30° for 48 h (4 %) [244].

-Also refer to: [1685].

m.p. 77–77.5° [2916], 76–76.5° [244], 72° [1685].

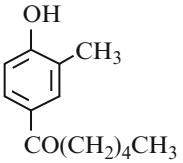
Phenyl ether [791615-78-6] $C_{19}H_{22}O_2$ mol. wt. 282.38

-Obtained by adding a mixture of m-phenoxytoluene and hexanoyl chloride to a suspension of aluminium chloride in methylene chloride at 0°, then the mixture stirred for 1.5–2 h at 3–5° (33 %) [2503].

b.p.$_{.3}$ 220–222° [2503]; ^{1}H NMR [2503], IR [2503], MS [2503].

1-(4-Hydroxy-3-methylphenyl)-1-hexanone

[132858-62-9] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses

-Obtained by Fries rearrangement of 2-methylphenyl caproate with aluminium chloride at 160° (25 %) [726] or 160–180° (20 %) [1644].

b.p.$_{.2}$ 180–182° [2679], b.p.$_{.15}$ 200–205° [726, 1916];

m.p. 79–80° [726, 2679].

Methyl ether [141036-68-2] $C_{14}H_{20}O_2$ mol. wt. 220.31

-Obtained by Friedel-Crafts acylation reaction of caproic anhydride with 2-methoxytoluene,

*using the combined catalyst system of $TiCl(OTf)_3$ and TfOH (97 %) [1483];

*in the presence of $SbCl_5$-$LiClO_4$ mixture in refluxing methylene chloride for 30 min (88 %) [2176].

-Also obtained by Friedel-Crafts acylation of 2-methylanisole in the presence of a Lewis acid catalyst while using carboxylic acid or trisubstituted-silyl carboxylate as acylating agent and carrying out the reaction in the presence of p-trifluoromethylbenzoic anhydride and, if necessary, a silver salt [2997].

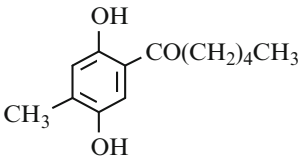
-Also refer to: [2172, 2999].

m.p. 34° [2999]; ^{1}H NMR [2999], ^{13}C NMR [2999], IR [2999].

Benzoate $C_{20}H_{22}O_3$ mol. wt. 310.39 m.p. 59–60° [726].

1-(2,5-Dihydroxy-4-methylphenyl)-1-hexanone

$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis

-Refer to: [1755].

Dimethyl ether [83893-24-7]

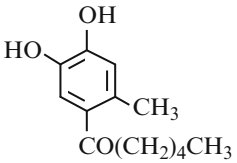
$C_{15}H_{22}O_3$ mol. wt. 250.34

-Prepared by Friedel-Crafts acylation (85 %) [1755].

b.p.$_{.3}$ 183° [1755]; ^{1}H NMR [1755], IR [1755].

1-(4,5-Dihydroxy-2-methylphenyl)-1-hexanone

$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Refer to: [305].

Dimethyl ether [3307-04-8]
$C_{15}H_{22}O_3$ mol. wt. 250.34
-Obtained by reaction of caproyl chloride with homoveratrole in the presence of aluminium chloride in carbon disulfide (73 %) [305].

-Also obtained by methylation of 1-(4,5-dihydroxy-2-methylphenyl)-1-hexanone [305].

b.p.$_{.8}$ 190° [305]; m.p. 48° [305].

Semicarbazone of the dimethyl ether [3787-68-6] $C_{16}H_{25}N_3O_3$ mol. wt. 307.39

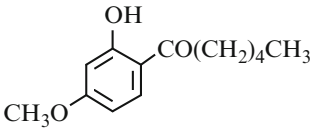
m.p. 128° [305].

Phenylhydrazone of the dimethyl ether [3307-23-1] $C_{21}H_{28}N_2O_2$ mol. wt. 340.47

m.p. 132° [305].

1-(2-Hydroxy-4-methoxyphenyl)-1-hexanone

[372486-19-6] $C_{13}H_{18}O_3$ mol. wt. 222.28



Syntheses
-Obtained by reaction of dimethyl sulfate with 2,4-dihydroxycaprophenone,
*in the presence of 20 % sodium hydroxide solution (72 %) [3160];

*in the presence of potassium carbonate in refluxing acetone for 4–6 h (85–90 %) [2501].

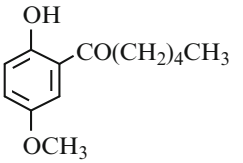
colourless oil [3160]; b.p.$_{12–13}$ 189–192° [3160].

Oxime [111625-07-1] $C_{13}H_{19}NO_3$ mol. wt. 237.30

GC [3012].

1-(2-Hydroxy-5-methoxyphenyl)-1-hexanone

$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Refer to: [285].

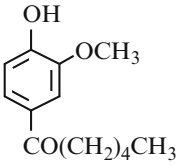
Oxime [140943-13-1]
$C_{13}H_{19}NO_3$ mol. wt. 237.30

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-(4-Hydroxy-3-methoxyphenyl)-1-hexanone

[114541-98-9] $C_{13}H_{18}O_3$ mol. wt. 222.28



Syntheses
-Obtained by refluxing a mixture (about 165°) of caproic acid, guaiacol and fused zinc chloride (Nencki reaction) [726].
-Also obtained by Fries rearrangement of 2-methoxyphenyl caproate with aluminium chloride [1990] in nitrobenzene (50 %) [726].

-Also obtained by adding DDQ to 1-(4-hydroxy-3-methoxyphenyl)-1-hexanol in benzene and the reaction mixture stirred for 4 h at r.t. [2989].
-Also refer to: [1427, 1429, 2075].

b.p.$_{15}$ 212–215° [726]; m.p. 60–62° [726], 53° [2989];
^{1}H NMR [2989].

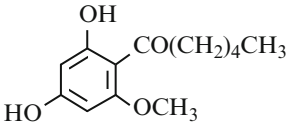
BIOLOGICAL ACTIVITY: Chloleretic [2989].

Benzoate $C_{20}H_{22}O_4$ mol. wt. 326.39

m.p. 54–55° [726].

1-(2,4-Dihydroxy-6-methoxyphenyl)-1-hexanone

[200878-64-4] $C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses
-Obtained by reaction of hexanonitrile with 3,5-dihydroxy-anisole in the presence of zinc chloride and hydrochloric acid (Hoesch reaction) [2012].

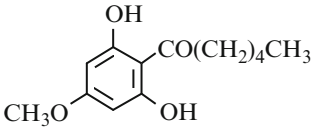
-Also refer to: [126–129].

m.p. 109° [126, 127];
^{1}H NMR [126, 127], MS [126, 127].

BIOLOGICAL ACTIVITY: Differentiation-inducing factor 1 (DIF-1) as protease-inhibitory and antiviral compound [129]; As cysteine protease activity modulator [128]; Picornavirus activity inhibitor [126]; 3C protease activity inhibitor [126]; Antiviral [126, 127]; Cytotoxicity [126].

1-(2,6-Dihydroxy-4-methoxyphenyl)-1-hexanone
(DMPH)

[142234-79-5] $C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses
-Obtained by reaction of hexanoyl chloride with 5-methoxyresorcinol in the presence of aluminium chloride in methylene chloride at r.t. for 3 h (58 %) [1129].
-Also obtained by reaction of hexanonitrile with 3,5-dihydroxyanisole in the presence of zinc chloride and hydrochloric acid (Hoesch reaction) [2012].

-Also refer to: [126–129, 1773, 2341, 3475].

m.p. 121° [126, 127];
^{1}H NMR [126, 127, 3475], ^{13}C NMR [3475], IR [3475], UV [3475], MS [126, 127, 3475]; GC-MS [1164].

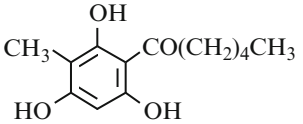
Isolation from natural sources

-From *Syzygium levinei* (Myrtaceae) [3475].
-From clove *Syzygium aromaticum* (Myrtaceae) [2108].
-Of *Populus tritis* bud exudate [955].
-In bud exudate of *Populus koreana*, *Populus maximowiczii* and *Populus suaveolens* (Salicaceae) [1164].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129]; Differentiation-inducing factor 1 (DIF-1) as protease-inhibitory and antiviral compound [129]; As cysteine protease activity modulator [128]; Caspase-3, inhibition of [127]; Picornavirus activity inhibitor [126]; 3C protease activity inhibitor [126]; Antiviral [126, 127]; Cytotoxicity [126].

1-(2,4,6-Trihydroxy-3-methylphenyl)-1-hexanone

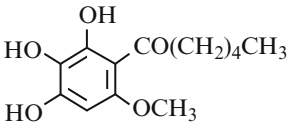
[101268-53-5] $C_{13}H_{18}O_4$ mol. wt. 238.28



Synthesis
-Obtained by reaction of capronitrile with methylphloroglucinol (Hoesch reaction) [1441].
-Also refer to: [1440].
m.p. 138–139° [1440, 1441].

1-(2,3,4-Trihydroxy-6-methoxyphenyl)-1-hexanone

[227946-82-9] $C_{13}H_{18}O_5$ mol. wt. 254.28

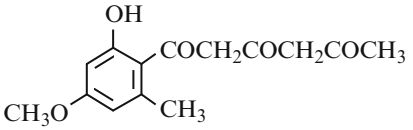


Synthesis
-Refer to: [128].

BIOLOGICAL ACTIVITY: As cysteine protease activity modulator [128].

1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1,3,5-hexanetrione

$C_{14}H_{16}O_5$ mol. wt. 264.28



Synthesis
-Obtained by hydrogenolysis of 1-(2-benzyloxy-4-methoxy-6-methylphenyl)-1,3,5-hexanetrione using a Pd-charcoal catalyst proceeded smoothly (93 %) [1259].

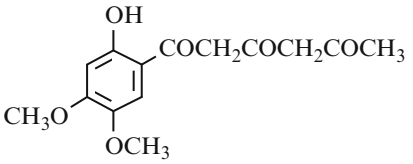
Benzyl ether [62643-39-4] $C_{21}H_{22}O_5$ mol. wt. 354.40

-Obtained by acylation of dilithioacetylacetone with methyl 2-*O*-benzyl-4-*O*-methylorsellinate for 15 h at 25° (74 %) [1259].

yellow crystals [1259]; m.p. 58.5–60.5° [1259];
^{1}H NMR [1259], IR [1259], UV [1259].

1-(2-Hydroxy-4,5-dimethoxyphenyl)-1,3,5-hexanetrione

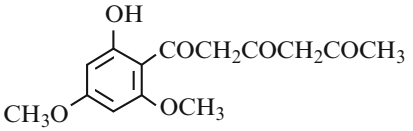
[856348-12-4] $C_{14}H_{16}O_6$ mol. wt. 280.28



Syntheses
-Refer to: [573, 834].
m.p. 100–102° [573].

1-(2,4-Dimethoxy-6-hydroxyphenyl)-1,3,5-hexanetrione

[76631-00-0] $C_{14}H_{16}O_6$ mol. wt. 280.28

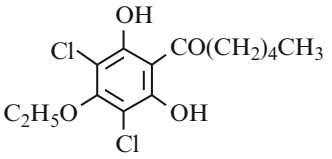


Synthesis
-Preparation by acylation of dianion of 2,4-pentanedione with methyl 2,4-dimethoxy-6-hydroxybenzoate (100 %) [2699].

apricot orange crystals [2699]; m.p. 95–98° [2699];
^{1}H NMR [2699], IR [2699], MS [2699].

1-(3,5-Dichloro-4-ethoxy-2,6-dihydroxyphenyl)-1-hexanone
(Et-DIF-1)

[861889-85-2] $C_{14}H_{18}Cl_2O_4$ mol. wt. 321.20



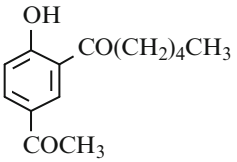
Syntheses
-Obtained by reaction of sulfuryl chloride (1.5 equiv.) with 4-ethoxy-2,6-dihydroxycaprophenone in a chloroform/ethanol mixture at r.t. [1129].
-Also refer to: [1772, 1773, 1777].

Yellow amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Et-DIF-1; Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(5-Acetyl-2-hydroxyphenyl)-1-hexanone

[92757-67-0] $C_{14}H_{18}O_3$ mol. wt. 234.30

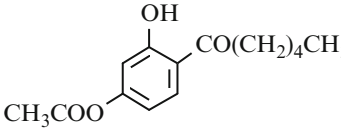


Syntheses
-Obtained by Fries rearrangement of p-(caproyloxy)-acetophenone with aluminium chloride (4 mol) without solvent at 150° for 3 h (37 %) [1305].
-Also obtained by Friedel-Crafts acylation of p-hydroxyacetophenone with caproyl chloride in the presence of aluminium chloride in tetrachloroethane at 130° for 4 h (39 %) [1305].

m.p. 52° [1305]; ^{1}H NMR [1305], IR [1305].

1-[4-(Acetyloxy)-2-hydroxyphenyl]-1-hexanone

[100972-54-1] $C_{14}H_{18}O_4$ mol. wt. 250.29

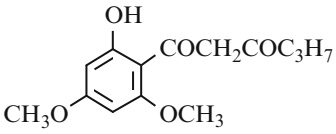


Syntheses
-Obtained by reaction of acetyl chloride with 2,4-dihydroxycaprophenone by heating on the water bath (76 %) [3160].
-Also refer to: [3008].

colourless oil [3160];
b.p.$_{14}$ 213–215° [3160]; m.p. 32.5–33.5° [3008].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-1,3-hexanedione

[60658-72-2] $C_{14}H_{18}O_5$ mol. wt. 266.29

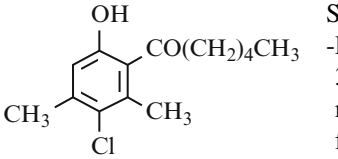


Synthesis
-Obtained by condensation of phloroacetophenone dimethyl ether with ethyl butyrate in the presence of sodium hydride for 0.25 h on the steam bath (92 %) [2602].

colourless needles [2602]; m.p. 104–105° [2602];
^{1}H NMR [2602], IR [2602], UV [2602].

1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-hexanone

[100792-79-8] $C_{14}H_{19}ClO_2$ mol. wt. 254.76



Synthesis
-Preparation by Fries rearrangement of 4-chloro-3,5-dimethylphenyl caproate with aluminium chloride in carbon disulfide at 80° for 2 h, then at 110° for 2 h after solvent elimination (86 %) [3114].

m.p. 80° [3114].

Semicarbazone [100952-80-5] $C_{15}H_{22}ClN_3O_2$ mol. wt. 311.81

m.p. 152° [3114].

Allyl ether [101598-23-6] $C_{17}H_{23}ClO_2$ mol. wt. 294.82

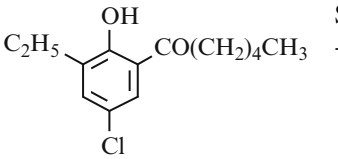
-Obtained by reaction of allyl bromide with the title ketone in the presence of potassium carbonate in refluxing acetone for 6 h (69 %) [3114].

b.p.$_{.2}$ 190° [3114].

USE: Insecticide [3114].

1-(5-Chloro-3-ethyl-2-hydroxyphenyl)-1-hexanone

[53347-28-7] $C_{14}H_{19}ClO_2$ mol. wt. 254.76



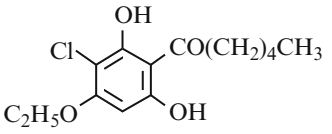
Synthesis
-Obtained by Fries rearrangement of 4-chloro-2-ethylphenyl caproate in the presence of aluminium chloride at 120° for 1.5 h (83 %) [2763].

b.p.$_{.0.2}$ 120–123.5° [2763]; $n_D^{20} = 1.5363$ [2763].

BIOLOGICAL ACTIVITY: Bacteriostatic [2763].

1-(3-Chloro-4-ethoxy-2,6-dihydroxyphenyl)-1-hexanone
(Et-DIF-3)

[861889-93-2] $C_{14}H_{19}ClO_4$ mol. wt. 286.76



Syntheses
-Obtained by reaction of sulfuryl chloride (1.5 equiv.) with 4-ethoxy-2,6-dihydroxycaprophenone in a chloroform/ethanol mixture at r.t. [1129].

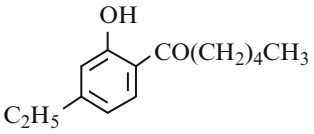
-Also refer to: [1772, 1773, 1777].

Colourless amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Et-DIF-3; Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(4-Ethyl-2-hydroxyphenyl)-1-hexanone

$C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses
-Obtained by Fries rearrangement of 3-ethylphenyl n-caproate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (88 %) [2801];
*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (87 %) [2801].

$b.p._{.18}$ 170° [2801].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 146° [2801].

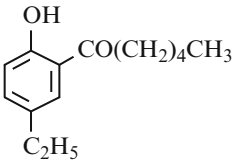
Methyl ether $C_{15}H_{22}O_2$ mol. wt. 234.34

-Obtained by reaction of dimethyl sulfate with 1-(4-ethyl-2-hydroxyphenyl)-1-hexanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (90 %) [2801].

$b.p._{.36}$ 165° [2801].

1-(5-Ethyl-2-hydroxyphenyl)-1-hexanone

$C_{14}H_{20}O_2$ mol. wt. 220.31



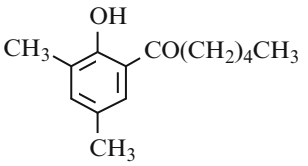
Synthesis
-Obtained by Fries rearrangement of 4-ethylphenyl caproate with aluminium chloride at 100° for 2 h (82 %) [2800].
b.p.$_{10}$ 162° [2800].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 178° [2800].

1-(2-Hydroxy-3,5-dimethylphenyl)-1-hexanone

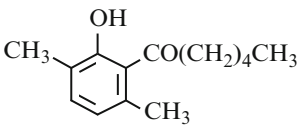
[107772-24-7] $C_{14}H_{20}O_2$ mol. wt. 220.31



Synthesis
-Refer to: [3466].
b.p.$_{12}$ 166–167° [3466].

1-(2-Hydroxy-3,6-dimethylphenyl)-1-hexanone

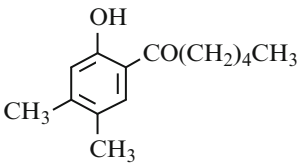
[107771-42-6] $C_{14}H_{20}O_2$ mol. wt. 220.31



Synthesis
-Refer to: [3466].
b.p.$_{12}$ 159–160° [3466].

1-(2-Hydroxy-4,5-dimethylphenyl)-1-hexanone

[856349-95-6] $C_{14}H_{20}O_2$ mol. wt. 220.31



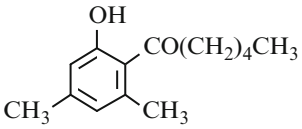
Synthesis
-Obtained by Fries rearrangement of 3,4-dimethylphenyl caproate with aluminium chloride at 110° without solvent (84 %) [3117].
b.p.$_4$ 180° [3117].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 197° [3117].

1-(2-Hydroxy-4,6-dimethylphenyl)-1-hexanone

$C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses

-Obtained by Fries rearrangement of 3,5-dimethylphenyl n-caproate (1 equiv.),

*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (83 %) [2801];

*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (75 %) [2801].

b.p.$_{20}$ 180° [2801].

Methyl ether $C_{15}H_{22}O_2$ mol. wt. 234.34

-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxy-4,6-dimethylphenyl)-1-hexanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (76 %) [2801].

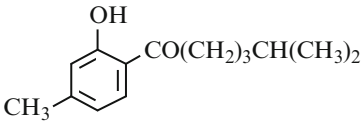
b.p.$_{56}$ 180° [2801].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 190° [2801].

1-(2-Hydroxy-4-methylphenyl)-5-methyl-1-hexanone

[88555-60-6] $C_{14}H_{20}O_2$ mol. wt. 220.31



Synthesis

-Obtained by reaction of isoheptanoyl chloride with m-cresol in the presence of aluminium chloride in nitrobenzene at 40° for 2.5 h [98].

^{1}H NMR [98], IR [98].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

-Refer to: [98].

m.p. 208–209° [98].

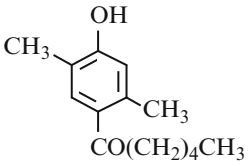
Methyl ether [88555-61-7] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Obtained by treatment of the title ketone with dimethyl sulfate in the presence of sodium hydroxide in refluxing ethanol for 3 h [98].

^{1}H NMR [98], IR [98].

1-(4-Hydroxy-2,5-dimethylphenyl)-1-hexanone

[95102-30-0] $C_{14}H_{20}O_2$ mol. wt. 220.31

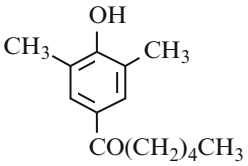


Syntheses
-Refer to: [1595, 2704, 3466].
m.p. 104.5–105.5° [3466].

USE: Colour developer for thermal recording materials [1595].

1-(4-Hydroxy-3,5-dimethylphenyl)-1-hexanone

[148516-07-8] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses
-Obtained by reaction of hexanoyl chloride with 2,6-dimethylphenol according to the method described previously [2871], (50 %) [119].
-Also refer to: [244, 3466].

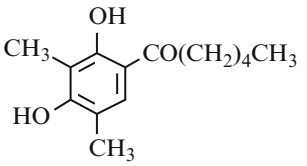
m.p. 108–109° [3466], 97.5–99° [119], 97–99° [244]; ^{1}H NMR [119], IR [119].

Methyl ether [104008-49-3] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Refer to: [3004].

1-(2,4-Dihydroxy-3,5-dimethylphenyl)-1-hexanone
(Tetrahydrosorbicillin)

[88924-67-8] $C_{14}H_{20}O_3$ mol. wt. 236.31



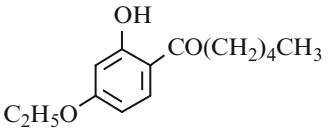
Syntheses
-Obtained by reaction of caproic acid with 3,5-dimethyl-resorcinol in the presence of boron trifluoride etherate at 120° for 1 h [2269].
-Also obtained by hydrogenation of sorbicillin (21 %) [3137].

-Also refer to: [743].

pale yellow crystals [2269];
m.p. 69–70° [743], 66–69° [3137], 66–68° [2269];
^{1}H NMR [2269, 3137], ^{13}C NMR [2269], IR [2269, 3137], UV [3137], MS [2269, 3137].

1-(4-Ethoxy-2-hydroxyphenyl)-1-hexanone

[19347-50-3] $C_{14}H_{20}O_3$ mol. wt. 236.31

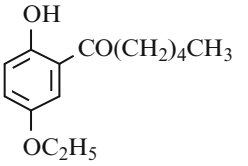


Synthesis
-Obtained by reaction of ethyl bromide with 4-caproyl-resorcinol in the presence of potassium hydroxide in ethanol for 2 h (68 %) [3473].

b.p.$_{0.5}$ 142–144° [3473].

1-(5-Ethoxy-2-hydroxyphenyl)-1-hexanone

[140943-32-4] $C_{14}H_{20}O_3$ mol. wt. 236.31

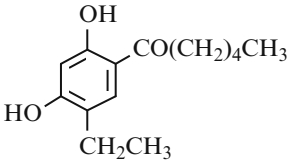


Synthesis
-Refer to: [285].

Oxime [140943-19-7]
$C_{14}H_{21}NO_3$ mol. wt. 251.33
-Refer to: [285].

1-(5-Ethyl-2,4-dihydroxyphenyl)-1-hexanone

[95102-17-3] $C_{14}H_{20}O_3$ mol. wt. 236.31

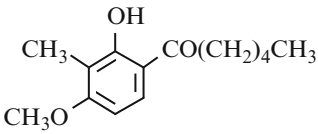


Syntheses
-Refer to: [2651, 2704].
b.p.$_{10}$ 220–225° [2651]; m.p. 93–94° [2651].

USE: Colour developer, for thermal recording materials [2704].

1-(2-Hydroxy-4-methoxy-3-methylphenyl)-1-hexanone

[647008-30-8] $C_{14}H_{20}O_3$ mol. wt. 236.31



Synthesis
-Refer to: [2492].

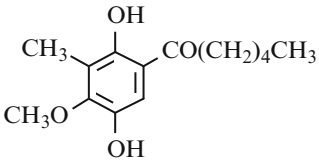
USE: Preparation of trichodimerol and related vertinoid polyketides [2492].

Acetate [647008-31-9] $C_{16}H_{22}O_4$ mol. wt. 278.35

USE: Preparation of trichodimerol and related vertinoid polyketides [2492].

1-(2,5-Dihydroxy-4-methoxy-3-methylphenyl)-1-hexanone

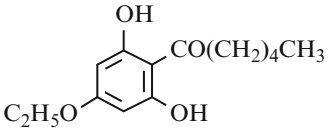
[647008-26-2] $C_{14}H_{20}O_4$ mol. wt. 252.31



Synthesis
-Refer to: [2492].

1-(4-Ethoxy-2,6-dihydroxyphenyl)-1-hexanone

[861889-80-7] $C_{14}H_{20}O_4$ mol. wt. 252.31

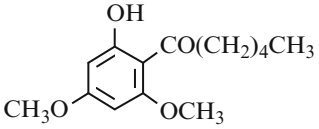


Synthesis
-Obtained by reaction of caproyl chloride with 5-ethoxy-resorcinol in the presence of aluminium chloride in methylene chloride at r.t. [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-hexanone

[1142936-17-1] $C_{14}H_{20}O_4$ mol. wt. 252.31

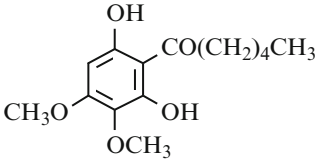


Synthesis
-Obtained by reaction of dimethyl sulfate with 1-(2,4,6-trihydroxyphenyl)-1-hexanone in the presence of potassium carbonate in acetone at 50–60° for 1.5 h under nitrogen (32 %) [2786].

m.p. 74–75° [2786];
^{1}H NMR [2786], ^{13}C NMR [2786], MS [2786].

1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-hexanone

[134081-94-0] $C_{14}H_{20}O_5$ mol. wt. 268.31



Synthesis
-Preparation by treatment of 1-[6-hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy) phenyl]-1-hexanone with potassium carbonate in refluxing methanol for 1–3 h (87 %) [1353].

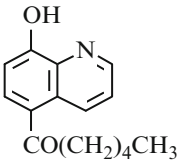
m.p. 96.5–97° [1353]; ^{1}H NMR [1353].

Dibenzyl ether $C_{28}H_{32}O_5$ mol. wt. 448.56

-Refer to: [1353].

1-(8-Hydroxy-5-quinolinyl)-1-hexanone

[246531-45-3] $C_{15}H_{17}NO_2$ mol. wt. 243.31



Synthesis
-Refer to: [1722].

Hydrochloride
$C_{15}H_{17}NO_2$, HCl mol. wt. 279.77

m.p. 172–174° [1725]; ^{1}H NMR [1725], IR [1725].

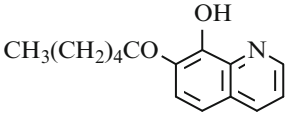
USE: Ion-flotation collector [1725].

Li salt [246531-44-2] $C_{15}H_{16}LiNO_2$ mol. wt. 249.24

-Refer to: [1722].

1-(8-Hydroxy-7-quinolinyl)-1-hexanone

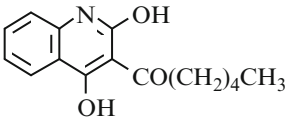
[246531-46-4] $C_{15}H_{17}NO_2$ mol. wt. 243.31



Synthesis
-Refer to: [1722].

1-(2,4-Dihydroxy-3-quinolinyl)-1-hexanone

[54289-79-1] $C_{15}H_{17}NO_3$ mol. wt. 259.30



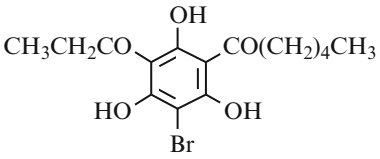
Synthesis
-Obtained by reaction of caproyl chloride with 2,4-dihydroxyquinoline in the presence of aluminium chloride in nitrobenzene on the steam bath for 3 h (12 %) [3123].

m.p. 183–184° [3123]; UV [3123].

BIOLOGICAL ACTIVITY: Antibacterial properties (Staphylococcus aureus and Escherichia coli) [3123].

1-[3-Bromo-5-(1-oxopropyl)-2,4,6-trihydroxyphenyl]-1-hexanone

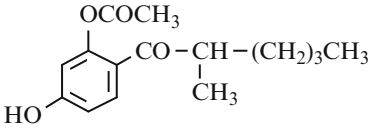
$C_{15}H_{19}BrO_5$ mol. wt. 359.22



Synthesis
-Obtained by acylating the phloroglucinol with appropriate acyl chloride or acid anhydride in the presence of boron trifluoride [3391].
m.p. 183° [3391].

1-[2-(Acetyloxy)-4-hydroxyphenyl]-2-methyl-1-hexanone (−)

[406174-72-9] $C_{15}H_{20}O_4$ mol. wt. 264.32

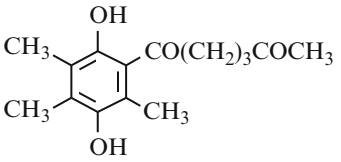


Synthesis
-Obtained by enzymatic enantioselective deacetylation of diester in the presence of PPL (54 %) [2829].

oil [2829];
^{1}H NMR [2829], ^{13}C NMR [2829], IR [2829], UV [2829],
MS [2829]; TLC [2829]; $(\alpha)_D^{25} = -41.6°$ (chloroform) [2829].

1-[2,5-Dihydroxy-3,4,6-trimethylphenyl]-1,5-hexanedione

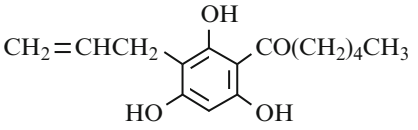
$C_{15}H_{20}O_4$ mol. wt. 264.32



Synthesis
-Refer to: [2642].
^{1}H NMR [2642], ^{13}C NMR [2642].

1-[2,4,6-Trihydroxy-3-(2-propenyl)phenyl]-1-hexanone
2-Caproyl-4-(propen-2-yl)phloroglucinol (**20**) [1026].

[74478-06-1] $C_{15}H_{20}O_4$ mol. wt. 264.32



Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and allyl chloride to a solution of phlorocaprophenone in ethyl ether at r.t., then to keep the mixturefor 12 h at this temperature [1026].

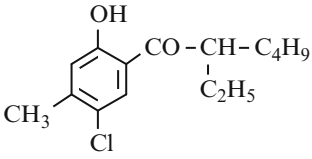
-Also obtained by reaction of allyl chloride with phlorovalerophenone in an alkaline two-phase (aqueous-ether) system and catalyzed by CuCl [838, 3193].
-Also refer to: [2111].

m.p. 118–120° [3193];
^{13}C NMR [1026, 3193], IR [1026].

BIOLOGICAL ACTIVITY: Bactericidal and fungicidal [1026, 3193]; Fungicide [2111].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-2-ethyl-1-hexanone

[57080-96-3] $C_{15}H_{21}ClO_2$ mol. wt. 268.78



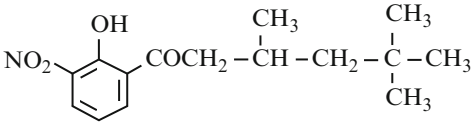
Synthesis
-Refer to: [1903].
b.p.$_{1-2}$ 150–160° [1903].

Oxime [57080-95-2] $C_{15}H_{22}ClNO_2$ mol. wt. 283.80

-Refer to: [1903].

1-(2-Hydroxy-3-nitrophenyl)-3,5,5-trimethyl-1-hexanone

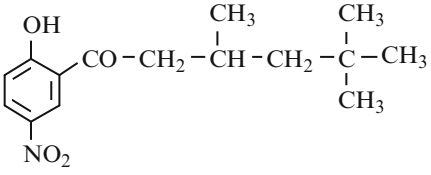
[176043-79-1] $C_{15}H_{21}NO_4$ mol. wt. 279.33



Synthesis
-Refer to: [628].

1-(2-Hydroxy-5-nitrophenyl)-3,5,5-trimethyl-1-hexanone

[154737-34-5] $C_{15}H_{21}NO_4$ mol. wt. 279.33

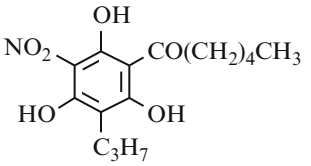


Syntheses
-Obtained by treatment of 1-(2-hydroxyphenyl)-3,5,5-trimethyl-1-hexanone with sodium nitrite in trifluoroacetic acid for 2 h at r.t. (45 %) [628].
-Refer to: [417].

m.p. 94–96° [628]; ^{1}H NMR [628].

1-(2,4,6-Trihydroxy-3-nitro-5-propylphenyl)-1-hexanone

[119692-02-3] $C_{15}H_{21}NO_6$ mol. wt. 311.33



Syntheses

-Obtained by adding a mixture of fuming nitric acid and acetic acid to the solution of 1-(2,4,6-trihydroxy-3-propyl-phenyl)-1-hexanone in acetic acid at 60° for 30 min (30–40 %) [3414].

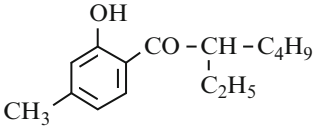
-Also refer to: [153].

m.p. 52–53° [3414]; ^{1}H NMR [3414], IR [3414], MS [3414].

BIOLOGICAL ACTIVITY: Germination inhibitory activity [3414]; PET inhibitory activity [3414]; Effect on gibberellin-inducible α-amylase synthesis in barley aleurone cells [153].

2-Ethyl-1-(2-hydroxy-4-methylphenyl)-1-hexanone

[57080-99-6] $C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis

-Refer to: [1903].

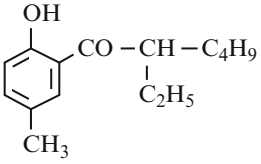
Oxime [57080-97-4]

$C_{15}H_{23}NO_2$ mol. wt. 249.35

-Refer to: [1903].

2-Ethyl-1-(2-hydroxy-5-methylphenyl)-1-hexanone

[74604-17-4] $C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis

-Obtained by Fries rearrangement of 4-methylphenyl 2-ethylhexanoate (b.p.$_{0.02}$ 90°) [2520].

b.p.$_{0.02}$ 90° [2520];

IR [2520], UV [2520].

Oxime [51528-15-5] $C_{15}H_{23}NO_2$ mol. wt. 249.35

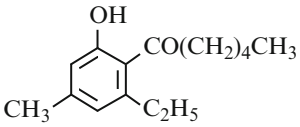
-Refer to: [2520, 3445].

crystals [2520]; m.p. 64–66° [2520];
IR [2520], UV [2520].

USE: Solvent extraction of copper (II) [2520].

1-(2-Ethyl-6-hydroxy-4-methylphenyl)-1-hexanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses

-Preparation by Fries rearrangement of 3-ethyl-5-methylphenyl caproate with aluminium chloride,
*without solvent at 130° for 2 h (82 %) [2802];
*in nitrobenzene at 25° for 6 h (83 %) [2802].

b.p.$_9$ 178° [2802].

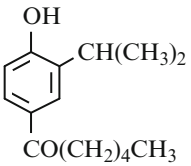
Methyl ether $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by methylation of the above ketone in the usual way (75 %) [2802].

b.p.$_{48}$ 215° [2802].

1-[4-Hydroxy-3-(1-methylethyl)phenyl]-1-hexanone

[95102-36-6] $C_{15}H_{22}O_2$ mol. wt. 234.34



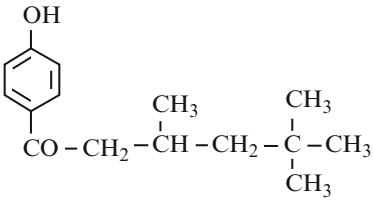
Syntheses

-Refer to: [1595, 2704].

USE: Colour developer for thermal recording materials [1595].

1-(4-Hydroxyphenyl)-3,5,5-trimethyl-1-hexanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis

-Refer to: [698].

Methyl ether

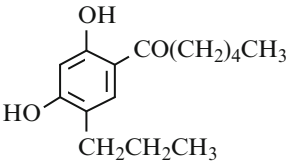
$C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by reaction of 4-chloroanisole with 3,5,5-trimethylhexanal (3,5,5-trimethylcaproaldehyde) in the presence of $Pd(dba)_2$ (2 mol%), Pd phosphine (6 mol%), 4 Å MS and pyrrolidine in DMA at 140° for 4 h (73 %) [698].

^{1}H NMR [698], ^{13}C NMR [698], IR [698], MS [698].

1-(2,4-Dihydroxy-5-propylphenyl)-1-hexanone

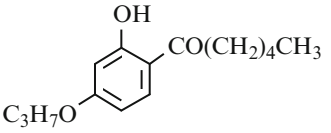
$C_{15}H_{22}O_3$ mol. wt. 250.34



Synthesis
-Refer to: [2651].
b.p.$_9$ 225–230° [2651]; m.p. 53° [2651].

1-(2-Hydroxy-4-propoxyphenyl)-1-hexanone

[92730-24-0] $C_{15}H_{22}O_3$ mol. wt. 250.34

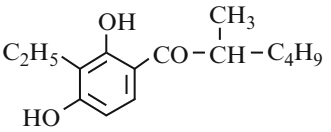


Synthesis
-Obtained by reaction of propyl bromide with 4-caproyl-resorcinol in the presence of potassium hydroxide in ethanol for 2 h (60 %) [3473].

b.p.$_2$ 169–171° [3473]; m.p. 28° [3473].

1-(3-Ethyl-2,4-dihydroxyphenyl)-2-methyl-1-hexanone

[820215-94-9] $C_{15}H_{22}O_3$ mol. wt. 250.34



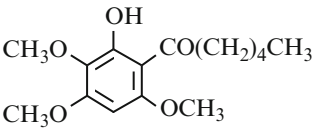
Isolation from natural sources
-From unidentified fungal strain CRM-51006 [2317].
-Novel strain MT90049 (KCTC 18043p), novel compound produced therefrom and use thereof [65].

^{1}H NMR [2317], ^{13}C NMR [2317].

BIOLOGICAL ACTIVITY: CRM-51006 as new phospholipase C inhibitor [65, 2317].

1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-hexanone

[134081-63-3] $C_{15}H_{22}O_5$ mol. wt. 282.34



Syntheses
-Obtained by partial selective demethylation of crude 2,3,4,6-tetramethoxyhexanophenone with aluminium chloride in acetonitrile at 50° for 1–2 h (80 %) [1353].
-Also refer to: [1351].

m.p. 62.5–64° [1353]; ^{1}H NMR [1353].

p-Toluenesulfonate [134081-78-0] $C_{22}H_{28}O_7S$ mol. wt. 436.53

-Obtained by reaction of p-toluenesulfonyl chloride with 2-hydroxy-3,4,6-trimethoxy-hexanophenone in the presence of potassium carbonate in refluxing acetone for 6–14 h (96 %) [1353].

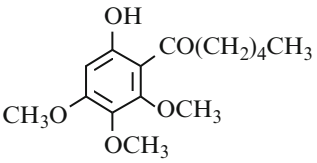
m.p. 91.5–92.5° [1353]; ^{1}H NMR [1353].

Methyl ether $C_{16}H_{24}O_5$ mol. wt. 296.36

-Obtained by reaction of caproyl chloride with 1,2,3,5-tetramethoxybenzene in the presence of aluminium chloride in ethyl ether at 0° for 30 min [1353].

1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-hexanone

[134081-70-2] $C_{15}H_{22}O_5$ mol. wt. 282.34



Syntheses

-Obtained by hydrogenation of (6-phenylmethoxy)-2,3,4-trimethoxycaprophenone over 10 % palladium on charcoal in ethyl acetate/methanol (1:1) until the uptake of hydrogen ceased (87 %) [1353].

-Also refer to: [1351].

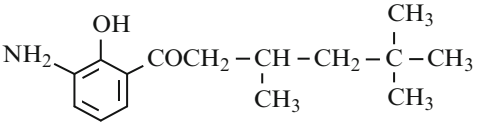
m.p. 46.5–48° [1353]; ^{1}H NMR [1353].

Benzyl ether $C_{22}H_{28}O_5$ mol. wt. 372.46

-Refer to: [1353].

1-(3-Amino-2-hydroxyphenyl)-3,5,5-trimethyl-1-hexanone

[176043-97-3] $C_{15}H_{23}NO_2$ mol. wt. 249.35

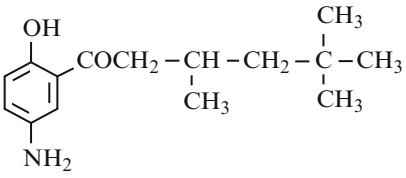


Synthesis

-Refer to: [628].

1-(5-Amino-2-hydroxyphenyl)-3,5,5-trimethyl-1-hexanone

[154737-35-6] $C_{15}H_{23}NO_2$ mol. wt. 249.35

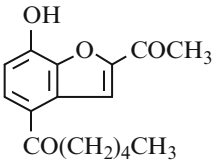


Syntheses

-Refer to: [417, 628].

1-(2-Acetyl-7-hydroxy-4-benzofuranyl)-1-hexanone

[59445-81-7] $C_{16}H_{18}O_4$ mol. wt. 274.32



Synthesis

-Obtained by treatment of its methyl ether with aluminium chloride (4 mol) in methylene chloride at r.t. for 24 h (85 %) [682].

m.p. 170° [682].

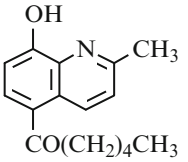
Methyl ether [59445-72-6] $C_{17}H_{20}O_4$ mol. wt. 288.34

-Obtained by reaction of caproyl chloride with 2-acetyl-7-methoxybenzofuran with aluminium chloride (2.4 mol) in methylene chloride at r.t. for 24 h (90 %) [682].

m.p. 101° [682].

1-(8-Hydroxy-2-methyl-5-quinolinyl)-1-hexanone

[217815-21-9] $C_{16}H_{19}NO_2$ mol. wt. 257.33



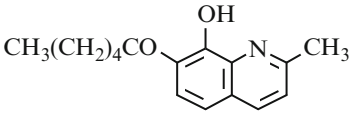
Synthesis

-Obtained by reaction of hexanoyl chloride with 8-hydroxyquinaldine in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

m.p. 60–62° [2261]; MS [2261].

1-(8-Hydroxy-2-methyl-7-quinolinyl)-1-hexanone

[217815-29-7] $C_{16}H_{19}NO_2$ mol. wt. 257.33



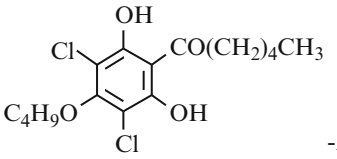
Synthesis

-Obtained by reaction of hexanoyl chloride with 8-hydroxyquinaldine in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

m.p. 56° [2261]; MS [2261].

1-(4-Butoxy-3,5-dichloro-2,6-dihydroxyphenyl)-1-hexanone
(Bu-DIF-1)

[861889-86-3] $C_{16}H_{22}Cl_2O_4$ mol. wt. 349.25



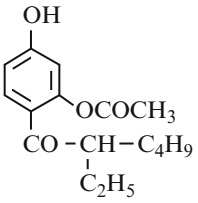
Syntheses
-Obtained by reaction of sulfuryl chloride (1.5 equiv.) with 4-butoxy-2,6-dihydroxycaprophenone in a chloroform/ethanol mixture at r.t. [1129].
-Also refer to: [1773, 1777].

Yellow amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: DIF-1(3 M); Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-[2-(Acetyloxy)-4-hydroxyphenyl]-2-ethyl-1-hexanone

[251463-60-2] $C_{16}H_{22}O_4$ mol. wt. 278.35

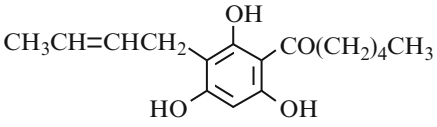


Synthesis
-Obtained by selective deacetylation of 2,4-diacetoxy-phenyl-1-ethylpentyl ketone mediated by porcine pancreatic lipase (PPL) in THF at 42–45° for 48 h in the presence of n-butanol (45 %) [2517].

viscous oil [2517]; $(\alpha)_D^{23} = -6.6°$ (chloroform) [2517];
^{1}H NMR [2517], ^{13}C NMR [2517], IR [2517], UV [2517], MS [2517].

1-[3-(2-Butenyl)-2,4,6-trihydroxyphenyl]-1-hexanone

[74478-07-2] $C_{16}H_{22}O_4$ mol. wt. 278.35

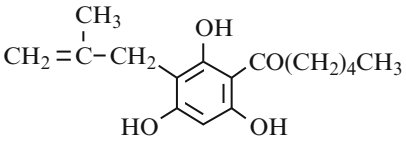


Synthesis
-Refer to: [2111].

BIOLOGICAL ACTIVITY: Fungicide [2111].

1-[2,4,6-Trihydroxy-3-(2-methyl-2-propenyl)phenyl]-1-hexanone

[74478-08-3] $C_{16}H_{22}O_4$ mol. wt. 278.35

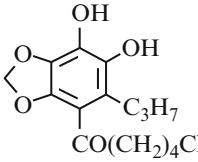


Synthesis
-Refer to: [2111].

USE: Fungicide [2111].

1-(6,7-Dihydroxy-5-propyl-1,3-benzodioxol-4-yl)-1-hexanone

$C_{16}H_{22}O_5$ mol. wt. 294.35



Synthesis
-Refer to: [2179].

Dimethyl ether [82652-26-4]
caproyl dihydrodillapiole
$C_{18}H_{26}O_5$ mol. wt. 322.40

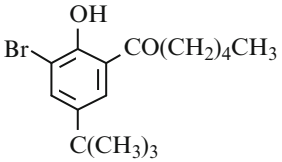
-Obtained by reaction of caproyl chloride with dihydrodillapiole in the presence of fused zinc chloride in methylene chloride for 3–4 h in an ice bath (70 %) [2179].

colourless solid [2179]; ^{1}H NMR [2179], IR [2179].

USE: Synergistic insecticidal activity of, with pyrethrum [2179].

1-[3-Bromo-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-hexanone

[101254-34-6] $C_{16}H_{23}BrO_2$ mol. wt. 327.26



Synthesis
-Preparation by Fries rearrangement of 2-bromo-4-tert-butylphenyl caproate in the presence of aluminium chloride at 110° for 2 h (68 %) [3113].
b.p.$_9$ 210° [3113].

2,4-Dinitrophenylhydrazone $C_{22}H_{27}BrN_4O_5$ mol. wt. 507.38

m.p. 136° [3113].

Allyl ether [108719-92-2] $C_{19}H_{27}BrO_2$ mol. wt. 367.33

-Obtained by reaction of allyl bromide with the title ketone in the presence of potassium carbonate in refluxing acetone for 8 h (76 %) [3113].

b.p.$_1$ 165° [3113].

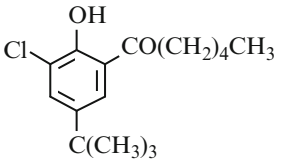
USE: Insecticide [3113].

2,4-Dinitrophenylhydrazone of the allyl ether $C_{25}H_{31}BrN_4O_5$ mol. wt. 547.75

m.p. 129° [3113].

1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-hexanone

[101254-66-4] $C_{16}H_{23}ClO_2$ mol. wt. 282.81



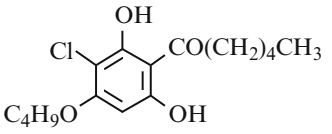
Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-tert-butylphenyl caproate with aluminium chloride at 110° (71 %) [3119].
b.p.$_{13}$ 163° [3119].

2,4-Dinitrophenylhydrazone [102475-97-8] $C_{22}H_{27}ClN_4O_5$ mol. wt. 462.93

m.p. 163° [3119].

1-(4-Butoxy-3-chloro-2,6-dihydroxyphenyl)-1-hexanone
(Bu-DIF-3)

[861889-94-3] $C_{16}H_{23}ClO_4$ mol. wt. 314.81



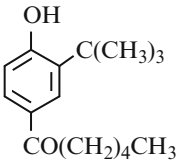
Syntheses
-Obtained by reaction of sulfuryl chloride (1.5 equiv.) with 4-butoxy-2,6-dihydroxycaprophenone in a chloroform/ethanol mixture at r.t. [1129].
-Also refer to: [1773, 1777].

Yellow amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Bu-DIF-3; Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-[4-Hydroxy-3-(1,1-dimethylethyl)phenyl]-1-hexanone

$C_{16}H_{24}O_2$ mol. wt. 248.37

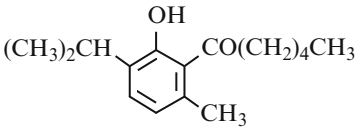


Synthesis
-Refer to: [2704] (Japanese patent).
m.p. 114° [2704].

USE: As colour developer [2704].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-hexanone

[856349-97-8] $C_{16}H_{24}O_2$ mol. wt. 248.37



Synthesis
-Obtained by Fries rearrangement of thymyl caproate with aluminium chloride at 120° (71 %) [2803].

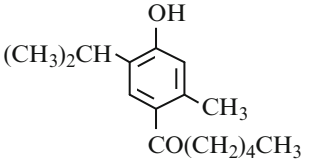
b.p.$_{38}$ 176° [2803].

2,4-Dinitrophenylhydrazone $C_{22}H_{28}N_4O_5$ mol. wt. 428.49

m.p. 188° [2803].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-hexanone

[95102-34-4] $C_{16}H_{24}O_2$ mol. wt. 248.37



Syntheses
-Obtained (**XXVI**) by treatment of 4-methoxy-2-methyl-5-isopropylcaprophenone (**VII**) with boiling pyridinium hydrochloride (205–215°) for 4.5 h (19 %) [2660].
-Also refer to: [2704] (Japanese patent).

b.p.$_{13}$ 220° [2660]; m.p. 103° [2660], 101° [2704].

USE: As colour developer [2704]; In preparation of thermographic recording material [1595].

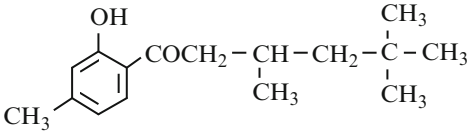
Methyl ether (**VII**) $C_{17}H_{26}O_2$ mol. wt. 262.39

-Obtained by reaction of caproyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (70 %) [2660].

b.p.$_{16}$ 196–198° [2660]; $n_D^{22.5} = 1.5205$ [2660].

1-(2-Hydroxy-4-methylphenyl)-3,5,5-trimethyl-1-hexanone

[52122-73-3] $C_{16}H_{24}O_2$ mol. wt. 248.37



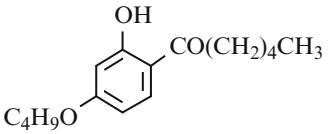
Syntheses
-Refer to: [108, 109].

Oxime [52122-64-2]
$C_{16}H_{25}NO_2$ mol. wt. 263.38

USE: In copper extraction from aqueous solutions [108]; Chelation with, of metals, [109].

1-(4-Butoxy-2-hydroxyphenyl)-1-hexanone

[19347-51-4] $C_{16}H_{24}O_3$ mol. wt. 264.36

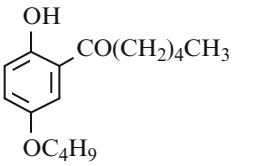


Syntheses
-Obtained by reaction of butyl bromide with 4-caproyl-resorcinol in the presence of potassium hydroxide in ethanol for 2 h (53 %) [3473].
-Also refer to: [1824, 1825].

b.p.$_2$ 176–180° [3473].

1-(5-Butoxy-2-hydroxyphenyl)-1-hexanone

[140943-37-9] $C_{16}H_{24}O_3$ mol. wt. 264.36



Synthesis
-Refer to: [285].

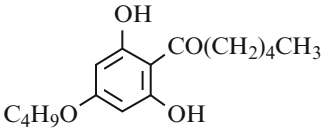
Oxime [140943-23-3]
$C_{16}H_{25}NO_3$ mol. wt. 279.38

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-(4-Butoxy-2,6-dihydroxyphenyl)-1-hexanone

[861889-81-8] $C_{16}H_{24}O_4$ mol. wt. 280.36

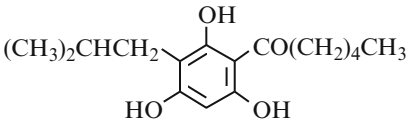


Synthesis
-Preparation by reaction of caproyl chloride with phloroglucinol monobutyl ether in the presence of aluminium chloride in methylene chloride at r.t. [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-[2,4,6-Trihydroxy-3-(2-methylpropyl)phenyl]-1-hexanone

[66711-56-6] $C_{16}H_{24}O_4$ mol. wt. 280.36

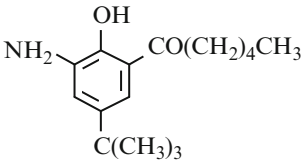


Synthesis
-Refer to: [2719].

BIOLOGICAL ACTIVITY: Fungicide [2719].

1-[3-Amino-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-hexanone

[85052-50-2] $C_{16}H_{25}NO_2$ mol. wt. 263.38

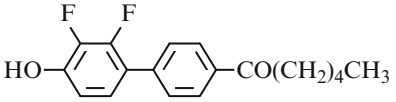


Synthesis
-Refer to: [2105].

Hydrochloride [85052-49-9]
$C_{16}H_{25}NO_2$, HCl mol. wt. 299.84
-Refer to: [2105].

1-(2′,3′-Difluoro-4′-hydroxy[1,1′-biphenyl]-4-yl)-1-hexanone

$C_{17}H_{18}F_2O_2$ mol. wt. 204.34



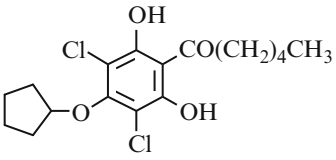
Synthesis
-Refer to: [2578].

Octyl ether [126163-53-9]
$C_{26}H_{34}F_2O_2$ mol. wt. 416.55

USE: Preparation of, for liquid-crystal media [2578].

1-[3,5-Dichloro-4-(cyclopentyloxy)-2,6-dihydroxyphenyl]-1-hexanone
(CP-DIF-1)

[861889-87-4] $C_{17}H_{22}Cl_2O_4$ mol. wt. 361.26



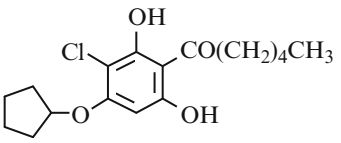
Syntheses
-Obtained by reaction of sulfuryl chloride (1.5 equiv.) with 4-cyclopentyloxy-2,6-dihydroxycaprophenone in a chloroform/ethanol mixture at r.t. [1129].
-Also refer to: [1773, 1777].

Yellow amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: CP-DIF-1; Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-[3-Chloro-4-(cyclopentyloxy)-2,6-dihydroxyphenyl]-1-hexanone
(CP-DIF-3)

[861889-95-4] $C_{17}H_{23}ClO_4$ mol. wt. 326.82



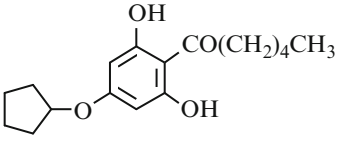
Syntheses
-Obtained by reaction of sulfuryl chloride (1.5 equiv.) with 4-cyclopentyloxy-2,6-dihydroxycaprophenone in a chloroform/ethanol mixture at r.t. [1129].
-Also refer to: [1773, 1777].

Yellow amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: CP-DIF-3; Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-[4-(Cyclopentyloxy)-2,6-dihydroxyphenyl]-1-hexanone

[861889-82-9] $C_{17}H_{24}O_4$ mol. wt. 292.37

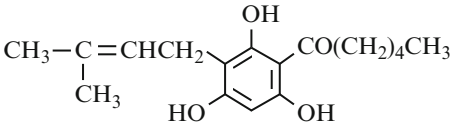


Synthesis
-Preparation by reaction of caproyl chloride with phloroglucinol monocyclopentyl ether in the presence of aluminium chloride in methylene chloride at r.t. [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-hexanone
2-Caproyl-4-(3-methylbuten-2-yl)phloroglucinol (**5**)

[69916-10-5] $C_{17}H_{24}O_4$ mol. wt. 292.37



Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and prenyl bromide to a solution of phlorocaprophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

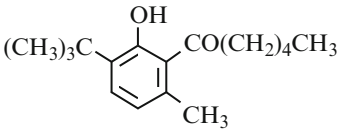
-Also prepared by adding prenyl bromide to a suspension of the sodium salt of phlorocaprophenone in benzene, then the mixture obtained was refluxed for 3 h [1026].
-Also obtained by reaction of prenyl chloride with phlorovalerophenone in an alkaline two-phase (aqueous-ether) system and catalyzed by CuCl [838, 3193].
-Also prepared by adding at 5° a solution of sodium methoxide in methanol, followed by isopentenyl bromide in ethyl ether to a solution of phlorocaprophenone in benzene and ethyl ether, then the mixture was stirred at r.t. for 6 h (15 %) [2113].

m.p. 135° [2113], 122–123° [3193].
N.B.: One of the reported melting point is obviously wrong.
^{13}C NMR [1026, 3193], IR [1026].

BIOLOGICAL ACTIVITY: Antifungal [2113]; Bactericidal and fungicidal [1026, 3193].

1-[3-(1,1-Dimethylethyl)-2-hydroxy-6-methylphenyl]-1-hexanone

$C_{17}H_{26}O_2$ mol. wt. 262.39



Syntheses
-Obtained by Fries rearrangement of 2-tert-butyl-5-methylphenyl caproate,
*in the presence of aluminium chloride (1.5 equiv.) in nitrobenzene at 25° for 6 h (81 %) [3118];

*in the presence of aluminium chloride (3 equiv.) at 110° for 2 h (78 %) [3118].

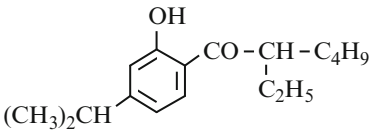
b.p.$_{.8}$ 146° [3118].

2,4-Dinitrophenylhydrazone $C_{23}H_{30}N_4O_5$ mol. wt. 442.52

m.p. 197° [3118].

2-Ethyl-1-[2-hydroxy-4-(1-methylethyl)phenyl]-1-hexanone

[57080-92-9] $C_{17}H_{26}O_2$ mol. wt. 262.39



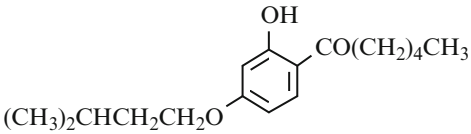
Synthesis
-Refer to: [1903].

Oxime [57080-91-8]
$C_{17}H_{27}NO_2$ mol. wt. 277.41

-Refer to: [1903].

1-[2-Hydroxy-4-(isopentyloxy)phenyl]-1-hexanone

[93542-41-7] $C_{17}H_{26}O_3$ mol. wt. 278.39

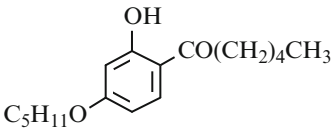


Synthesis
-Obtained by reaction of *iso*-amyl bromide with 4-caproylresorcinol in the presence of potassium hydroxide in ethanol for 2 h (53 %) [3473].

b.p.$_{0.5}$ 161–162° [3473]; m.p. 36–37° [3473]; IR [3473].

1-[2-Hydroxy-4-(pentyloxy)phenyl]-1-hexanone

[101002-32-8] $C_{17}H_{26}O_3$ mol. wt. 278.39



Synthesis
-Obtained by reaction of pentyl bromide with 2,4-dihydroxycaprophenone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 41–42° [284].

Oxime [101002-19-1] $C_{17}H_{27}NO_3$ mol. wt. 293.41

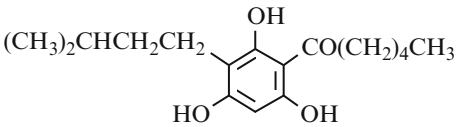
-Obtained by reaction of hydroxylamine hydrochloride with 1-[2-hydroxy-4-(pentyloxy)phenyl]-1-hexanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].
-Also refer to: [2742].

m.p. 80° [284, 3077]; ^{1}H NMR [284].

BIOLOGICAL ACTIVITY: Topical preparations comprising at least one aryloxime and bisabolol [483]; As lipoxygenase inhibitor [3077].

1-[2,4,6-Trihydroxy-3-(3-methylbutyl)phenyl]-1-hexanone

[74478-05-0] $C_{17}H_{26}O_4$ mol. wt. 294.39



Syntheses
-Preparation by hydrogenation of 2,4,6-trihydroxy-3-(3-methyl-2-butenyl)-isovalerophenone in the presence of PtO_2 in methanol under an hydrogen atmosphere at r.t. for 1 h (82 %) [2113].

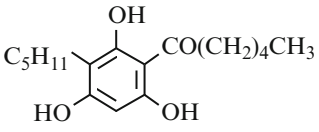
-Also refer to: [2111].

m.p. 159° [2113].

BIOLOGICAL ACTIVITY: Antifungal [2111, 2113].

1-(2,4,6-Trihydroxy-3-pentylphenyl)-1-hexanone

[74478-04-9] $C_{17}H_{26}O_4$ mol. wt. 294.39



Syntheses

-Obtained by adding a solution of hexanoyl chloride in nitrobenzene to a suspension, of 2,4,6-trihydroxy-pentylbenzene and aluminium chloride in carbon disulfide at r.t., then stirring the mixture for 6 h at 30–35° (55 %) [2113].

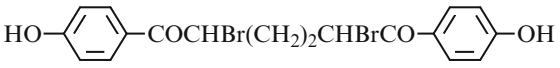
-Also refer to: [2111].

m.p. 124° [2113].

BIOLOGICAL ACTIVITY: Antifungal [2111, 2113].

1,6-Bis(4-hydroxyphenyl)-2,5-dibromo-1,6-hexanedione

$C_{18}H_{16}Br_2O_4$ mol. wt. 456.13



Synthesis

-Refer to: [1073].

Dimethyl ether [71248-64-1] 1,4-dibromo-1,4-dianisoylbutane (**XI**)

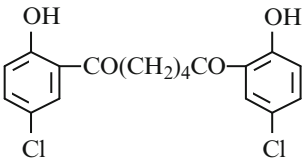
$C_{20}H_{20}Br_2O_4$ mol. wt. 484.18

-Obtained by reaction of bromine with 1,6-bis(4-methoxyphenyl)-1,6-hexanedione in hot carbon tetrachloride (67–90 %) [1073].

m.p. 158–169° (d) [1073].

1,6-Bis-(5-chloro-2-hydroxyphenyl)-1,6-hexanedione

[101735-99-3] $C_{18}H_{16}Cl_2O_4$ mol. wt. 367.23



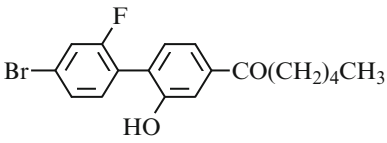
Synthesis

-Obtained by Fries rearrangement of bis-4-chlorophenyl adipate with aluminium chloride at 150° for 1 h (36 %) [3235].

m.p. 196.5° [3235].

1-(4′-Bromo-2′-fluoro[1,1′-biphenyl]-4-yl)-2-hydroxy-1-hexanone

[792709-04-7] $C_{18}H_{18}BrFO_2$ mol. wt. 365.24

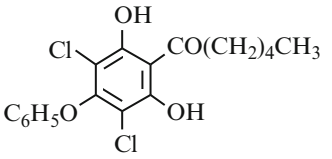


Synthesis

-Refer to: [2553].

1-(3,5-Dichloro-2,6-dihydroxy-4-phenoxyphenyl)-1-hexanone
(Ph-DIF-1)

[861889-73-8] $C_{18}H_{18}Cl_2O_4$ mol. wt. 369.24



Syntheses
-Preparation by adding triphenylbismuth diacetate and copper powder to a solution of 3,5-dichloro-2,4,6-trihydroxyhexanophenone in methylene chloride at r.t. (41 %) [1129].
-Also refer to: [1772, 1773, 1777].

Yellow amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Ph-DIF-1; Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

6-(4-Hydroxyphenyl)-1-phenyl-1,6-hexanedione

$C_{18}H_{18}O_3$ mol. wt. 282.33

Synthesis
-Refer to: [3247].

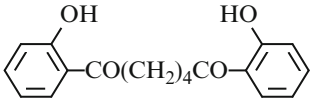
Methyl ether [51067-61-9] $C_{19}H_{20}O_3$ mol. wt. 296.36

-Refer to: [3247 (30 %), 3249].

off-white solid [3247]; m.p. 111–112.5° [3247];
^{1}H NMR [3247], ^{13}C NMR [3247], IR [3247], MS [3247];
phosphorescence spectroscopy [3249].

1,6-Bis(2-hydroxyphenyl)-1,6-hexanedione

[109471-10-5] $C_{18}H_{18}O_4$ mol. wt. 298.34



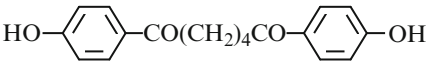
Syntheses
-Obtained by Fries rearrangement of phenyl adipate with aluminium chloride,
-in the presence of solvents:

*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];
*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].

m.p. 160–161° [902].

1,6-Bis(4-hydroxyphenyl)-1,6-hexanedione

[20837-37-0] $C_{18}H_{18}O_4$ mol. wt. 298.34



Syntheses

-Obtained by Fries rearrangement of phenyl adipate with aluminium chloride,

-in the presence of solvents:
*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];
*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].
-Also refer to: [470, 471, 1148, 1176, 2530].

m.p. 240–242° [902], 237–240° [1148].

Diacetate [114399-84-7] $C_{22}H_{22}O_6$ mol. wt. 382.41

-Obtained by reaction of acetic anhydride with 1,6-bis(4-hydroxyphenyl)-1,6-hexanedione [902].

m.p. 142° [902].

Dimethyl ether [4280-49-3] $C_{20}H_{22}O_4$ mol. wt. 326.39

-Obtained by reaction of dimethyl sulfate with 1,6-bis(4-hydroxyphenyl)-1,6-hexanedione in the presence of 2 N sodium hydroxide [902].
-Also obtained by reaction of adipic acid dichloride with anisole in the presence of aluminium chloride, (60 %) [210],
*in carbon disulfide at a temperature $< 60°$ [1073];
*in nitrobenzene/tetrachloroethane mixture (1:2) at 0° (55 %) [593];
*in dichloromethane at 0° for 4 h (93 %) [1724];
*without solvent at $< 40°$ (75 %) [905].
-Also obtained by reaction of adipic anhydride with anisole in the presence of aluminium chloride in refluxing carbon disulfide for 3 h (14 %) [2494].
-Also obtained by adding dropwise adiponitrile over 30 min to an ether solution of the Grignard reagent prepared from p-bromoanisole and magnesium. Then, the solution was refluxed for 4 h (74 %) [3247].
-Also refer to: [41, 348, 681 (35 %), 843, 1014 (55 %), 1148, 1688, 1833, 2168, 2519, 2577, 2596 (85 %), 3197].

colourless prisms [2494];
m.p. 147–149° [2577], 147° [902], 146–147° [1148], 145–146° [2596], 145° [593], 144.5–145.5° [210], 144–146° [1014], 144–145° [843, 905], 144° [2494], 142° [681], 141.5–142.5° [1073, 3247], 140–142° [2519], 140° [3197], 137–138° [1724], 136° [1688];
^{1}H NMR [348, 681, 1724, 3247],
^{13}C NMR [681, 3247], IR [681, 843, 1724, 3247], UV [3247], MS [681, 3247].

Dihydrazone of the dimethyl ether $C_{20}H_{26}N_4O_2$ mol. wt. 354.45

m.p. 109–111° [905].

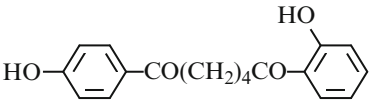
Diethyl ether [88167-05-9] $C_{22}H_{26}O_4$ mol. wt. 354.45

-Refer to: [41, 2467, 2494, 3197].

colourless plates [2494]; m.p. 131–132° [3197], 127° [2494].

1-(2-Hydroxyphenyl)-6-(4-hydroxyphenyl)-1,6-hexanedione

[101790-34-5] $C_{18}H_{18}O_4$ mol. wt. 298.34



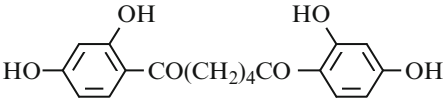
Syntheses
-Obtained by Fries rearrangement of phenyl adipate with aluminium chloride,
-in the presence of solvents:

*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];
*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].

m.p. 190–192° [902].

1,6-Bis(2,4-dihydroxyphenyl)-1,6-hexanedione

[19343-47-6] $C_{18}H_{18}O_6$ mol. wt. 330.34



Syntheses
-Obtained by adding resorcinol into adiponitrile and hydrogen chloride in ethyl ether in the presence of zinc chloride.

Then, the diketimine dichlorhydrate obtained was hydrolyzed by boiling water (40 %) [2674].
-Also refer to: [1735, 2504, 3374].

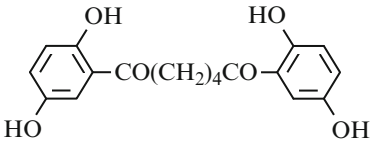
m.p. 285–286° [3374], 285° (d) [2504, 2674]; UV [2504].

Di-2,4-Dinitrophenylhydrazone [115963-79-6] $C_{30}H_{26}N_8O_{12}$ mol. wt. 690.58

m.p. 360° [2674].

1,6-Bis(2,5-dihydroxyphenyl)-1,6-hexanedione

[91453-26-8] $C_{18}H_{18}O_6$ mol. wt. 330.34



Syntheses

-Obtained by treatment of 1,6-bis(2-hydroxy-5-methoxyphenyl)-1,6-hexanedione with boron tribromide in methylene chloride (85 %) [2103].

-Also refer to: [2331].

yellow solid [411]; m.p. 236–238° [2103].

Tetramethyl ether [10365-23-8] $C_{22}H_{26}O_6$ mol. wt. 386.45

-Obtained by reaction of adipic acid with hydroquinone dimethyl ether in the presence of thionyl chloride (32 %) [2331].

-Also obtained by reaction of adipic acid dichloride (1 mol) with hydroquinone dimethyl ether (2.5 mol) in the presence of aluminium chloride (1 mol) (65 %) [1575].

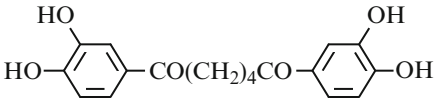
-Also obtained by reaction of adipic acid dichloride with hydroquinone dimethyl ether in the presence of aluminium chloride in carbon disulfide or methylene chloride (53–56 %).

-Also refer to: [1575, 3175] (5 %).

needles [2331]; white needles [3175];
m.p. 112–113° [3175], 110° [1575], 105–106° [2331].

1,6-Bis(3,4-dihydroxyphenyl)-1,6-hexanedione

$C_{18}H_{18}O_6$ mol. wt. 330.34



Synthesis

-Refer to: [3061].

Tetramethyl ether [50766-16-0]

$C_{22}H_{26}O_6$ mol. wt. 386.45

-Obtained by hydrogenating 1-veratroyl-4-(3,4-dimethoxy-6-bromophenyl)butane with Raney Nickel and KOH in ethanol at 12 atm. and 63° (90 %) [3061].

-Also obtained by hydrogenating its oxime in acetic acid, in the presence of 10 % Pd/C in a Parr apparatus at r.t. and 45–50 psig for 12–36 h (68 %) [1014].

-Obtained by reaction of adipyl chloride with veratrole in the presence of aluminium chloride in carbon disulfide first at 0°, then at reflux for 3 h [1124].

-Also refer to: [1013, 2342, 3364 (70 %)].

m.p. 149–150° [1014, 1124];
^{1}H NMR [2342], ^{13}C NMR [2342], IR [3364].

Dioxime of the tetramethyl ether [50766-28-4] $C_{22}H_{28}N_2O_6$ mol. wt. 416.47

-Refer to: [1012, 1014].

m.p. 154° [1012], 151–153° [1014].

Tetraethyl ether [50766-18-2] $C_{26}H_{34}O_6$ mol. wt. 442.55

-Obtained by hydrogenating its oxime in acetic acid, in the presence of 10 % Pd/C in a Parr apparatus at r.t. and 45–50 psig for 12–36 h (39 %) [1014].
-Also refer to: [1012].

m.p. 135–138° [1012], 132–134° [1014].

Dioxime of the tetraethyl ether [50766-34-2] $C_{26}H_{36}N_2O_6$ mol. wt. 472.58

m.p. 135–139° [1014].

Tetrapropyl ether [50766-19-3] $C_{30}H_{42}O_6$ mol. wt. 498.66

-Obtained by hydrogenating its oxime in acetic acid, in the presence of 10 % Pd/C in a Parr apparatus at r.t. and 45–50 psig for 12–36 h (48 %) [1014].
-Also refer to: [1012].

m.p. 147–149° [1012], 144–146° [1014].

Dioxime of the tetrapropyl ether [50766-35-3] $C_{30}H_{44}N_2O_6$ mol. wt. 528.69

m.p. 142–143° [1014].

Tetrabutyl ether [50766-20-6] $C_{34}H_{50}O_6$ mol. wt. 554.77

-Obtained by hydrogenating its oxime in acetic acid, in the presence of 10 % Pd/C in a Parr apparatus at r.t. and 45–50 psig for 12–36 h (61 %) [1014].
-Also refer to: [1012].

m.p. 126–128° [1012], 123–125° [1014].

Dioxime of the tetrabutyl ether [50766-36-4] $C_{34}H_{52}N_2O_6$ mol. wt. 584.80

m.p. 123–124° [1014].

Dimethylenedioxy [6268-56-0] $C_{20}H_{18}O_6$ mol. wt. 354.36

1,6-Bis(3,4-methylenedioxyphenyl)-1,6-hexanedione

-Obtained by adding 1,6-bis(3,4-methylenedioxyphenyl)-1,6-hexanediol to a suspension of chromium (VI) oxide in pyridine and Celite at r.t. under an argon atmosphere. After the mixture was stirred for 8 h at r.t. (77 %) [1132].
-Also refer to: [1014, 2693 (38 %)].

m.p. 179.4–180.4° [2693], 179–180° [1014];
^{1}H NMR [1132], IR [1132].

Di-2,4-dinitrophenylhydrazone of the dimethylenedioxy $C_{32}H_{26}N_8O_{12}$ mol. wt. 714.61

m.p. 316–317° (d) [2693].

Dimethyloxime of the dimethylenedioxy [50766-33-1] $C_{22}H_{24}N_2O_6$ mol. wt. 412.44

m.p. 117–121° [1014].

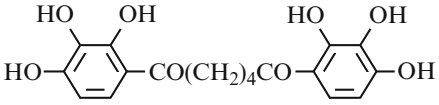
1,6-Bis(3,5-dihydroxyphenyl)-1,6-hexanedione

$C_{18}H_{18}O_6$ mol. wt. 330.34

Synthesis
-Refer to: [1316].
m.p. 251–255° [1316].

1,6-Bis(2,3,4-trihydroxyphenyl)-1,6-hexanedione

$C_{18}H_{18}O_8$ mol. wt. 362.33



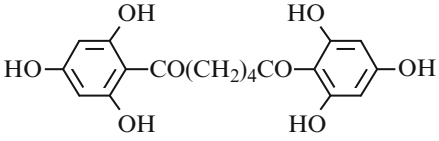
Synthesis
-Refer to: [1575].
Hexamethyl ether [10373-31-6]
$C_{24}H_{30}O_8$ mol. wt. 446.50

-Obtained by reaction of dimethyl sulfate with 1,6-bis(2-hydroxy-3,4-dimethoxyphenyl)-1,6-hexanedione in the presence of 30 % sodium hydroxide (65–90 %) [1574].
-Also refer to: [1575].

m.p. 116° [1574, 1575].

1,6-Bis(2,4,6-trihydroxyphenyl)-1,6-hexanedione

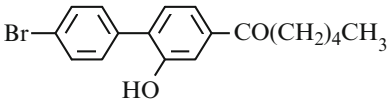
[19343-46-5] $C_{18}H_{18}O_8$ mol. wt. 362.33



Syntheses
-Refer to: [2673, 3374].
m.p. 290° [2673], 265° [3374];
IR [2673].

1-(4′-Bromo[1,1′-biphenyl]-4-yl)-2-hydroxy-1-hexanone

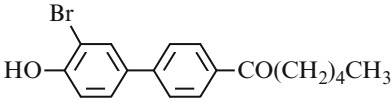
[792708-89-5] $C_{18}H_{19}BrO_2$ mol. wt. 347.25



Synthesis
-Refer to: [2553].

1-(3′-Bromo-4′-hydroxy[1,1′-biphenyl]-4-yl)-1-hexanone

$C_{18}H_{19}BrO_2$ mol. wt. 347.25

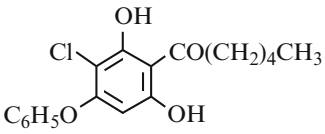


Synthesis
-Refer to: [2993].
Methyl ether [83258-17-7]
$C_{19}H_{21}BrO_2$ mol. wt. 361.27

-Refer to: [2993].

1-(3-Chloro-2,6-dihydroxy-4-phenoxyphenyl)-1-hexanone
(Ph-DIF-3)

[861889-74-9] $C_{18}H_{19}ClO_4$ mol. wt. 334.80



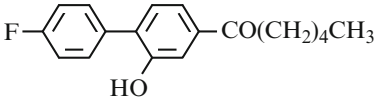
Syntheses
-Preparation by adding triphenylbismuth diacetate and copper powder to a solution of 3-chloro-2,4,6-trihydroxy-hexanophenone in methylene chloride at r.t. [1129].
-Also refer to: [1772, 1773, 1777].

colourless amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Ph-DIF-3; Dictyostelium differentiation-inducing factor-1 derivs. promotion of glucose consumption in mammalian cells [1777]; DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(4′-Fluoro[1,1′-biphenyl]-4-yl)-2-hydroxy-1-hexanone

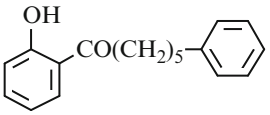
[792708-75-9] $C_{18}H_{19}FO_2$ mol. wt. 286.35



Synthesis
-Refer to: [2553].

1-(2-Hydroxyphenyl)-5-phenyl-1-hexanone

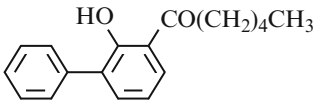
[1396756-63-0] $C_{18}H_{20}O_2$ mol. wt. 268.36



Synthesis
-Refer to: [3242].
^{1}H NMR [3242], ^{13}C NMR [3242], MS [3242].

1-[1,1′-Biphenyl]-3-yl-2-hydroxy-1-hexanone

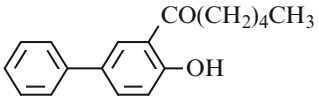
$C_{18}H_{20}O_2$ mol. wt. 268.36



Synthesis
-Obtained (by-product) by Fries rearrangement of 2-hydroxydiphenyl caproate with aluminium chloride at 160° for 30–45 min (7 %) [1256].

1-[1,1′-Biphenyl]-3-yl-4-hydroxy-1-hexanone

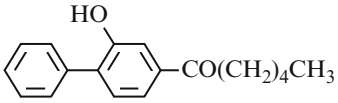
$C_{18}H_{20}O_2$ mol. wt. 268.36



Synthesis
-Obtained by Fries rearrangement of 4-hydroxydiphenyl caproate with aluminium chloride at 160° for 30–45 min (47 %) [1256].
m.p. 86–88° [1256].

1-[1,1′-Biphenyl]-4-yl-2-hydroxy-1-hexanone

[792705-86-3] $C_{18}H_{20}O_2$ mol. wt. 268.36



Synthesis
-Refer to: [2553].

Acetate [792708-61-3]
$C_{20}H_{22}O_3$ mol. wt. 310.39

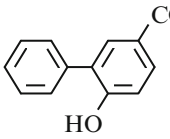
-Refer to: [2553].

O-Methyloxime [792708-48-6] $C_{19}H_{23}NO_2$ mol. wt. 297.40

-Refer to: [2553].

1-(6-Hydroxy[1,1′-biphenyl]-3-yl)-1-hexanone

[95102-42-4] $C_{18}H_{20}O_2$ mol. wt. 268.36

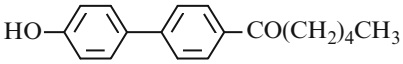


Syntheses
-Refer to: [1256, 1595].
m.p. 86–88° [1256].

USE: Colour developer for thermal recording materials [1595].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-hexanone

$C_{18}H_{20}O_2$ mol. wt. 268.36



Synthesis
-Obtained by Fries rearrangement of 4-hexanoyl-oxybiphenyl with aluminium chloride in nitrobenzene, first at 20° for 12 h, then at 60° for 1 h [522].

Methyl ether [56116-78-0] $C_{19}H_{22}O_2$ mol. wt. 282.38

-Obtained from hexanoyl chloride and 4-methoxybiphenyl [522].
-Also refer to: [514, 847, 2994].

smooth nacreous [522];
$b.p._{.15}$ 258–262° [514, 522]; m.p. 123° [514, 522].

Various ethers (10)

-Preparations and liquid crystalline properties of, [847].

Ethyl ether [56116-87-1] $C_{20}H_{24}O_2$ mol. wt. 296.41 Refer to: [847].

Propyl ether [56116-95-1] $C_{21}H_{26}O_2$ mol. wt. 310.44 Refer to: [847].

Butyl ether [56117-03-4] $C_{22}H_{28}O_2$ mol. wt. 324.46 Refer to: [847].

Pentyl ether [56117-12-5] $C_{23}H_{30}O_2$ mol. wt. 338.49 Refer to: [847].

Hexyl ether [56117-21-6] $C_{24}H_{32}O_2$ mol. wt. 352.52

-Obtained by reaction of hexanoyl chloride with 4-hexyloxybiphenyl in the presence of aluminium chloride in nitrobenzene (23 %) [1799].
-Also refer to: [847].

Heptyl ether [56117-30-7] $C_{25}H_{34}O_2$ mol. wt. 366.54 Refer to: [847].

Octyl ether [56117-38-5] $C_{26}H_{36}O_2$ mol. wt. 380.57 Refer to: [847].

Nonyl ether [56117-47-6] $C_{27}H_{38}O_2$ mol. wt. 394.60 Refer to: [847].

Decyl ether [56117-56-7] $C_{28}H_{40}O_2$ mol. wt. 408.62 Refer to: [847].

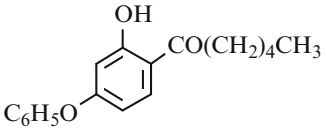
Dodecyl ether [56117-65-8] $C_{30}H_{44}O_2$ mol. wt. 436.68 Refer to: [847].

Hexanoate [72057-94-4] $C_{24}H_{30}O_3$ mol. wt. 366.49 Refer to: [847].

-Obtained by Friedel-Crafts reaction of 4-hydroxybiphenyl with caproyl chloride in the presence of aluminium chloride (72 %) [287].

1-(2-Hydroxy-4-phenoxyphenyl)-1-hexanone

[307000-38-0] $C_{18}H_{20}O_3$ mol. wt. 284.35



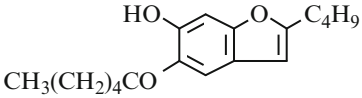
Syntheses
-Refer to: [250, 1345].

USE: For composition of deodorant and antiperspirant [250].

BIOLOGICAL ACTIVITY: Antimicrobial [1345].

1-(2-Butyl-6-hydroxy-5-benzofuranyl)-1-hexanone

[1002158-21-5] $C_{18}H_{24}O_3$ mol. wt. 288.39

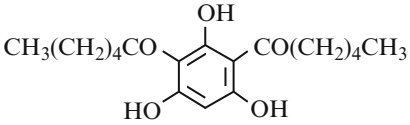


Synthesis
-Obtained by treatment of 2,4-bis (butylethynyl)-1,5-diacetoxybenzene with NaOH (6 equiv.) in THF/MeOH/H_2O at 80° (16 %) [1875].

^{1}H NMR [1875], ^{13}C NMR [1875], IR [1875], MS [1875].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-hexanone

[3118-34-1] $C_{18}H_{26}O_5$ mol. wt. 322.40



Syntheses
-Obtained by reaction of hexanoic acid with phloroglucinol in the presence of boron trifluoride etherate [3019].
-Also obtained by reaction of hexanoyl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene for 3 days at r.t. (5–10 %) [421].

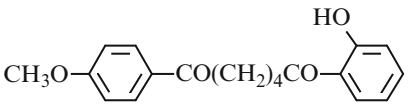
-Also obtained by reaction of caproic anhydride with phloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].
-Also refer to: [457, 600, 644, 962, 2911, 3018, 3033].

m.p. 105° [421], 97–98° [457, 2911];
^{1}H NMR [421, 3019], ^{13}C NMR [3019], IR [421, 3019], UV [3019], MS [421].

BIOLOGICAL ACTIVITY: Antagonist both thromboxane A_2 and Leukotriene D_4 [3019]; Inhibitory effects of treatment with this acylphenol on TPA Induced EBV-EA Activation [3033]; Antiviral activity towards the replication of vesicular stomatitis virus in HEL cell cultures [644]; Germination inhibition in cress (*Lepidium sativum*) seeds [421]; Industrial bactericidal and fungicidal agent, algicide and biofouling inhibitor [962]; For treatment of immune dysfunction associated with human immunodeficiency virus infection [600]; Anthelmintic [457].

6-(2-Hydroxyphenyl)-1-(4-methoxyphenyl)-1,6-hexanedione

$C_{19}H_{20}O_4$ mol. wt. 312.36

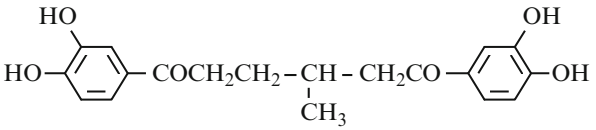


Synthesis
-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxyphenyl)-6-(4-hydroxyphenyl)-1,6-hexanedione in the presence of 2 N NaOH [902].

m.p. 118° [902].

1,6-Bis(3,4-dihydroxyphenyl)-3-methyl-1,6-hexanedione

$C_{19}H_{20}O_6$ mol. wt. 344.36



Synthesis
-Refer to: [1014].

Tetramethyl ether [50766-25-1] $C_{23}H_{28}O_6$ mol. wt. 400.47

-Obtained by hydrogenating its oxime in acetic acid, in the presence of 10 % Pd/C in a Parr apparatus at r.t. and 45–50 psig for 12–36 h (38 %) [1014].
-Also refer to: [1012].

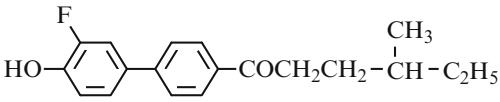
m.p. 91–94° [1014], 83–86° [1012].

Dioxime of the tetramethyl ether [50766-42-2] $C_{23}H_{30}N_2O_6$ mol. wt. 430.50

m.p. 127–130° [1014].

1-(3′-Fluoro-4′-hydroxy[1,1′-biphenyl]-4-yl)-4-methyl-1-hexanone

$C_{19}H_{21}FO_2$ mol. wt. 300.37



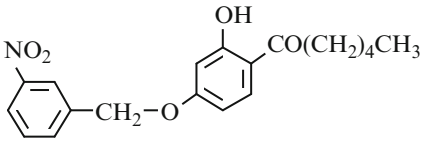
Synthesis
-Refer to: [2107].

Decyl ether (S) [112780-62-8] $C_{29}H_{41}FO_2$ mol. wt. 440.64

USE: Liq.-crystal compnds. contg., for display devices [2107].

1-[2-Hydroxy-4-[(3-nitrophenyl)methoxy]phenyl]-1-hexanone

[103981-28-8] $C_{19}H_{21}NO_5$ mol. wt. 343.38



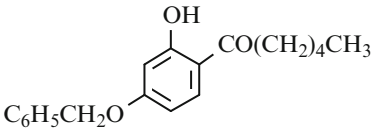
Synthesis
-Obtained by reaction of 3-nitrobenzyl bromide with 2,4-dihydroxycaprophenone in the presence of potassium carbonate and cesium carbonate (cat.) [1657].

Methyl ether [103981-30-2] $C_{20}H_{23}NO_5$ mol. wt. 357.41

-Refer to: [1657].

1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-hexanone

[143287-04-1] $C_{19}H_{22}O_3$ mol. wt. 298.38



Synthesis
-Obtained by reaction of benzyl chloride with 2,4-dihydroxycaprophenone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

-Also refer to: [3410].

m.p. 62–67° [284].

Oxime [143286-81-1] $C_{19}H_{23}NO_3$ mol. wt. 313.40

-Obtained by reaction of hydroxylamine hydrochloride with 1-[2-hydroxy-4-(phenylmethoxy)phenyl]-1-hexanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

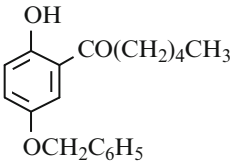
m.p. 88–94° [284]; ^{1}H NMR [284].

Methyl ether [177426-78-7] $C_{20}H_{24}O_3$ mol. wt. 312.40

-Refer to: [3410].

1-[2-Hydroxy-5-(phenylmethoxy)phenyl]-1-hexanone

$C_{19}H_{22}O_3$ mol. wt. 298.38

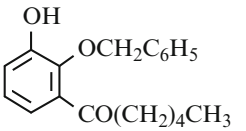


Synthesis
-Refer to: [3409].

Methyl ether [186246-05-9]
$C_{20}H_{24}O_3$ mol. wt. 312.40
-Refer to: [3409, 3411].

1-[3-Hydroxy-2-(phenylmethoxy)phenyl]-1-hexanone

$C_{19}H_{22}O_3$ mol. wt. 298.38



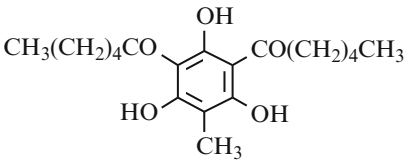
Synthesis
-Refer to: [3411].

Methyl ether [195158-14-6]
$C_{20}H_{24}O_3$ mol. wt. 312.40

-Refer to: [3411].

1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-hexanone

[3118-38-5] $C_{19}H_{28}O_5$ mol. wt. 336.43



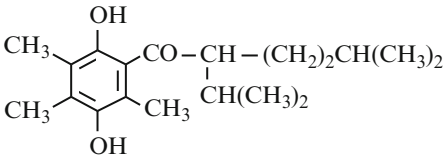
Syntheses
-Obtained by reaction of caproic anhydride with 2-methylphloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].
-Also refer to: [457, 600, 2730, 2731, 2911].

m.p. 108–110° [457, 2911].

BIOLOGICAL ACTIVITY: For treatment of immune dysfunction associated with human immunodeficiency virus infection [600]; Mitochondria of ascarid in response to [2730]; Anthelmintic [457]; Phosphorylation response to, in roundworm mitochondria, [2731].

1-(2,5-Dihydroxy-3,4,6-trimethylphenyl)-5-methyl-2-(1-methylethyl)-1-hexanone

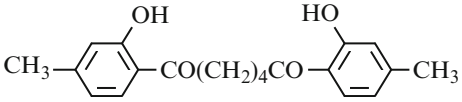
[357172-20-4] $C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Refer to: [2352].

1,6-Bis(2-hydroxy-4-methylphenyl)-1,6-hexanedione

[13320-65-5] $C_{20}H_{22}O_4$ mol. wt. 326.39



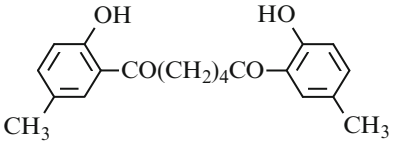
Syntheses
-Obtained by Fries rearrangement of m-cresyl adipate with aluminium chloride, first at 100°, then at 165° for 50 min [2774].

-Also refer to: [618].

m.p. 122–123° [2774]; ^{1}H NMR [618].

1,6-Bis(2-hydroxy-5-methylphenyl)-1,6-hexanedione

[13282-24-1] $C_{20}H_{22}O_4$ mol. wt. 326.39

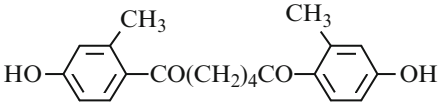


Syntheses
-Obtained by Fries rearrangement of di (4-methyl-phenyl) adipate with aluminium chloride,
*without solvent at 130° for 4 h (28 %) [3107];
*in refluxing chlorobenzene for 6 h (72 %) [3107].

m.p. 163–164° [3107]; IR [3107].

1,6-Bis(4-hydroxy-2-methylphenyl)-1,6-hexanedione

[5550-54-9] $C_{20}H_{22}O_4$ mol. wt. 326.39



Synthesis
-Obtained by reaction of adipyl chloride with m-cresol in the presence of aluminium chloride in nitrobenzene at 0° [593].

m.p. 114° [593].

Dioxime [5538-13-6] $C_{20}H_{24}N_2O_4$ mol. wt. 356.42

m.p. 131° [593].

Dimethyl ether [5550-56-1] $C_{22}H_{26}O_4$ mol. wt. 354.45

-Obtained by reaction of adipyl chloride with m-cresol methyl ether in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture (1:1) at 0° [593].

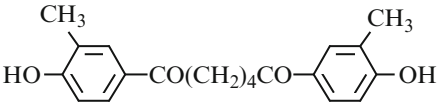
m.p. 130° [593].

Oxime of the dimethyl ether [5538-16-9] $C_{22}H_{28}N_2O_4$ mol. wt. 384.48

m.p. 145° [593].

1,6-Bis(4-hydroxy-3-methylphenyl)-1,6-hexanedione

[6016-44-0] $C_{20}H_{22}O_4$ mol. wt. 326.39



Synthesis

-Obtained by reaction of adipyl chloride with o-cresol in the presence of aluminium chloride in nitrobenzene at 0° (10 %) [593].

m.p. 204° [593].

Dioxime [5538-08-9] $C_{20}H_{24}N_2O_4$ mol. wt. 356.42

m.p. 175° [593].

Dimethyl ether [5538-10-3] $C_{22}H_{26}O_4$ mol. wt. 354.45

-Obtained by reaction of adipyl chloride with o-cresol methyl ether in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture (1:1) at 0° [593].

-Also refer to: [1014 Method D (81 %), 2246, 3378].

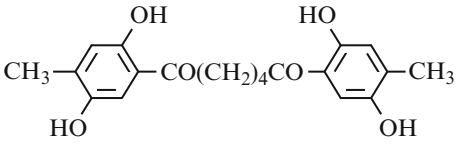
m.p. 164–165° [3378], 163° [2246], 160–161° [1014], 160° [593];
^{1}H NMR [3378], IR [3378], UV [2246].

Dioxime of the dimethyl ether [5550-53-8] $C_{22}H_{28}N_2O_4$ mol. wt. 384.48

m.p. 185° [593], 178–179° [1014].

1,6-Bis(2,5-dihydroxy-4-methylphenyl)-1,6-hexanedione

[91453-27-9] $C_{20}H_{22}O_6$ mol. wt. 358.39

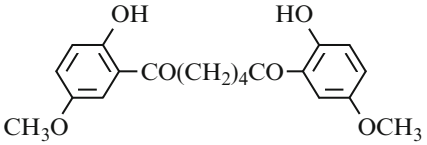


Synthesis
-Obtained by treatment of 1,6-bis (2-hydroxy-5-methoxy-4-methyl-phenyl)-1,6-hexane-dione with boron tribromide in methylene chloride (85 %) [2103].

yellow solid [2103]; m.p. 137–139° [2103];
^{1}H NMR [2103], IR [2103].

1,6-Bis(2-hydroxy-5-methoxyphenyl)-1,6-hexanedione

[10365-28-3] $C_{20}H_{22}O_6$ mol. wt. 358.39



Syntheses
-Obtained by reaction of adipoyl dichloride with p-dimethoxybenzene in the presence of aluminium chloride [1575] in refluxing 1,2-dichloroethane for 8 h [2103].

-Also refer to: [1575, 3175].

yellow crystals [3175]; m.p. 157–158° [3175], 157° [1575].

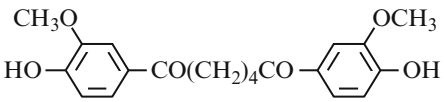
Diacetate [10365-33-0] $C_{24}H_{26}O_8$ mol. wt. 442.47

-Obtained by reaction of acetic anhydride (4 vol) with the title ketone in the presence of 1–2 drops concentrated sulfuric acid, the mixture warmed 5 min [1575].

m.p. 152° [1575].

1,6-Bis(4-hydroxy-3-methoxyphenyl)-1,6-hexanedione

$C_{20}H_{22}O_6$ mol. wt. 358.39



Synthesis
-Refer to: [1014].

Diethyl ether [50766-21-7] $C_{24}H_{30}O_6$ mol. wt. 414.50

-Refer to Method D: [1014] (85 %).

m.p. 130–131° [1014].

Dioxime of the diethyl ether [50766-37-5] $C_{24}H_{32}N_2O_6$ mol. wt. 444.53

m.p. 187–189° [1014].

Dibenzyl ether [50766-22-8] $C_{34}H_{34}O_6$ mol. wt. 538.64

-Refer to Method D: [1014] (70 %).

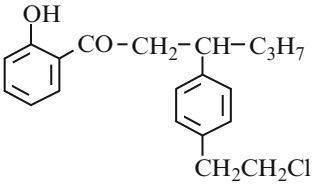
m.p. 163–164° [1014].

Dioxime of the dibenzyl ether [50766-38-6] $C_{36}H_{40}N_2O_6$ mol. wt. 596.72

m.p. 125–126° [1014].

3-[4-(2-Chloroethyl)phenyl]-1-(2-hydroxyphenyl)-1-hexanone

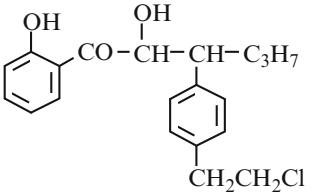
[70206-42-7] $C_{20}H_{23}ClO_2$ mol. wt. 330.85



Synthesis
-Obtained from degradation of clocoumarol [3205].
^{1}H NMR [3205], IR [3205], UV [3205], MS [3205].

3-[4-(2-Chloroethyl)phenyl]-2-hydroxy-1-(2-hydroxyphenyl)-1-hexanone

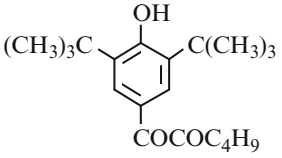
[70206-43-8] $C_{20}H_{23}ClO_3$ mol. wt. 346.85
[72793-41-0]
[72793-42-1]



Synthesis
-Obtained from degradation of clocoumarol [3205].
^{1}H NMR [3205], IR [3205], UV [3205], MS [3205].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1,2-hexanedione

[96251-00-2] $C_{20}H_{30}O_3$ mol. wt. 318.46

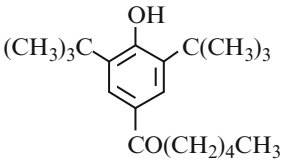


Syntheses
-Obtained by oxygenation of 1-[3,5-(dimethylethyl)-4-hydroxyphenyl]-1-hexyne with Co(Salpr) in methylene chloride at 0° (70 %) [2290].
-Also refer to: [2007, 2289].

colourless prisms [2290]; m.p. 187–188° [2289, 2290];
^{1}H NMR [2007, 2289, 2290], ^{13}C NMR [2007, 2289, 2290],
IR [2289, 2290], UV [2290].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-hexanone

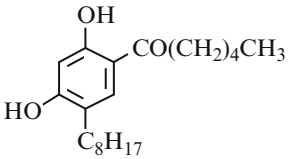
$C_{20}H_{32}O_2$ mol. wt. 304.47



Synthesis
-Refer to: [1408].
O-Methyloxime [169888-14-6]
$C_{21}H_{35}NO_2$ mol. wt. 333.51
-Refer to: [1408].

1-(2,4-Dihydroxy-5-octylphenyl)-1-hexanone

$C_{20}H_{32}O_3$ mol. wt. 320.47

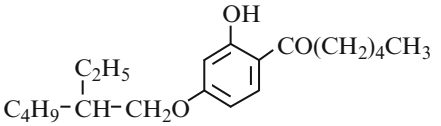


Synthesis
-Refer to: [1051].
Oxime, **nickel complex** [82307-87-7]

USE: Colour photog. stabilizer [1051].

1-[4-[(2-Ethylhexyl)oxy]-2-hydroxyphenyl]-1-hexanone

[80851-64-5] $C_{20}H_{32}O_3$ mol. wt. 320.47

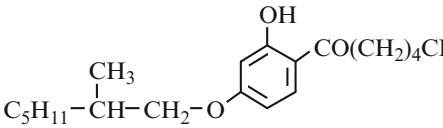


Synthesis
-Refer to: [1050].
Oxime, **nickel complex** [80848-70-0]

USE: Photog. stabilizer compns. contg. phenol derivs. and, for magenta images [1050].

1-[2-Hydroxy-4-(sec-octyloxy)phenyl]-1-hexanone

[127313-65-9] $C_{20}H_{32}O_3$ mol. wt. 320.47

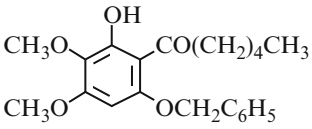


Synthesis
-Refer to: [3427].
Oxime [127313-53-5]
$C_{20}H_{33}NO_3$ mol. wt. 335.49

USE: Copper extn. reactivity of [3427].

1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-hexanone

[134082-02-3] $C_{21}H_{26}O_5$ mol. wt. 358.43



Synthesis

-Obtained by elimination of one phenylmethyl group in 2-position by treatment of 1-(2,6-dibenzyloxy-3,4-dimethoxyphenyl)-1-hexanone with concentrated hydrochloric acid and acetic acid at r.t. for 2–3 h (81 %) [1353].

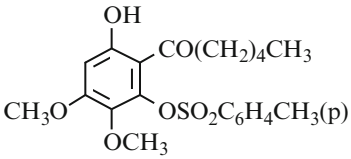
m.p. 104.5–105.5° [1353]; ^{1}H NMR [1353].

Methyl ether $C_{22}H_{28}O_5$ mol. wt. 372.46

-Refer to: [1353].

1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-hexanone

[134081-86-0] $C_{21}H_{26}O_7S$ mol. wt. 422.50



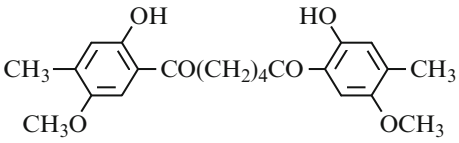
Synthesis

-Obtained by treatment of 1-(2-tosyloxy-3,4,6-trimethoxyphenyl)-1-hexanone with 25 % aluminium bromide in acetonitrile at r.t. for 2–3 h (80 %) [1353].

m.p. 53–54° [1353]; ^{1}H NMR [1353].

1,6-Bis(2-hydroxy-5-methoxy-4-methylphenyl)-1,6-hexanedione

[344574-57-8] $C_{22}H_{26}O_6$ mol. wt. 386.45



Synthesis

-Obtained by reaction of adipoyl dichloride with 2,5-dimethoxytoluene in the presence of aluminium chloride in refluxing 1,2-dichloroethane for 8 h [2103].

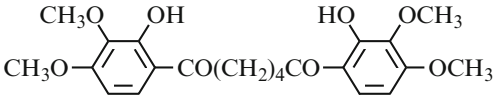
Dimethyl ether [180578-80-7] $C_{24}H_{30}O_6$ mol. wt. 414.50

-Obtained by reaction of adipic acid dichloride with 2,5-dimethoxytoluene in the presence of aluminium chloride in dichloromethane first at 0° under an argon atmosphere, then at r.t. for 16 h (61 %) [2570], (56 %) [1402].

colourless needles [1402];
m.p. 167° [1402], 164–165° [2570];
^{1}H NMR [2570], ^{13}C NMR [2570], IR [2570].

1,6-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,6-hexanedione

[10351-90-3] $C_{22}H_{26}O_8$ mol. wt. 418.44



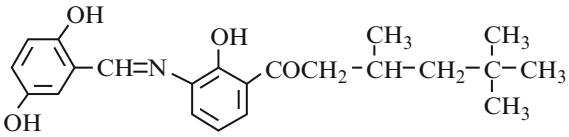
Syntheses
-Obtained by reaction of adipic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride [3058] in tetrachloroethane [1574].
-Also refer to: [1575, 3058].

m.p. 175° [1574, 1575], 174–175° [3058].

1-[3-[[(2,5-Dihydroxyphenyl)methylene]amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone

1-[3-(2,5-Dihydroxybenzylideneamino)-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone
1-[3-[(2,5-Dihydroxybenzylidene)amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone

[176044-11-4] $C_{22}H_{27}NO_4$ mol. wt. 369.46



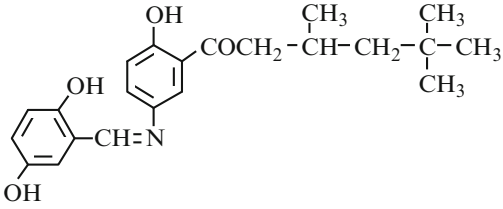
Synthesis
-Refer to: [628].

BIOLOGICAL ACTIVITY: As inhibitor of EGF receptor-assocd. tyrosine kinase [628].

1-[5-[[(2,5-Dihydroxyphenyl)methylene]amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone

1-[5-(2,5-Dihydroxybenzylideneamino)-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone
1-[5-[(2,5-Dihydroxybenzylidene)amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone

[154737-36-7] $C_{22}H_{27}NO_4$ mol. wt. 369.46



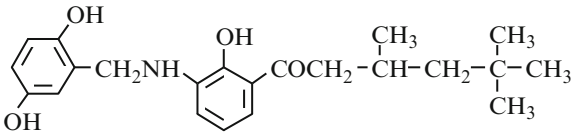
Synthesis
-Refer to: [628].

BIOLOGICAL ACTIVITY: As inhibitor of EGF receptor-assocd. tyrosine kinase [628].

1-[3-[[(2,5-Dihydroxyphenyl)methyl]amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone

1-[3-(2,5-Dihydroxybenzylamino)-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone

[176044-29-4] $C_{22}H_{29}NO_4$ mol. wt. 371.47



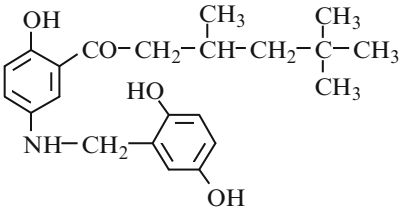
Synthesis
-Refer to: [628].

BIOLOGICAL ACTIVITY: As inhibitor of EGF receptor-assocd. tyrosine kinase [628].

1-[5-[[(2,5-Dihydroxyphenyl)methyl]amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone

1-[5-(2,5-Dihydroxybenzylamino)-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone

[154736-91-1] $C_{22}H_{29}NO_4$ mol. wt. 371.47

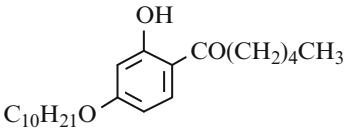


Syntheses
-Refer to: [417, 628].

BIOLOGICAL ACTIVITY: As inhibitor of EGF receptor-assocd. tyrosine kinase [628].

1-[4-(Decyloxy)-2-hydroxyphenyl]-1-hexanone

[101002-33-9] $C_{22}H_{36}O_3$ mol. wt. 348.53



Syntheses
-Obtained by reaction of decyl bromide with 2,4-dihydroxycaprophenone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

-Also refer to: [3077].

m.p. 45–47° [284].

Oxime [101002-20-4] $C_{22}H_{37}NO_3$ mol. wt. 363.54

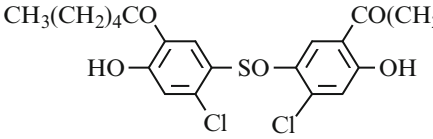
-Obtained by reaction of hydroxylamine hydrochloride with 1-[4-(decyloxy)-2-hydroxyphenyl]-1-hexanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].
-Also refer to: [3077].

m.p. 58–60° [284, 3077]; ^{1}H NMR [284].

USE: Topical preparations comprising at least one aryloxime and bisabolol [483]; As lipoxygenase inhibitor [3077].

1,1′-[Sulfonylbis(6-chloro-4-hydroxy-3,1-phenylene)]bis-1-hexanone

[50444-97-8] $C_{24}H_{28}Cl_2O_5S$ mol. wt. 499.45



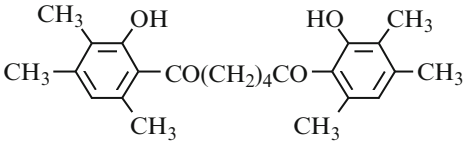
Synthesis
-Obtained by treatment of 4-chloro-2-hydroxycaprophenone with thionyl chloride in the presence of aluminium chloride in carbon disulfide (52 %) [2430].

m.p. 123° [2430]; IR [2430].

USE: Antifungal [2430].

1,6-Bis(2-hydroxy-3,4,6-trimethylphenyl)-1,6-hexanedione

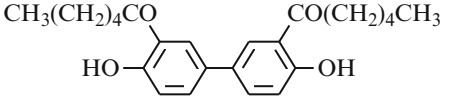
[84978-15-4] $C_{24}H_{30}O_4$ mol. wt. 382.50



Synthesis
-Refer to: [2325].
m.p. 186–187.5° [2325];
^{1}H NMR [2325], IR [2325].

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-hexanone

[103758-73-2] $C_{24}H_{30}O_4$ mol. wt. 382.50



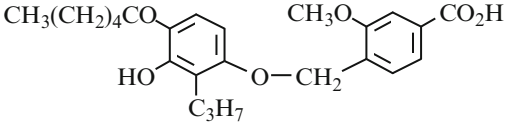
Syntheses
-Preparation by Fries rearrangement of 4,4′-biphenyl dicaproate with aluminium chloride,

*in the presence of sodium chloride at 140° (99 %) [2091];
*in refluxing chlorobenzene for 24 h (53 %) [2377].

m.p. 92.5–93.5° [2377]; IR [2377].

4-[3-Hydroxy-4-(1-hexanoyl)-2-propylphenoxymethyl]-3-methoxybenzoic acid

[118683-27-5] $C_{24}H_{30}O_6$ mol. wt. 414.50

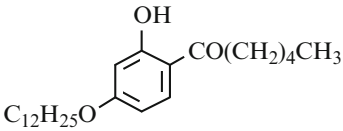


Synthesis
-Refer to: [466].
m.p. 204–206° [466].

BIOLOGICAL ACTIVITY: Antagonist of the peptidoleukotrienes [466].

1-[4-(Dodecyloxy)-2-hydroxyphenyl]-1-hexanone

$C_{24}H_{40}O_3$ mol. wt. 376.58



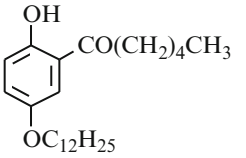
Synthesis
-Refer to: [2742].

Oxime [110647-47-7]
$C_{24}H_{41}NO_3$ mol. wt. 391.59

-Refer to: [2742].

1-[5-(Dodecyloxy)-2-hydroxyphenyl]-1-hexanone

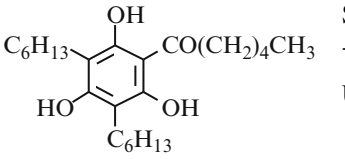
[140466-94-0] $C_{24}H_{40}O_3$ mol. wt. 376.58



Synthesis
-Refer to: [3322].

1-(3,5-Dihexyl)-2,4,6-(trihydroxyphenyl)-1-hexanone

[54556-08-0] $C_{24}H_{40}O_4$ mol. wt. 392.58

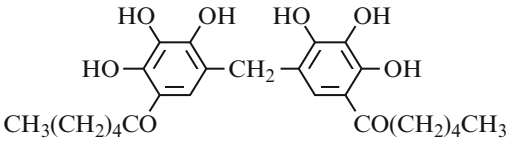


Synthesis
-Refer to: [3339].

USE: Oxidation of, [3339].

1,1′-[Methylenebis(2,3,4-trihydroxy-5,1-phenylene)]bis-1-hexanone

$C_{25}H_{32}O_8$ mol. wt. 460.52

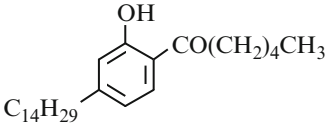


Synthesis
-Obtained by treatment of 4-caproyl-pyrogallol with 35 % aqueous solution of formaldehyde in refluxing ethanol for 10 min [506].

m.p. 171° [506].

1-(2-Hydroxy-4-tetradecylphenyl)-1-hexanone

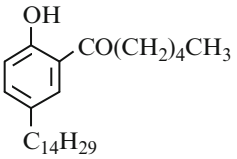
[118469-92-4] $C_{26}H_{44}O_2$ mol. wt. 388.63



Synthesis
-Refer to: [3323].
m.p. 44–45° [3323].

1-(2-Hydroxy-5-tetradecylphenyl)-1-hexanone

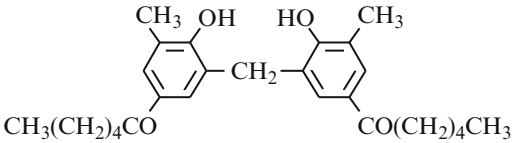
[118469-84-4] $C_{26}H_{44}O_2$ mol. wt. 388.63



Synthesis
-Refer to: [3323].
m.p. 41–42° [3323].

1,1′-[Methylenebis(2-hydroxy-3-methyl-5,1-phenylene)]bis-1-hexanone

$C_{27}H_{36}O_4$ mol. wt. 424.58

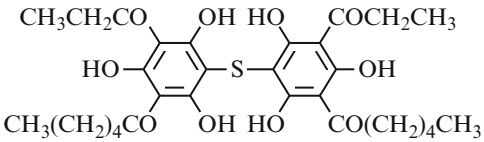


Syntheses
-Obtained by reaction of hexanoyl chloride with bis(2-hydroxy-3-methyl-phenyl) methane according to the method described previously [2871], (55 %) [119].

m.p. 141–142° [119]; ^{1}H NMR [119], IR [119].

1,1′-Thiobis[2,4,6-trihydroxy-3-(1-oxopropyl)-5,1-phenylene]bis-1-hexanone

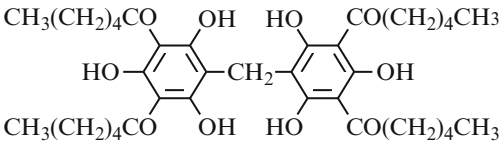
$C_{30}H_{33}O_{10}S$ mol. wt. 585.65



Synthesis
-Refer to: [3391].
m.p. 124° [3391].

1,1′-Methylenebis(2,4,6-trihydroxy-3,5,1-phenylene)bis-1-hexanone

[68223-34-7] $C_{37}H_{52}O_{10}$ mol. wt. 656.81



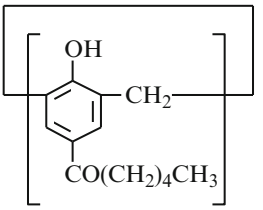
Syntheses
-Preparation by condensation of two molecules of acylphloroglucinol with formaldehyde or methoxymethyl acetate [3391].

-Also refer to: [1571].

m.p. 116–118° [3391], 95–97° [1571].

5,11,17,23,29,35-Hexahexanoyl-37,38,39,40,41,42-hexahydroxycalix [6]arene

$C_{78}H_{96}O_{12}$ mol. wt. 1225.61



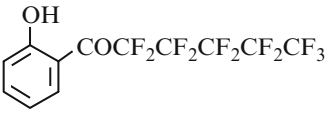
Synthesis
-Obtained by Fries rearrangement of 37,38,39,40,41,42-hexakis(hexanoyloxy)calix[6]arene (**2a**) with aluminium chloride in chlorobenzene at 45–50° for 17 h under a nitrogen atmosphere (29 %) (**3a**) [135].
m.p. 227–230° [135];
^{1}H NMR [135], IR [135].

2 Aromatic Hydroxyketones Derived from Various Halogenohexanoic Acids

2.1 Unsubstituted Hydroxyketones

2,2,3,3,4,4,5,5,6,6,6-Undecafluoro-1-(2-hydroxyphenyl)-1-hexanone

[173979-31-2] $C_{12}H_5F_{11}O_2$ mol. wt. 390.15

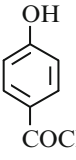


Synthesis
-Obtained by treatment of 4-(perfluoro-n-hexyl) anisole with 48 % hydrobromic acid in glacial acetic acid at 110° for 22 days (30 %) [626].

^{1}H NMR [626], ^{19}F NMR [626], IR [626], MS [626].

2,2,3,3,4,4,5,5,6,6,6-Undecafluoro-1-(4-hydroxyphenyl)-1-hexanone

[173979-30-1] $C_{12}H_5F_{11}O_2$ mol. wt. 390.15

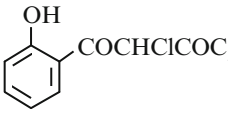


Synthesis
-Obtained by treatment of 4-(perfluoro-n-hexyl)anisole with 48 % hydrobromic acid in glacial acetic acid at 110° for 6 days (79 %) [626].
$b.p._{.70}$ 185° [626]; m.p. 67° [626];

^{1}H NMR [626], ^{19}F NMR [626], IR [626], MS [626].

2-Chloro-1-(2-hydroxyphenyl)-1,3-hexanedione

$C_{12}H_{13}ClO_3$ mol. wt. 240.69



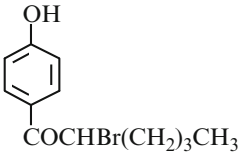
Synthesis
-Refer to: [3400].
Methyl ether [1001024-96-9]
$C_{13}H_{15}ClO_3$ mol. wt. 254.71

-Obtained by reaction of N-chlorosuccinimide with 1-(2-hydroxyphenyl)-1,3-hexanedione in refluxing carbon tetrachloride for 4 h at 75–80° (81 %) [3400].

yellowish oil [3400];
^{1}H NMR [3400], ^{13}C NMR [3400], IR [3400], MS [3400];
GC-MS [3400].

2-Bromo-1-(4-hydroxyphenyl)-1-hexanone

[1245904-83-9] $C_{12}H_{15}BrO_2$ mol. wt. 271.15



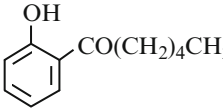
Syntheses
-Refer to: [1114, 1888].
Methyl ether [33809-55-1]
$C_{13}H_{17}BrO_2$ mol. wt. 285.18

-Obtained by treatment of 1-(4-methoxyphenyl)-1-hexanone with bromine,
*in ethyl ether and glacial acetic acid at r.t. (89 %) [1114];
*in a mixture of ethyl ether/dioxane at r.t. (46 %) [3232].
-Also obtained by treatment of 1-(4-methoxyphenyl)-1-hexanone with bromine in the presence of a catalytic amount of aluminium chloride (nearly quantitative yield) [2157].
-Also refer to: [1186, 1870, 2157].

b.p.$_{14}$ 182–184° [3232];
m.p. 54–55° [1186, 1870], 51–52° [1114];
^{1}H NMR [1114, 1186, 1870, 2157, 3232], ^{13}C NMR [2157], IR [3232], MS [1114, 1186, 1870].

6-Bromo-1-(2-hydroxyphenyl)-1-hexanone

[51821-14-8] $C_{12}H_{15}BrO_2$ mol. wt. 271.15



Synthesis
-Obtained by demethylation of ether below with boron tribromide in methylene chloride at −20° (73 %) [1430].
m.p. 44.5–45° [1430]; ^{1}H NMR [1430], IR [1430].

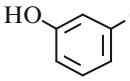
Methyl ether [51795-94-9] $C_{13}H_{17}BrO_2$ mol. wt. 285.18

-Obtained by interaction of 6-bromohexanenitrile with the Grignard reagent derived from o-bromoanisole, followed by acid hydrolysis (52 %) [1430].

IR [1430].

6-Bromo-1-(3-hydroxyphenyl)-1-hexanone

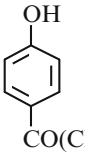
$C_{12}H_{15}BrO_2$ mol. wt. 271.15



Synthesis
-Refer to: [154].
^{1}H NMR [154].

6-Bromo-1-(4-hydroxyphenyl)-1-hexanone

[188973-67-3] $C_{12}H_{15}BrO_2$ mol. wt. 271.15



Syntheses
-Obtained by Friedel-Crafts acylation of phenol with 6-bromohexanoyl chloride in the presence of aluminium chloride [2459] in methylene chloride at 25° [2919].
-Also refer to: [154, 217, 1314, 1473, 2459, 3419].

^{1}H NMR [154, 3419].

USE: Polymeric prodrugs having temporary linkages to amino groups [1314].

Methyl ether [57840-61-6] $C_{13}H_{17}BrO_2$ mol. wt. 285.18

-Obtained by Friedel-Crafts acylation of anisole,
*with 6-bromohexanoic acid using alkylhalosilanes and indium halides or triflates [217];
*with 6-bromohexanoyl chloride in the presence of aluminium chloride (85 %) [1509], in 1,2-dichloroethane at −10° for 1 h (87 %) [2943], at 25° [2919] or in dichloromethane at −10° for 1–2 h under nitrogen (73 %) [572].
-From 6-bromo-1-fluoro-1-(p-methoxyphenyl)-1-hexene in $CDCl_3$ or neat (H_2O) [90].
-Also refer to: [572, 620, 1123, 1473, 1509, 1630, 2298, 2950].

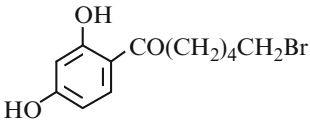
m.p. 50–52° [2943], 43–44° [572], 41–43° [620];
^{1}H NMR [572, 1509, 2943], ^{13}C NMR [2943],
MS [1509, 2943]; GC-MS [1509].

Phenyl ether [164396-78-5] $C_{18}H_{19}BrO_2$ mol. wt. 347.25

-Refer to: [717].

6-Bromo-1-(2,4-dihydroxyphenyl)-1-hexanone

$C_{12}H_{15}BrO_3$ mol. wt. 287.15



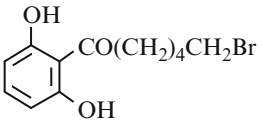
Syntheses
-Refer to: [154, 308].
^{1}H NMR [154].

Dimethyl ether [118018-78-4] $C_{14}H_{19}BrO_3$ mol. wt. 315.20

-Refer to: [308, 1123].

6-Bromo-1-(2,6-dihydroxyphenyl)-1-hexanone

[1111652-08-4] $C_{12}H_{15}BrO_3$ mol. wt. 287.15

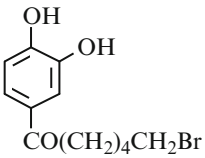


Synthesis
-Refer to: [1219] (Chinese patent).

USE: Preparation of low swelling sulfonated polyimide proton exchange membrane for fuel cell [1219].

6-Bromo-1-(3,4-dihydroxyphenyl)-1-hexanone

$C_{12}H_{15}BrO_3$ mol. wt. 287.15



Synthesis
-Refer to: [2919].
Dimethyl ether [123014-46-0]
$C_{14}H_{19}BrO_3$ mol. wt. 315.20

-Obtained by Friedel-Crafts acylation of veratrole with 6-bromohexanoyl chloride in the presence of aluminium chloride in methylene chloride at 25° [2919].
-Also refer to: [154, 560, 561, 1473, 1542, 1543, 3419].

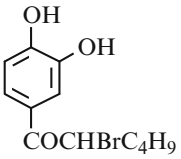
m.p. 44–45° [1543], 38–40° [154, 3419];
^{1}H NMR [1543], ^{13}C NMR [1543].

Methylenedioxy $C_{13}H_{15}BrO_3$ mol. wt. 299.16

^{1}H NMR [3419].

2-Bromo-1-(3,4-dihydroxyphenyl)-1-hexanone

$C_{12}H_{15}BrO_3$ mol. wt. 287.15

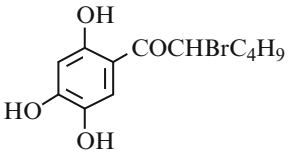


Synthesis
-Refer to: [2657].
Dibenzyl ether $C_{26}H_{27}BrO_3$ mol. wt. 467.40
-Obtained by reaction of N-bromosuccinimide with 3,4-(dibenzyloxy)caprophenone in carbon tetrachloride in the presence of benzoyl peroxide at 50° (85–90 %) [2657].

m.p. 98° [2657].

2-Bromo-1-(2,4,5-trihydroxyphenyl)-1-hexanone

$C_{12}H_{15}BrO_4$ mol. wt. 303.15

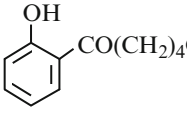


Synthesis
-Refer to: [2696].
Trimethyl ether [90834-09-6]
$C_{15}H_{21}BrO_4$ mol. wt. 345.23
-Obtained by reaction of bromine with 2,4,5-trimethoxycaprophenone in acetic acid at 35–40°, then at 25° for 40 min [2695].
-Also refer to: [2696].

m.p. 55–58° [2696], 55–56° [2695];
^{1}H NMR [2695, 2696], IR [2695, 2696], MS [2695, 2696].

6-Chloro-1-(2-hydroxyphenyl)-1-hexanone

[501083-62-1] $C_{12}H_{15}ClO_2$ mol. wt. 226.70



Synthesis
-Refer to: [2459].
^{1}H NMR [2459], MS [2459].

Methyl ether [501083-60-9] $C_{13}H_{17}ClO_2$ mol. wt. 240.73

-Refer to: [2459].

^{1}H NMR [2459], MS [2459].

6-Chloro-1-(3-hydroxyphenyl)-1-hexanone

[501083-64-3] $C_{12}H_{15}ClO_2$ mol. wt. 226.70

Synthesis
-Refer to: [2459].
^{1}H NMR [2459], MS [2459].

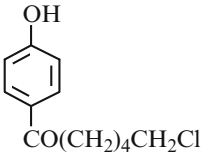
Methyl ether [258882-50-7] $C_{13}H_{17}ClO_2$ mol. wt. 240.73

-Preparation by treatment of 6-chloro-1-(3-methoxyphenyl)-1-hexanol with chromium trioxide in dilute sulfuric acid (Jones' reagent) in acetone first at 0°, then at r.t. for 6 h [2460].
-Also refer to: [2459].

^{1}H NMR [2460], MS [2460].

6-Chloro-1-(4-hydroxyphenyl)-1-hexanone

$C_{12}H_{15}ClO_2$ mol. wt. 226.70



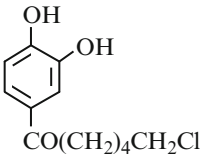
Synthesis
-Refer to: [2287].
Methyl ether [278619-91-3]
$C_{13}H_{17}ClO_2$ mol. wt. 240.73

-Obtained by Friedel-Crafts acylation of anisole,
*with tert-butyl 6-chlorohexanoate in the presence of indium tribromide using dimethylchlorosilane (**1 t**) (64 %) [2287];
*with 6-chlorohexanoic acid using alkylhalosilanes, and indium halides or triflates [217].

b.p.$_{0.1}$ 130° [2287];
^{1}H NMR [2287], ^{13}C NMR [2287], IR [2287], MS [2287].

6-Chloro-1-(3,4-dihydroxyphenyl)-1-hexanone

$C_{12}H_{15}ClO_3$ mol. wt. 242.70

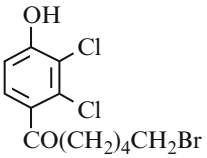


Synthesis
-Refer to: [2560].
Dimethyl ether [19347-74-1]
$C_{14}H_{19}ClO_3$ mol. wt. 270.76
-Refer to: [2560].

2.2 Substituted Hydroxyketones

6-Bromo-1-(2,3-dichloro-4-hydroxyphenyl)-1-hexanone

$C_{12}H_{13}BrCl_2O_2$ mol. wt. 340.04



Synthesis
-Refer to: [3333].

Methyl ether [53107-64-5]
$C_{13}H_{15}BrCl_2O_2$ mol. wt. 354.07

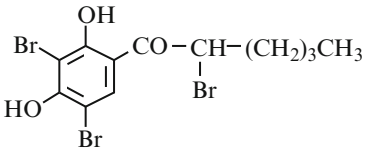
-Obtained by reaction of 6-bromohexanoyl chloride with 2,3-dichloroanisole in the presence of aluminium chloride (21 %) [3333].
-Also refer to: [732, 736–738, 740, 2052, 2053].

m.p. 52–53° [2051, 2052], 50° [3333].

USE: Prepn. and cyclization of, [736, 737, 2053]; Prepn. and reaction of, with formaldehyde [738, 2052].

2-Bromo-1-(3,5-dibromo-2,4-dihydroxyphenyl)-1-hexanone

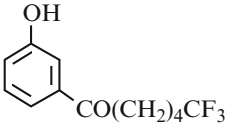
[238074-78-7] $C_{12}H_{13}Br_3O_3$ mol. wt. 444.95



Synthesis
-Refer to: [998].

6,6,6-Trifluoro-1-(3-hydroxyphenyl)-1-hexanone

[104325-65-7] $C_{12}H_{13}F_3O_2$ mol. wt. 246.23

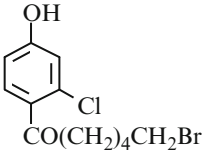


Syntheses
-Refer to: [2197, 2198].

USE: In preparation of antiinflammatory and antiallergic agents [2198].

6-Bromo-1-(2-chloro-4-hydroxyphenyl)-1-hexanone

$C_{12}H_{14}BrClO_2$ mol. wt. 305.60

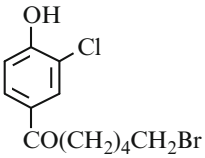


Synthesis
-Refer to: [1123].

Methyl ether [118108-79-5]
$C_{13}H_{16}BrClO_2$ mol. wt. 319.63
-Refer to: [1123].

6-Bromo-1-(3-chloro-4-hydroxyphenyl)-1-hexanone

$C_{12}H_{14}BrClO_2$ mol. wt. 305.60



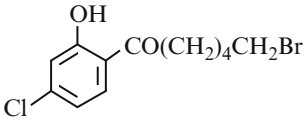
Synthesis
-Refer to: [2919].
Methyl ether [188973-65-1]
$C_{13}H_{16}BrClO_2$ mol. wt. 319.63

-Obtained by Friedel-Crafts acylation of 2-chloroanisole with 6-bromohexanoyl chloride in the presence of aluminium chloride in methylene chloride at 25° [2919].
-Also refer to: [154, 3419].

m.p. 104–106° [154, 3419].

6-Bromo-1-(4-chloro-2-hydroxyphenyl)-1-hexanone

$C_{12}H_{14}BrClO_2$ mol. wt. 305.60

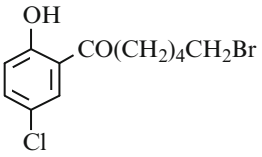


Synthesis
-Refer to: [706].
Methyl ether [57840-53-6]
C13$H_{16}BrClO_2$ mol. wt. 319.63

-Refer to: [706].

6-Bromo-1-(5-chloro-2-hydroxyphenyl)-1-hexanone

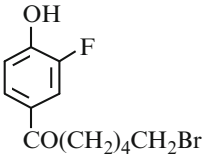
[173055-27-1] $C_{12}H_{14}BrClO_2$ mol. wt. 305.60



Synthesis
-Refer to: [2623].

6-Bromo-1-(3-fluoro-4-hydroxyphenyl)-1-hexanone

$C_{12}H_{14}BrFO_2$ mol. wt. 289.14



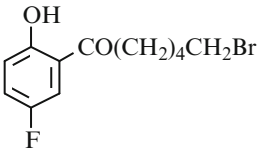
Synthesis
-Refer to: [2919].
Methyl ether [188973-66-2]
$C_{13}H_{16}BrFO_2$ mol. wt. 303.17

-Obtained by Friedel-Crafts acylation of 2-fluoroanisole with 6-bromohexanoyl chloride in the presence of aluminium chloride in methylene chloride at 25° [2919].
-Also refer to: [154, 1473, 3419].

m.p. 47–48° [154, 3419].

6-Bromo-1-(5-fluoro-2-hydroxyphenyl)-1-hexanone

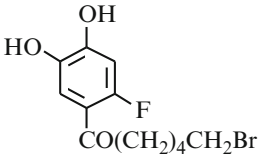
[173055-25-9] $C_{12}H_{14}BrFO_2$ mol. wt. 289.14



Synthesis
-Refer to: [2623].

6-Bromo-1-(2-fluoro-4,5-dihydroxyphenyl)-1-hexanone

$C_{12}H_{14}BrFO_3$ mol. wt. 305.14



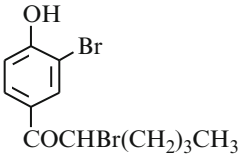
Synthesis
-Refer to: [560].

Dimethyl ether [123015-34-9]
$C_{14}H_{18}BrFO_3$ mol. wt. 333.20
-Refer to: [560].

m.p. 81–83° [558, 559]; MS [558, 559].

2-Bromo-1-(3-bromo-4-hydroxyphenyl)-1-hexanone

$C_{12}H_{14}Br_2O_2$ mol. wt. 350.05



Synthesis
-Refer to: [441].

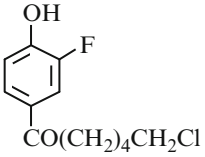
Methyl ether (2S) [306972-96-3]
$C_{13}H_{16}Br_2O_2$ mol. wt. 364.08

-Preparation of nonracemic α-bromoketones by stereoselective bromination of aryl alkyl tartrate acetals followed by hydrolysis (67 %, 66 % ee) [441].

m.p. 58–60° [441]; ^{1}H NMR [441], IR [441], MS [441].

6-Chloro-1-(3-fluoro-4-hydroxyphenyl)-1-hexanone

$C_{12}H_{14}ClFO_2$ mol. wt. 244.69



Synthesis
-Refer to: [217].

Methyl ether [927911-86-2]
$C_{13}H_{16}ClFO_2$ mol. wt. 258.72

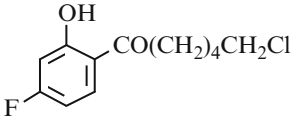
-Obtained by Friedel-Crafts acylation of 2-fluoroanisole with 6-chlorohexanoic acid using alkylhalosilanes, and indium halides or triflates [217].

-Also obtained by reaction of 6-chlorohexanoic acid with 2-fluoroanisole in the presence of $HSiMe_2Cl$ and $InCl_3$ in 1,2-dichloroethane, first 1 h at r.t., then heated at 80° for 4 h (72 %) [218].

m.p. 35–37° [218];
^1H NMR [218], ^{13}C NMR [218], IR [218], MS [218].

6-Chloro-1-(4-fluoro-2-hydroxyphenyl)-1-hexanone

[263545-26-2] $C_{12}H_{14}ClFO_2$ mol. wt. 244.69



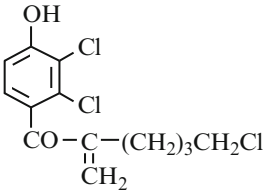
Syntheses
-Refer to: [1662, 1663].

Oxime [263545-27-3]
$C_{12}H_{15}ClFNO_2$ mol. wt. 259.71

-Refer to: [1662, 1663].

6-Chloro-1-(2,3-dichloro-4-hydroxyphenyl)-2-methylene-1-hexanone

$C_{13}H_{13}Cl_3O_2$ mol. wt. 307.60



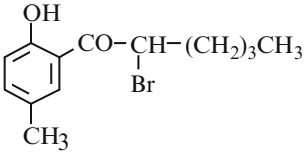
Syntheses
-Refer to: [732, 738, 2052].

Methyl ether [54343-87-2]
$C_{14}H_{15}Cl_3O_2$ mol. wt. 321.63
-Refer to: [732, 738, 2052].

-Prepn. and cyclization of, [738, 2052].

2-Bromo-1-(2-hydroxy-5-methylphenyl)-1-hexanone

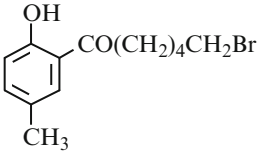
$C_{13}H_{17}BrO_2$ mol. wt. 285.18



Synthesis
-Refer to: [181].
m.p. 30.5–31.5° [181].

6-Bromo-1-(2-hydroxy-5-methylphenyl)-1-hexanone

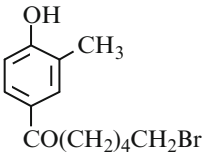
[173055-29-3] $C_{13}H_{17}BrO_2$ mol. wt. 285.18



Synthesis
-Refer to: [2623].

6-Bromo-1-(4-hydroxy-3-methylphenyl)-1-hexanone

[868521-08-8] $C_{13}H_{17}BrO_2$ mol. wt. 285.18

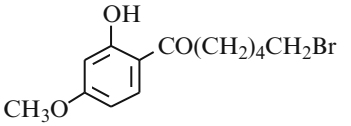


Synthesis
-Refer to: [1314].

USE: Polymeric prodrugs having temporary linkages to amino groups [1314].

6-Bromo-1-(2-hydroxy-4-methoxyphenyl)-1-hexanone

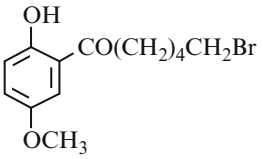
[173055-23-7] $C_{13}H_{17}BrO_3$ mol. wt. 301.18



Syntheses
-Refer to: [308, 2623, 3284].

6-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-hexanone

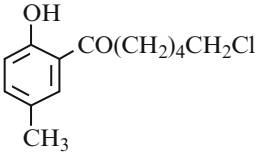
[173055-21-5] $C_{13}H_{17}BrO_3$ mol. wt. 301.18



Syntheses
-Refer to: [2623, 2918].

6-Chloro-1-(2-hydroxy-5-methylphenyl)-1-hexanone

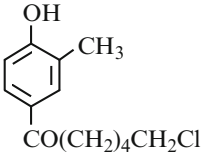
[51317-86-3] $C_{13}H_{17}ClO_2$ mol. wt. 240.73



Synthesis
-Obtained by reaction of 6-chlorocaproic acid with p-cresol in the presence of boron trifluoride (86 %) [2311].
m.p. 36° [2311]; pK = 4.64 [2311].

6-Chloro-1-(4-hydroxy-3-methylphenyl)-1-hexanone

$C_{13}H_{17}ClO_2$ mol. wt. 240.73



Synthesis
-Refer to: [218].

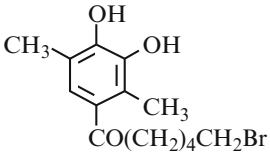
Methyl ether [927911-85-1]
$C_{14}H_{19}ClO_2$ mol. wt. 254.76

-Obtained by reaction of 6-chlorohexanoic acid with 2-methylanisole in the presence of $HSiMe_2Cl$ and $InCl_3$ (or $InBr_3$) in 1,2-dichloroethane, first 1 h at r.t., then heated at 80° for 4 h (78 %) (or 83 %) [218].

m.p. 44–46° [218];
^1H NMR [218], ^{13}C NMR [218], IR [218], MS [218].

6-Bromo-1-(3,4-dihydroxy-2,5-dimethylphenyl)-1-hexanone

$C_{14}H_{19}BrO_3$ mol. wt. 315.20



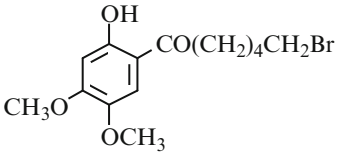
Synthesis
-Refer to: [560].

Dimethyl ether [123015-22-5]
$C_{16}H_{23}BrO_3$ mol. wt. 343.26
-Refer to: [560].

MS [558, 559].

6-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-hexanone

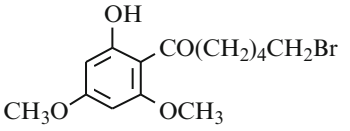
[173055-31-7] $C_{14}H_{19}BrO_4$ mol. wt. 331.20



Syntheses
-Refer to: [2623, 2918].
^1H NMR [2918].

6-Bromo-1-(2-hydroxy-4,6-dimethoxyphenyl)-1-hexanone

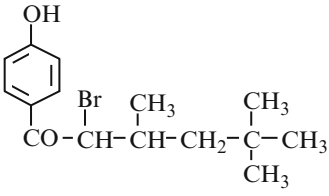
[173055-33-9] $C_{14}H_{19}BrO_4$ mol. wt. 331.20



Synthesis
-Refer to: [2623].

2-Bromo-3,5,5-trimethyl-1-(4-hydroxyphenyl)-1-hexanone

$C_{15}H_{21}BrO_2$ mol. wt. 313.23

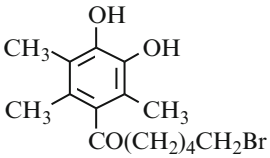


Synthesis
-Refer to: [1140].

Pentyl ether [97744-24-6]
$C_{20}H_{31}BrO_2$ mol. wt. 383.37
-Refer to: [1140].

6-Bromo-1-(3,4-dihydroxy-2,5,6-trimethylphenyl)-1-hexanone

$C_{15}H_{21}BrO_3$ mol. wt. 329.23



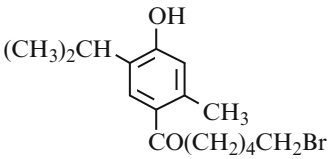
Synthesis
-Refer to: [560].

Dimethyl ether [123015-39-4]
$C_{17}H_{25}BrO_3$ mol. wt. 357.28
-Refer to: [560].

MS [558, 559].

6-Bromo-1-[4-hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-hexanone

$C_{16}H_{23}BrO_2$ mol. wt. 327.26



Synthesis
-Refer to: [220].

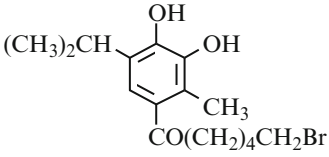
Methyl ether [72236-94-3]
$C_{17}H_{25}BrO_2$ mol. wt. 341.29
$n_D^{20} = 1.5424$ [220].

-Obtained by reaction of 6-bromohexanoyl chloride with thymol methyl ether in the presence of aluminium chloride in methylene chloride at r.t. (90 %) [220].

BIOLOGICAL ACTIVITY: Amebicidal and bactericidal and molluscicidal [220].

6-Bromo-1-[3,4-dihydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-hexanone

$C_{16}H_{23}BrO_3$ mol. wt. 343.26

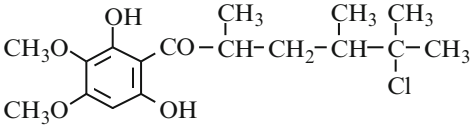


Synthesis
-Refer to: [560].

Dimethyl ether [123015-21-4]
$C_{18}H_{27}BrO_3$ mol. wt. 371.31
-Refer to: [560].

5-Chloro-1-(2,6-dihydroxy-3,4-dimethoxyphenyl)-2,4,5-trimethyl-1-hexanone

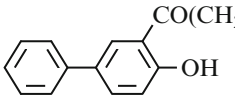
[1049661-48-4] $C_{17}H_{25}ClO_5$ mol. wt. 344.83



Synthesis
-Refer to: [802].

6-Bromo-1-(4-hydroxy[1,1′-biphenyl]-3-yl)-1-hexanone

$C_{18}H_{19}BrO_2$ mol. wt. 347.25



Synthesis
-Refer to: [308].

Methyl ether [187396-83-4]
$C_{19}H_{21}BrO_2$ mol. wt. 361.27

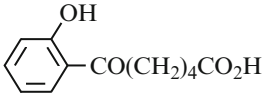
-Refer to: [308].

3 Aromatic Hydroxyketones Derived from 6-Oxohexanoic Acid

3.1 Unsubstituted Hydroxyketones

6-(2-Hydroxyphenyl)-6-oxo-1-hexanoic acid

[100118-19-2] $C_{12}H_{14}O_4$ mol. wt. 222.24



Syntheses
-Obtained by Fries rearrangement of phenyl adipate with aluminium chloride,
-in the presence of solvents:

*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];
*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].
-Also obtained by treatment of hexahydrodiphenyl oxide with chromium trioxide in acetic acid on a water bath (30 %) [444].
-Also obtained by diazotization of δ-o-aminobenzoylvaleric acid [2419].
-Also obtained by degradation of 2,3-dihydropentachromone (m.p. 120–121°) with KOH in dilute ethanol (69 %) [1211].
-Also refer to: [936 (80 %), 3370].

b.p.$_{12}$ 240–242° [444];
m.p. 94° [444, 902, 2419], 93–94° [1211], 90° [936].

Oxime [100391-90-0] $C_{12}H_{15}NO_4$ mol. wt. 237.26

m.p. 128° [444].

Semicarbazone [100706-52-3] $C_{13}H_{17}N_3O_4$ mol. wt. 279.30

m.p. 186° [444].

Phenylhydrazone $C_{18}H_{20}N_2O_3$ mol. wt. 312.37

m.p. 173° [444, 2419].

Benzoate $C_{19}H_{18}O_5$ mol. wt. 326.35

m.p. 82° [444].

Methyl ether [107151-39-3] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by treatment of title ketone with methyl iodide [444].
-Also refer to: [2495].

m.p. 82° [444, 2495].

Semicarbazone of the methyl ether $C_{14}H_{19}N_3O_4$ mol. wt. 293.32

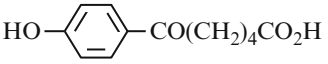
m.p. 175–176° [444].

Methyl ester of the methyl ether $C_{14}H_{18}O_4$ mol. wt. 250.29

m.p. 28° [444].

6-(4-Hydroxyphenyl)-6-oxo-1-hexanoic acid

[5537-75-7] $C_{12}H_{14}O_4$ mol. wt. 222.24



Syntheses
-Obtained by Fries rearrangement of phenyl adipate with aluminium chloride,

-in the presence of solvents:
*in the tetrachloroethane/nitrobenzene mixture (500 ml/125 ml) for 4 h at 50–60° [902];
*in nitrobenzene for 4 h at 50°, then 30 min at 60° [902];
*in tetrachloroethane at 80° [902].
-without solvent at 120° [902].
-Also obtained by reaction of adipyl chloride with phenol in the presence of aluminium chloride in nitrobenzene, first at 0–5°, then at r.t. for 12 h (36 %) [593].
-Also obtained by reaction of δ-carbomethoxyvaleroyl chloride with phenol in the presence of aluminium chloride in chlorobenzene, first at 10–15°, then at 60° for 6 h (45 %) [2519].
-Also refer to: [445, 1073, 3135].

m.p. 150° [593], 149–150° [2519], 148° [902, 3135], 147° [445].

2,4-Dinitrophenylhydrazone [5485-73-4] $C_{18}H_{18}N_4O_7$ mol. wt. 402.36

m.p. 166° [593].

Methyl ether [5537-76-8] $C_{13}H_{16}O_4$ mol. wt. 236.27

-Obtained by reaction of adipyl chloride with anisole in the presence of aluminium chloride in nitrobenzene/tetrachloroethane mixture (1:2) at 0° (45 %) [593].
-Also obtained (by-product) in the preparation of 1,6-bis(4-methoxyphenyl)-1,6-hexanedione (12–16 %) [1073].
-Also obtained by reaction of δ-carbomethoxyvaleroyl chloride with anisole in the presence of aluminium chloride,
*in a mixture of tetrachloroethane and chlorobenzene at 0–5° for 3 h and left overnight (79 %) [2519];
*in a mixture of tetrachloroethane and nitrobenzene (79 %) [2519];
*in tetrachloroethane at 0° for 3–4 h (95 %) [2392].
-Also obtained by reaction of adipic anhydride with anisole in the presence of aluminium chloride,
*in refluxing carbon disulfide for 3 h (23 %) [2494];
*in a mixture of nitrobenzene and tetrachloroethane for two days at 5° (33 %) [2519].
-Also obtained by treatment of its methyl ester in THF with 2 N sodium hydroxide at r.t. overnight (87 %) [1724].
-Also refer to: [178, 242, 701, 988, 1131, 2168, 3195].

colourless plates [2494];
m.p. 129° [593], 128–129° [2494], 128° [2392], 127–129° [242], 127–127.5° [2168, 3195], 127° [988, 2494], 126° [1073], 123–125° [178], 122–124° [2519];
^{1}H NMR [701, 1724], IR [242, 701, 1724].

BIOLOGICAL ACTIVITY: Delivery of human zinc insulin [1131].

Methyl ester of the methyl ether [29389-23-9] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of adipic acid monochloride monomethyl ester with anisole in the presence of aluminium chloride in methylene chloride at 0° for 30 min [1724].
-Refer to: [1274, 1512].

m.p. 65° [1274], 64–65° [1512];
^{1}H NMR [1512, 1724], ^{13}C NMR [1512], IR [1512, 1724], MS [1512].

Ethyl ester of the methyl ether [42916-80-3] $C_{15}H_{20}O_4$ mol. wt. 264.32

-Obtained by reaction of ethyl 5-(chloroformyl)pentanoate with anisole in the presence of aluminium chloride in tetrachloroethane (50 %) [2689].
-Also refer to: [878 (49 %), 1865, 2689, 3254].

b.p.$_{0.05}$ 142–155° [878];
m.p. 54° [3254], 52–54° [2689], 44–45° [878]; UV [3254],
ESR spectroscopy [3254]; phosphorescence spectroscopy [3254].

Ethyl ether [854659-09-9] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of adipic acid dichloride with phenetole in the presence of aluminium chloride in carbon disulfide first at −10°, then at r.t. for 5 h (16 %) [3196].
-Also refer to: [2494].

colourless plates [2494]; m.p. 111–112° [3196], 110° [2494].

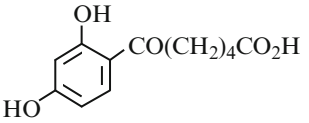
Ethyl ester [119348-65-1] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by treatment of 6-(4-hydroxyphenyl)-6-oxo-1-hexanoic acid in ethanol with methanesulfonic acid at 25° for 25 h (74 %) [878].

m.p. 66–67° [878].

6-(2,4-Dihydroxyphenyl)-6-oxo-1-hexanoic acid

[133535-20-3] $C_{12}H_{14}O_5$ mol. wt. 238.24



Syntheses
-Obtained by reaction of adipic acid with resorcinol in the presence of zinc chloride at 140° for 5 h (20 %) [445].
-Also refer to: [2606, 3370].

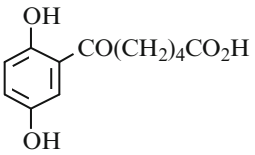
b.p.$_{0.5}$ 250° [445]; m.p. 171° [445], 169° [2606].

Methyl ester $C_{13}H_{16}O_5$ mol. wt. 252.27

b.p.$_{0.4}$ 230° [445]; m.p. 113° [445].

6-(2,5-Dihydroxyphenyl)-6-oxo-1-hexanoic acid

[108515-73-7] $C_{12}H_{14}O_5$ mol. wt. 238.24



Syntheses
Obtained by treatment of its dimethyl ether with hydrobromic acid in refluxing acetic acid for 1 h (67 %) [3175].
-Also obtained by condensation of quinol with adipic acid [469].
-Also refer to: [2331].

pale yellow leaflets [469];
m.p. 130–131.5° [3175], 130° [469].

2,4-Dinitrophenylhydrazone $C_{18}H_{18}N_4O_8$ mol. wt. 418.36

orange plates [469]; m.p. 194° [469].

Dimethyl ether [79381-16-1] $C_{14}H_{18}O_5$ mol. wt. 266.29

-Obtained by reaction of polymeric adipic anhydride with hydroquinone dimethyl ether in the presence of aluminium chloride (53 %) [2331].
-Also obtained by reaction of adipoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride,
*in carbon disulfide at < 10° (48 %) [3175];
*in nitrobenzene at 0° for 5 h (60 %) [3128].
-Also refer to: [3056].

needles [2331]; white prisms [3175]; colourless solid [3128];
m.p. 80.5–82° [3175], 78–80° [2331, 3056], 75–77° [3128];
^{1}H NMR [3128], ^{13}C NMR [3128].

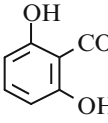
Methyl ester of the dimethyl ether [374808-50-1] $C_{15}H_{20}O_5$ mol. wt. 280.32

-Obtained by treatment of dimethyl ether with methanol in the presence of concentrated sulfuric acid (2 drops) at reflux for 18 h (94 %) [3128].

pale yellow oil [3128]; ^{1}H NMR [3128], ^{13}C NMR [3128].

6-(2,6-Dihydroxyphenyl)-6-oxo-1-hexanoic acid

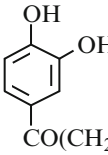
$C_{12}H_{14}O_5$ mol. wt. 238.24



Synthesis
-Refer to: [2483].
m.p. 138–140° [2483].

6-(3,4-Dihydroxyphenyl)-6-oxo-1-hexanoic acid

$C_{12}H_{14}O_5$ mol. wt. 238.24



Synthesis
-Refer to: [1013].
Dimethyl ether [38767-74-7]
$C_{14}H_{18}O_5$ mol. wt. 266.29

-Obtained by heating of its methyl ester below with 10 % aqueous NaOH on the steam bath for 1.5 h (90 %) [1013].
-Also obtained (by-product) by reaction of adipyl chloride with veratrole in the presence of aluminium chloride in carbon disulfide first at 0°, then at reflux for 3 h [1124].
-Also obtained by treatment of ethyl 6-(3,4-dimethoxyphenyl)-6-oxo-1-hexanoate with 10 % ethanolic NaOH at r.t. for 3 h (97 %) [306].
-Also refer to: [1080, 2982, 3057, 3363, 3364].

m.p. 123–125° [306], 123° [2982, 3057], 122–123.5° [3363],
122–123° [1013, 1124], 111–115° [1080];
^{1}H NMR [306], IR [1013, 3364].

Methyl ester of the dimethyl ether [57641-18-6] $C_{15}H_{20}O_5$ mol. wt. 280.32

-Obtained by reaction 6-chloro-6-oxohexanoic acid methyl ester with 1,2-dimethoxybenzene in the presence of aluminium chloride in 1,1,2,2-tetrachloroethane first at 0–3° for 2.5 h, then overnight to 2° (82 %) [1013].

b.p.$_{0.1}$ 175–176° [1013]; m.p. 65–66° [1013]; IR [1013].

Ethyl ester of the dimethyl ether [167159-65-1] $C_{16}H_{22}O_5$ mol. wt. 294.35

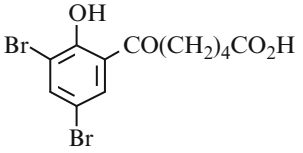
-Refer to: [306].

m.p. 50–52° [306]; ^{1}H NMR [306].

3.2 Substituted Hydroxyketones

6-(3,5-Dibromo-2-hydroxyphenyl)-6-oxo-1-hexanoic acid

$C_{12}H_{12}Br_2O_4$ mol. wt. 380.03



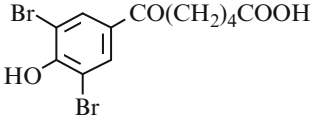
Synthesis

-Obtained by treatment of 1-(2-hydroxyphenyl)-6-oxo-1-hexanoic acid with a potassium bromate/potassium bromide mixture in dilute hydrochloric acid [936].

m.p. 128° [936].

6-(3,5-Dibromo-4-hydroxyphenyl)-6-oxo-1-hexanoic acid

[100121-89-9] $C_{12}H_{12}Br_2O_4$ mol. wt. 380.03



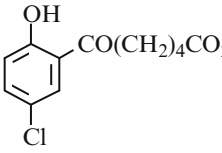
Synthesis

-Refer to: [2471].

m.p. 158° [2471].

6-(5-Chloro-2-hydroxyphenyl)-6-oxo-1-hexanoic acid

[857480-74-1] $C_{12}H_{13}ClO_4$ mol. wt. 256.69



Syntheses

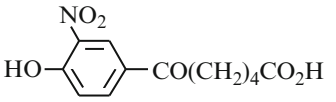
-Obtained by Fries rearrangement of bis(4-chlorophenyl) adipate (m.p. 110.5°) with aluminium chloride (1 mol) at 150° for 1 h (31 %) [3235].

-Also obtained by hydrolysis of 6-chloro-2,3-"dihydropentachromone" [2495].

m.p. 136° [2495, 3235].

6-(4-Hydroxy-3-nitrophenyl)-6-oxo-1-hexanoic acid

$C_{12}H_{13}NO_6$ mol. wt. 267.24



Synthesis
-Refer to: [2494].
Methyl ether
$C_{13}H_{15}NO_6$ mol. wt. 281.26

-Obtained by treatment of δ-anisoylvaleric acid in concentrated sulfuric acid with potassium nitrate between −5 and 0° (70 %) [2494].

pale yellow plates; m.p. 107–109° [2494].

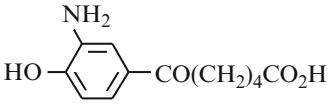
Ethyl ether [867134-00-7] $C_{14}H_{17}NO_6$ mol. wt. 295.29

-Refer to: [2494].

colourless prisms [2494]; m.p. 110° [2494].

6-(3-Amino-4-hydroxyphenyl)-6-oxo-1-hexanoic acid

$C_{12}H_{15}NO_4$ mol. wt. 237.26



Synthesis
-Refer to: [2494].
Methyl ether
$C_{13}H_{17}NO_4$ mol. wt. 251.28

-Obtained by adding a hot solution of 4-methoxy-3-nitrobenzoylvaleric acid in dilute ammonia to a boiling solution of ferrous sulfate to which an excess ammonia been added. The whole was boiled 10 min (41 %) [1531].

brown plates; m.p. 116° [2494].

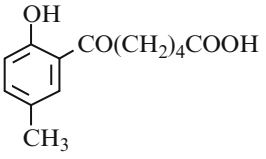
Ethyl ether $C_{14}H_{19}NO_4$ mol. wt. 265.31

-Refer to: [2494].

pink plates; m.p. 102° [2494].

6-(2-Hydroxy-5-methylphenyl)-6-oxo-1-hexanoic acid

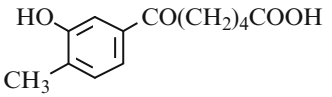
$C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Refer to: [1827].
UV [1827].

6-(3-Hydroxy-4-methylphenyl)-6-oxo-1-hexanoic acid

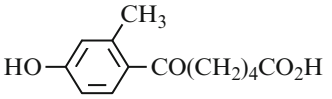
[124016-88-2] $C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Refer to: [2972].

6-(4-Hydroxy-2-methylphenyl)-6-oxo-1-hexanoic acid

[5538-11-4] $C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Obtained by reaction of adipyl chloride with m-cresol in the presence of aluminium chloride in nitrobenzene at 0° [593].

m.p. 100° [593].

2,4-Dinitrophenylhydrazone [5538-12-5] $C_{19}H_{20}N_4O_7$ mol. wt. 416.39

m.p. 185° [593].

Methyl ether [5538-14-7] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of adipyl chloride with m-cresol methyl ether in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture (1:1) at 0° [593].

$b.p._{.0.2}$ 160° [593].

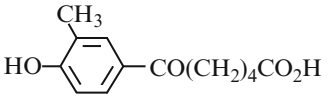
2,4-Dinitrophenylhydrazone of the methyl ether

[5550-55-0] $C_{20}H_{22}N_4O_7$ mol. wt. 430.42

m.p. 175° [593].

6-(4-Hydroxy-3-methylphenyl)-6-oxo-1-hexanoic acid

[5538-07-8] $C_{13}H_{16}O_4$ mol. wt. 236.27



Synthesis
-Obtained by reaction of adipyl chloride with o-cresol in the presence of aluminium chloride in nitrobenzene at 0° (90 %) [593].

m.p. 125° [593].

2,4-Dinitrophenylhydrazone [5550-52-7] $C_{19}H_{20}N_4O_7$ mol. wt. 416.39

m.p. 165° [593].

Methyl ether [5485-77-8] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Obtained by reaction of adipyl chloride with o-cresol methyl ether in the presence of aluminium chloride in a nitrobenzene/tetrachloroethane mixture (1:1) at 0° [593].

m.p. 95° [593].

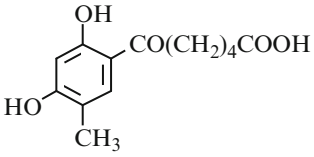
2,4-Dinitrophenylhydrazone of the methyl ether

[5538-09-0] $C_{20}H_{22}N_4O_7$ mol. wt. 430.42

m.p. 162° [593].

6-(2,4-Dihydroxy-5-methylphenyl)-6-oxo-1-hexanoic acid

[1344146-37-7] $C_{13}H_{16}O_5$ mol. wt. 252.27

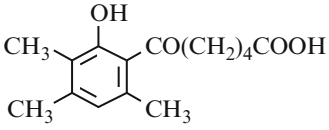


Synthesis
-Refer to: [1940].
m.p. 210–212° [1940]; ^{1}H NMR [1940], ^{13}C NMR [1940], IR [1940], MS [1940].

BIOLOGICAL ACTIVITY: Cytotoxic [1940].

6-(2-Hydroxy-3,4,6-trimethylphenyl)-6-oxo-1-hexanoic acid

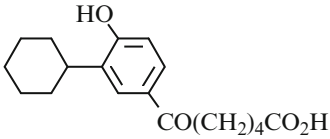
[58185-73-2] $C_{15}H_{20}O_4$ mol. wt. 264.32



Synthesis
-Refer to: [2149, 2325].
m.p. 146–148° [2149, 2325], ^{1}H NMR [2149, 2325], IR [2149, 2325].

6-(3-Cyclohexyl-4-hydroxyphenyl)-6-oxo-1-hexanoic acid

$C_{18}H_{24}O_4$ mol. wt. 304.39



Synthesis
-Preparation by demethylation of its methyl ether [496].
m.p. 137° [496].

Methyl ether $C_{19}H_{26}O_4$ mol. wt. 318.41

-Obtained by reaction of δ-carbomethoxyvaleryl chloride with o-cyclohexylanisole in the presence of aluminium chloride in benzene, first for 4 h between 3 and 8°, then at r.t. for 18 h. After hydrolysis, the residual crude methyl ester, after solvent elimination, was saponified with sodium hydroxide in refluxing methanol (50 %) [496].

colourless crystals [496]; m.p. 96° [496].

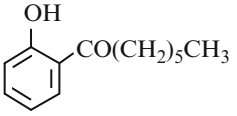
Chapter 5
Heptanones

1 Aromatic Hydroxyketones Derived from Heptanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-1-heptanone

[22362-59-0] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses

-Obtained by Fries reaction of phenyl enanthate with aluminium chloride,

*(58 %) [726];

*in nitrobenzene at 37.5° for 44.5 h (19 %) [244];

*without solvent at 140° for 45 min (51 %) [932].

-Also obtained by reaction of enanthoyl chloride with phenol in the presence of aluminium chloride,

*without solvent, first at 100°, then at 125–130° for 1 h (48 %) [2700];

*in nitrobenzene, first at 0°, then at r.t. overnight (33 %) [2700].

-Also obtained by stirring a solution of salicylaldehyde, 1-hexene, $RhCl(PPh_3)_3$ [1435], acetonitrile and sodium acetate in methylene chloride at r.t. for 8 h under an argon atmosphere (86 %) [1434].

-Also obtained by treatment of 4-chromanone with n-butyllithium in hexane/THF first at 0° for 4 h, then at r.t. overnight (16.3 %) [248].

-Also obtained by zeolite-catalyzed Friedel-Crafts reaction of anisole with heptanoic acid [3266].

-Also refer to: [1447, 2259, 2478, 2584, 3066].

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yellow semi-solid mass [248];
$b.p._{.0.1}$ 94° [932], $b.p._{.0.4}$ 104–106° [2478], $b.p._{.10}$ 155–156° [2700], $b.p._{.20}$ 172–174° [726];
m.p. 24° [726], 9.8° [2700];
^{1}H NMR [248, 1435, 1447, 3066], IR [1447, 3066],
UV [1996], MS [248, 1447]; TLC [248].
$n_D^{25} = 1.5205$ [2478], $n_D^{25} = 1.5211$ [932].

USE: Cyclization of, with chloroacetamide or chloroacetonitrile [2584].

Oxime $C_{13}H_{19}NO_2$ mol. wt. 221.30

-Obtained by treatment of 4-chromanone oxime with n-butyllithium in hexane/THF first at 0° for 4 h, then at r.t. overnight (54.8 %) [248].

white crystals [248]; m.p. 88–90° [248];
^{1}H NMR [248], ^{13}C NMR [248], IR [248], MS [248].

2,4-Dinitrophenylhydrazone $C_{19}H_{22}N_4O_5$ mol. wt. 386.41

m.p. 153° [932].

Phenylhydrazone $C_{19}H_{24}N_2O$ mol. wt. 296.41

m.p. 91–92° [726].

Methyl ether [118476-18-9] $C_{14}H_{20}O_2$ mol. wt. 220.31

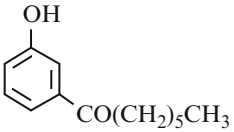
-Obtained by hydration of 1-(2-methoxyphenyl)-1-heptyne on treatment with sodium sulfide followed by aqueous HCl in methanol at 65° for 60 h (95 %) [611].
-Also refer to: [1648, 1649 (3 %)].

Ethyl ether [52922-74-4] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Obtained (by-product) by adding levulinic acid to the mixture of o-ethoxybenzoyl chloride and triethylamine at 0–5°. After, the reaction with hexylmagnesium bromide was carried at −20° (11 %) [130].

1-(3-Hydroxyphenyl)-1-heptanone

[132858-49-2] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses
-Synthesis of 3-hydroxyheptanophenone by means of organocadmium derivatives (60 %) [2586].
-Also obtained by treatment of its methyl ether with aluminium chloride in benzene by heating on a water bath for 2 h (80 %) [966].

-Also obtained by diazotization of 3-aminoheptanophenone (42 %) [551].
-Also obtained by treatment of its methyl ether with aluminium bromide in boiling benzene for 4–5 h [551].
-Also obtained by heating an emulsion of N,N-diethyl-2-heptanoyl-6-methoxybenzamide in 48 % hydrobromic acid and acetic acid under reflux for 48 h (20 %) [2321].
-Also refer to: [967].

orange oil [2321];
b.p.$_{1}$ 165–167° [2586], b.p.$_{0.6–0.7}$ 170–177° [551];
m.p. 66° [551], 62° [966, 967, 2586];
^{1}H NMR [2321], ^{13}C NMR [2321], IR [2321].

4-Nitrophenylhydrazone $C_{19}H_{23}N_3O_3$ mol. wt. 341.41

m.p. 143° [967].

2,4-Dinitrophenylhydrazone [110051-30-4] $C_{19}H_{22}N_4O_5$ mol. wt. 386.41

m.p. 193° [551], 191° [2586].

Acetate $C_{15}H_{20}O_3$ mol. wt. 248.32 b.p.$_{1}$ 144–146° [2586].

Methyl ether [100863-37-4] $C_{14}H_{20}O_2$ mol. wt. 220.31

-Obtained by treatment of 3-hydroxyenantophenone with dimethyl sulfate in 2 N sodium hydroxide on a water bath for 90 min (35 %) [551].
-Also obtained by adding a solution of hexylmagnesium bromide in ethyl ether to a solution of N,3-dimethoxy-N-methylbenzamide in THF and the reaction solution refluxing for 6 h (61 %) [436].
-Also obtained by condensation of hexylmagnesium bromide with m-methoxybenzamide in ethyl ether. The reaction was carried out at 60° for 48 h under hydrogen atmosphere (60–70 %) [966].
-Also obtained by hydration of 1-(3-methoxyphenyl)-1-heptyne on treatment with sodium sulfide followed by aqueous HCl in methanol at 65° for 60 h (<25 %) [611].
-Also obtained by treatment of 1-(3-methoxyphenyl)-1-heptanol with CrO_3 in aqueous sulfuric acid in acetone at 5°, then at r.t. for 30 h (98 %) [635].
-Also refer to: [2789].

colourless oil [436]; pale yellow oil [551];
b.p.$_{0.6}$ 139–144° [551], b.p.$_{20}$ 235° [966, 967];
^{1}H NMR [436, 635, 2789], ^{13}C NMR [635, 2789],
MS [635, 2789]; $n_D^{20} = 1.5153$ [551], $n_D^{35} = 1.5171$ [967].

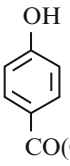
2,4-Dinitrophenylhydrazone of the methyl ether

[102458-44-6] $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 110.5–111° [551], 107° [967].

1-(4-Hydroxyphenyl)-1-heptanone

[14392-72-4] $C_{13}H_{18}O_2$ mol. wt. 206.28



Syntheses

-Phenol was energetically mixed with finely divided aluminium chloride (1 mol) and heated to 100° (1 mol of hydrochloric acid is evolved); 1 mol of n-enantoyl chloride was then added and heated to 125–130° for 1 h (41 %) [2700].

-Also obtained by reaction of heptanoyl chloride with phenol in the presence of aluminium chloride in methylene chloride for 14 h at r.t. (45 %) [1910].
-Also obtained by reaction of enanthic acid with phenol in the presence of zinc chloride (9 %) [726].
-Also obtained by Fries reaction of phenyl enanthate with aluminium chloride,
*in nitrobenzene (60 %) [379] at 37.5° for 44.5 h (72 %) [244] at 38° for 2 days (45 %) [414] or at 40° for 48 h under an argon atmosphere (73.4 %) [1116];
*without solvent at 140° for 45 min (34 %) [932].
-Also obtained [2478] by the method [2074].
-Also refer to: [62, 499, 513, 914, 1057, 1536 (92 %), 1872].

$b.p._{.0.4}$ 166° [2478], $b.p._{.1}$ 171° [932, 1536], $b.p._{.9}$ 214° [2700], $b.p._{.15}$ 220° [726]; white solid [1910];
m.p. 95.2–95.7° [1910], 93–94° [726], 92–94° [414], 92° (Sadtler standard N° 65674K),
91–92° [379], 91–91.5° [2700], 90° [932, 1116], 88° [2478];
^{1}H NMR [1910] (Sadtler standard N° 38625M), ^{13}C NMR [1910],
IR [1910] (Sadtler standard N° 65674K), UV [1995], MS [1910]; TLC [1910].

BIOLOGICAL ACTIVITY: Inhibition of 17-β hydroxysteroid dehydrogenase 3 [1910]; Fungicides, for coatings, for kitchens and ship bulls [499].

2,4-Dinitrophenylhydrazone $C_{19}H_{22}N_4O_5$ mol. wt. 386.41

m.p. 199–200° [379], 174° [932].

Nicotinylhydrazone [102011-49-4] $C_{19}H_{23}N_3O_2$ mol. wt. 325.41

m.p. 155° [520, 521].

USE: In chemotherapy of leprosy [520, 521].

isoNicotinylhydrazone [108984-69-6] $C_{19}H_{23}N_3O_2$ mol. wt. 325.41

m.p. 203° [520, 521].

USE: In chemotherapy of leprosy [520, 521].

Acetate $C_{15}H_{20}O_3$ mol. wt. 248.32

b.p.$_9$ 194–195° [2700]; m.p. 46.5° [2700].

Benzoate $C_{20}H_{22}O_3$ mol. wt. 310.39

m.p. 96.5–97° [2700], 92–93° [726].

Methyl ether [69287-13-4] $C_{14}H_{20}O_2$ mol. wt. 220.31

-Obtained by adding a solution of hexylmagnesium bromide in ethyl ether to a solution of N,4-dimethoxy-N-methylbenzamide in THF and the reaction solution refluxing for 6 h (89 %) [436].
-Other preparation: n-hexyl triphenylphosphonium bromide and lithium iodide were suspended in THF. The reaction flask was wrapped with aluminium foil. At ice-water temperature, butyllithium in hexane was added, producing the red solution of the phosphorane. After 20 min, THF containing 4-methoxybenzonitrile was added. The reaction mixture was then maintained at 50° for 8 h (95 %) [3014].
-Also obtained by Friedel-Crafts acylation of anisole with n-heptanoic acid in the presence of [$Eu(NTf_2)_3$] at 250° for 6 h (87 %) [2709], (84 %) [1649].
-Also obtained by direct acylation of 4-bromoanisole with enanthic aldehyde by palladium catalysis (88 %) [2668].
-Also obtained by reaction of heptanoyl chloride with 4-methoxyphenylmagnesium chloride in the presence of $Fe(acac)_3$ as catalyst in THF at −78° (99 %) [2739].
-Also obtained by Friedel-Crafts acylation of anisole using metal triflates in ionic liquid [2654].
-Obtained by reaction of dimethyl sulfate with 4-heptanoylphenol in the presence of aqueous sodium hydroxide for 4 h at reflux [2478].
-Also obtained by reaction of 4-methoxybenzyl alcohol with 1-hexene in the presence of $RhCl_3$, x H_2O, polystyrene-based diphenylphosphine and PPh_3 with co-catalyst 2-amino-4-picoline in toluene at 130° for 72 h (58–68 %) [1555].
-Also obtained by reaction of heptanoic acid with anisole,
*in the presence of $HNTf_2$ in refluxing toluene for 36 h, using a Dean-Stark apparatus (89 %) [1648];
*in the presence of $Eu(NTf_2)_3$ at 250° for 6 h (84 %) [1648];
*over HZSM-5 catalyst for 48 h at 423° K (7 %) [3265];
*in the presence of an ultrastable Y zeolite (USY) catalyst [1941];
*in the presence of HY zeolite as catalyst [3264].
-Also obtained by hydration of 1-(4-methoxyphenyl)-1-heptyne on treatment with sodium sulfide followed by aqueous HCl in methanol at 65° for 60 h (92 %) [611].
-Also obtained by zeolite-catalyzed Friedel-Crafts reaction of anisole with heptanoic acid [3266].

-Also refer to: [605, 698 (74 %), 1009, 1200, 1202, 1558 (79 %), 1679, 1749 (81 %), 1750, 2080, 2399, 2478, 2866, 2901, 3214, 3262].

b.p.$_{0.4}$ 120–121° [2478], b.p.$_{17}$ 192° [2901], b.p.$_{25}$ 203° [251], b.p.$_{50}$ 240° [2399]; white solid [1648];
m.p. 44–45° [2739], 43° [251], 41–43° [3214], 40° [2901], 39–40° [2478], 38.6–39.8° [1750], 38–39° [1648];
^{1}H NMR [436, 698, 1649, 1749, 1750, 2668, 2709, 2739, 3014],
^{13}C NMR [698, 2668, 2739, 3014],
IR [698, 1749, 1750, 2668, 2709, 2739],
MS [698, 2668, 2739]; $n_D^{28} = 1.5114$ [2399].

Phenylhydrazone of the methyl ether $C_{20}H_{26}N_2O$ mol. wt. 310.44

m.p. 35° [2901].

2-Bromoethyl ether [60985-68-4] $C_{15}H_{21}BrO_2$ mol. wt. 313.23

USE: Preparation and condensation with (methylphenethyl)amine [2484].

Propyl ether $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by reaction of heptanoyl chloride with phenyl propyl ether in the presence of zinc chloride at reflux for 30 min (30.6 %) [1237].

b.p.$_{15}$ 217–221° [1237]; m.p. 31–32° [1237].

Oxime of the propyl ether $C_{16}H_{25}NO_2$ mol. wt. 263.38

m.p. 53.5° [1237].

1,1,2,2-Tetrafluoroethyl ether [56426-10-9] $C_{15}H_{18}F_4O_2$ mol. wt. 306.44

USE: Reaction of, with halogenated heterocycles [297].

4-Heptanoylphenyl ether [149454-86-4] $C_{26}H_{34}O_3$ mol. wt. 394.55

-Obtained by reaction of heptanoyl chloride with diphenyl ether in the presence of aluminium chloride in refluxing carbon disulfide for 30 min (85 %) [463].

m.p. 102–103° [463].

Dioxime of the 4-heptanoylphenyl ether $C_{26}H_{36}N_2O_3$ mol. wt. 424.58

-Preparation: A suspension of the diketone, 100 % excess of hydroxylamine hydrochloride, and powdered anhydrous sodium carbonate in butanol [463].

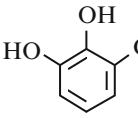
m.p. 102–103° [721], 95–96° [463].
m.p. 95–96° [463].

Dihydrazone of the 4-heptanoylphenyl ether $C_{26}H_{38}N_4O$ mol. wt. 422.61

b.p.$_{0.02}$ 212–218° [721]; m.p. 95–96° [721].

1-(2,3-Dihydroxyphenyl)-1-heptanone

[862666-35-1] $C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis

-Obtained by deprotection of its dimethyl ether with boron tribromide in methylene chloride at 0°. Then, the mixture was stirred overnight at r.t. (70 %) [82].

brown solid [82]; m.p. 46° [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

USE: Reactant for preparation of lithium gallium/titanium ketone complexes [82].

Dimethyl ether [1854-69-9] $C_{15}H_{22}O_3$ mol. wt. 250.34

-Obtained by treatment of 1-(2,3-dimethoxyphenyl)-1-heptanol in acetone with potassium dichromate in dilute sulfuric acid (Jones reagent) at r.t. for 3 h (28 %) [82].
-Also obtained by treatment of 2,3-dimethoxyphenylhexylcarbinol with potassium dichromate in dilute sulfuric acid at 30° (73.5 %) [3148].

colourless oil [82]; b.p.$_{10}$ 179–181° [3148];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

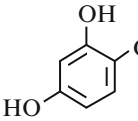
2,4-Dinitrophenylhydrazone of the dimethyl ether

[1854-68-8] $C_{21}H_{26}N_4O_6$ mol. wt. 430.46

m.p. 127° [3148].

1-(2,4-Dihydroxyphenyl)-1-heptanone
(Res-oenanthophenone)

[27883-47-2] $C_{13}H_{18}O_3$ mol. wt. 222.28



Syntheses

-Obtained by reaction of enanthic nitrile with resorcinol (Hoesch reaction) [1608].
-Also obtained by reaction of heptanoic acid with resorcinol in the presence of zinc chloride (68–78 %) [2501].

-Also obtained by reaction of heptanoyl chloride with resorcinol in the presence of aluminium chloride in 1,2-ethylene chloride for 5 h at 65° [284].
-Also refer to: [893, 1500, 1655, 1673, 1798, 2112, 2114, 2790, 2842, 3168].

b.p.$_{6-7}$ 204–206° [893, 2842];
m.p. 48–50° [893, 1673, 2842], 48–49° [1608].

USE: Polyamide fibers modified with, transparency of, [2790]; Wine preservation by, [3168].

BIOLOGICAL ACTIVITY: Antiseptic and germicidal product [2734]; Antifungal [2112, 2114]; Nematocide [1798].

Hemihydrate $C_{13}H_{18}O_3$, 0.5 H_2O mol. wt. 231.29

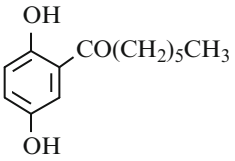
m.p. 41–43° [1608].

Oxime [165740-65-8] $C_{13}H_{19}NO_3$ mol. wt. 237.30

USE: Silver halide photog. material [1472].

1-(2,5-Dihydroxyphenyl)-1-heptanone

[18787-33-2] $C_{13}H_{18}O_3$ mol. wt. 222.28



Syntheses
-Obtained by Friedel-Crafts acylation of hydroquinone with heptanoyl chloride [1442].
-Also obtained by Fries reaction of hydroquinone diheptanoate [1442].
-Also obtained by treatment of its dimethyl ether with hydrobromic acid in acetic acid, first at 0°, then at reflux for 6 h [1442].

-Preparation by reaction of heptanoic acid with hydroquinone in the presence of boron trifluoride for 2 h at 125° [2063].
-Also refer to: [3168, 3460, 3462].

m.p. 118° [1442], 50° [2063].
N.B.: One of the reported melting point is obviously wrong.

USE: Electroluminescent devices employing complex fluorene-containing compounds [3461]; Wine preservation by, [3168].

Oxime [165740-62-5] $C_{13}H_{19}NO_3$ mol. wt. 237.30

USE: Silver halide photog. material [1472].

Dimethyl ether [719315-63-6] $C_{15}H_{22}O_3$ mol. wt. 250.34

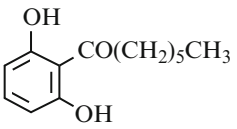
-Preparation by reaction of heptanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in nitrobenzene at r.t. overnight [1442].
-Also refer to: [550 (by-product), 3460, 3462].

b.p.$_{.5}$ 175–180° [1442]; m.p. 34–35° [1442].

USE: Electroluminescent devices employing complex fluorene-containing compounds [3461].

1-(2,6-Dihydroxyphenyl)-1-heptanone

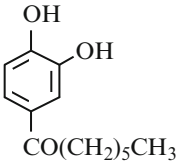
$C_{13}H_{18}O_3$ mol. wt. 222.28



Synthesis
-Refer to: [2672].
m.p. 75° [2672].

1-(3,4-Dihydroxyphenyl)-1-heptanone
(4-Heptanoylcatechol)

[2525-08-8] $C_{13}H_{18}O_3$ mol. wt. 222.28



Syntheses
-Obtained by adding heptanoyl chloride (1 mol) to a solution of pyrocatechol (1 mol) and aluminium chloride (1.5 mol) in carbon disulfide. After heating at 40–50° the solvent was removed and the residue heated at 150° for 4 h (50 %) [1283].
-Also obtained by treatment of guaiacol heptanoate with aluminium chloride in carbon disulfide at 90° for 50 min, then at 135–140° for 2 h after solvent elimination [2075].
-Also refer to: [2508].

m.p. 93–94° [1283], 78–79° [2075]; paper chromatography [2508].

O-Methyloxime [474668-95-6] $C_{14}H_{21}NO_3$ mol. wt. 251.33

-Refer to: [3177].

Dimethyl ether [101100-86-1] $C_{15}H_{22}O_3$ mol. wt. 250.34

-Obtained by reaction of heptoyl chloride with veratrole in the presence of zinc chloride in refluxing carbon disulfide for 4 h and then left overnight (60 %) [2836], (59 %) [1486].
-Also refer to: [2505].

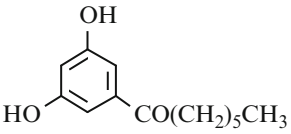
b.p.$_{.4}$ 178–180° [2836], b.p.$_{.1}$ 180° [1486].

Semicarbazone of the dimethyl ether [101427-26-3] $C_{16}H_{25}N_3O_3$ mol. wt. 307.39

white needles [2836]; m.p. 141° [1486], 140–141° [2836].

1-(3,5-Dihydroxyphenyl)-1-heptanone

[39192-54-6] $C_{13}H_{18}O_3$ mol. wt. 222.28



Syntheses

-Obtained by treatment of its diacetate with 5 % sodium hydroxide (quantitatif yield) [1880], at reflux for 4.5 h (62 %) [1406].

Isolation from natural sources

-From the roots and stems of *Ardisia virens* Kurz (Myrsinaceae) [607].
-From the roots of *Ardisia cornudentata* Mez. [604].

m.p. 94° [1406], 88–89° [1880].

2,4-Dinitrophenylhydrazone [102161-23-9] $C_{19}H_{22}N_4O_6$ mol. wt. 402.41

m.p. 230° [1406].

Diacetate [39192-52-4] $C_{17}H_{22}O_5$ mol. wt. 306.36

-Preparation by reaction of dihexylcadmium with 3,5-diacetoxybenzoyl chloride (quantitatif yield) [1880], in refluxing benzene for 1 h (82 %) [1406].

$b.p._{.0.8}$ 205° [1406].

2,4-Dinitrophenylhydrazone of the diacetate

[102655-30-1] $C_{23}H_{26}N_4O_8$ mol. wt. 486.48

m.p. 132° [1406].

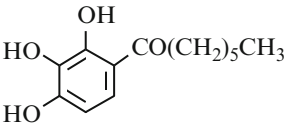
Dimethyl ether [39192-51-3] $C_{15}H_{22}O_3$ mol. wt. 250.34

-Preparation by reaction of hexylmagnesium bromide with 3,5-dimethoxybenzamide in refluxing ethyl ether for 5 h (85 %) [2990].
-Preparation by reaction of hexyl bromide with 3,5-dimethoxybenzonitrile [2017].
-Preparation by reaction of hexylmagnesium bromide with (3,5-dimethoxyphenyl)-*N*-methoxy-*N*-methylcarboxamide (90 %) [1252].
-Also obtained by adding a solution of chromic acid in dilute sulfuric acid (Jone's reagent) to a cold solution (0 °C) of 1-(3,5-dimethoxyphenyl)-1-heptanol in acetone. Then, the reaction mixture was stirred at r.t. for 30 min (79.6 %) [2394].
-Also refer to: [1880 (quantitatif yield), 2144, 2395, 2396, 2575, 2899].

white solid [1252];
$b.p._{.3}$ 161–161.5° [2990]; m.p. 30.5–31° [2990], 27–28° [1252];
^{1}H NMR [1252, 2394], ^{13}C NMR [1252], IR [1252], MS [1252];
$n_D^{25} = 1.5175$ [2990].

1-[2,3,4-Trihydroxyphenyl]-1-heptanone

[43043-27-2] $C_{13}H_{18}O_4$ mol. wt. 238.28

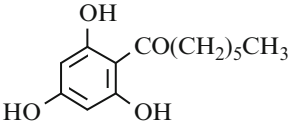


Synthesis
-Refer to: [1260, 1500, 3168].
m.p. 78–78.5° [1260].

USE: Wine preservation by, [3168].

1-[2,4,6-Trihydroxyphenyl]-1-heptanone

[43043-31-8] $C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses
-Obtained by reaction of enanthic nitrile with phloroglucinol (Hoesch reaction) [1608].
-Also obtained by reaction of heptanoyl chloride with phloroglucinol in the presence of aluminium chloride,

*in nitrobenzene for 3 days at r.t. (60–70 %) [421];
*in nitrobenzene and carbon disulfide mixture (58 %) [2113].
-Also refer to: [1026, 1439, 2111, 2719, 3168].

m.p. 108° [2113], 107–108° [1608], 107° [421, 1439];
^{1}H NMR [421], IR [421], MS [421].

USE: Assembly and photodimerization of bis(pyridyl)ethylene with phloroglucinols [1038]; Wine preservation by, [3168].

BIOLOGICAL ACTIVITY: Antifungal [2111, 2113, 2719]; Anthelmintic and bactericide [1439].

Monohydrate $C_{13}H_{18}O_4, H_2O$ mol. wt. 256.30

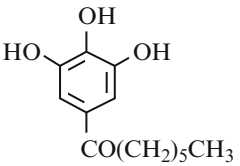
m.p. 98–100° [1608].

Polymer with formaldehyde [108080-61-1].

-Refer to: [1366].

1-(3,4,5-Trihydroxyphenyl)-1-heptanone

[100079-25-2] $C_{13}H_{18}O_4$ mol. wt. 238.28



Syntheses
-Refer to: [151, 2315].

BIOLOGICAL ACTIVITY: As platelet aggregation inhibitor and antiallergic agent [2315].

Trimethyl ether $C_{16}H_{24}O_4$ mol. wt. 280.36

-Obtained by treatment of ethyl 3,4,5-trimethoxybenzoylamylacetate with 5 % alc. KOH at 40° [151].

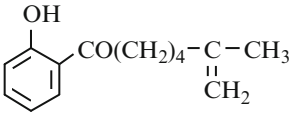
b.p.$_{.4}$ 175–176° [151]; m.p. 29° [151].

Tribenzyl ether [100079-28-5] $C_{34}H_{36}O_4$ mol. wt. 444.66

-Refer to: [2315].

1-(2-Hydroxyphenyl)-6-methylene-1-heptanone

$C_{14}H_{18}O_2$ mol. wt. 218.30



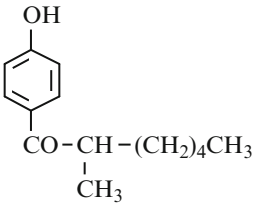
Synthesis

-Obtained by intermolecular hydroacylation between salicylaldehyde and 2-methyl-1,5-hexadiene (6 equiv.) in the presence of $RhCl(PPh_3)_3$ (0.2 equiv.) in methylene chloride for 24 h at r.t. (5 %) [1435].

^{1}H NMR [1435].

1-(4-Hydroxyphenyl)-2-methyl-1-heptanone (+)

[120837-02-7] (+) $C_{14}H_{20}O_2$ mol. wt. 220.31

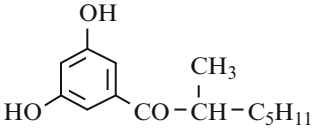


Synthesis

-Refer to: [1321].

1-(3,5-Dihydroxyphenyl)-2-methyl-1-heptanone

$C_{14}H_{20}O_3$ mol. wt. 236.31



Synthesis

-Refer to: [25].

Dimethyl ether [10586-43-3]

$C_{16}H_{24}O_3$ mol. wt. 264.36

-Preparation from 3,5-dimethoxybenzamide and $BrMgCH(CH_3)C_5H_{11}$ in ethyl ether (93 %) [479], (82 %) [25, 31].

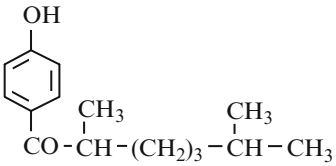
-Also refer to: [870, 2348].

b.p.$_{.0.2}$ 130° [479], b.p.$_{0.2}$ 133–138° [870], b.p.$_{.1}$ 147° [25, 31];
^{1}H NMR [479]; $n_D^{20} = 1.5136$ [25].

USE: Preparation of soft cannabinoid analogues as potential antiglaucoma agents [479]; Preparation and Grignard reaction with methyl iodide [2348].

1-(4-Hydroxyphenyl)-2,6-dimethyl-1-heptanone

[117692-93-0] $C_{15}H_{22}O_2$ mol. wt. 234.34

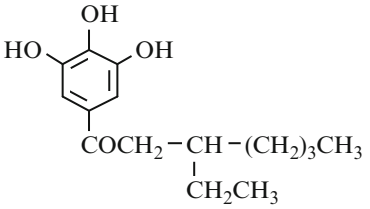


Synthesis
-Refer to: [2095].

Benzyl ether [117692-92-9]
$C_{22}H_{28}O_2$ mol. wt. 324.46
-Refer to: [2095].

3-Ethyl-1-(3,4,5-trihydroxyphenyl)-1-heptanone-

[353499-11-3] $C_{15}H_{22}O_4$ mol. wt. 266.34

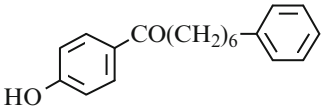


Syntheses
-Refer to: [1969, 2688].

USE: Developing agent for making lithographic plates [2688].

1-(4-Hydroxyphenyl)-5-phenyl-1-heptanone

[14392-75-7] $C_{19}H_{22}O_2$ mol. wt. 282.38

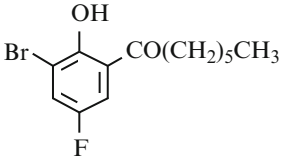


Synthesis
-Refer to: [414, 415].
m.p. 76° [415], 74–76° [414].

1.2 Substituted Hydroxyketones

1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-heptanone

[2342-47-4] $C_{13}H_{16}BrFO_2$ mol. wt. 303.17



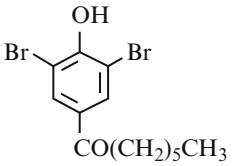
Synthesis
-Obtained by Fries rearrangement of 2-bromo-4-fluorophenyl enanthate with aluminium chloride at 130–140° for 3 h (90 %) [1550].
$b.p._{.0.2–0.5}$ 148° [1550].

2,4-Dinitrophenylhydrazone [2317-60-4] $C_{19}H_{20}BrFN_4O_5$ mol. wt. 483.29

m.p. 140–141° [1550].

1-(3,5-Dibromo-4-hydroxyphenyl)-1-heptanone

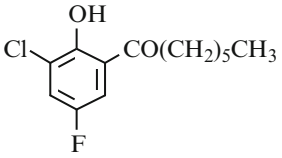
[20683-50-5] $C_{13}H_{16}Br_2O_2$ mol. wt. 364.08



Synthesis
-Obtained by reaction of bromine with 4-hydroxyenanthophenone in aqueous acetic acid [516].
m.p. 71° [516].

1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-heptanone

[2342-49-6] $C_{13}H_{16}ClFO_2$ mol. wt. 258.72



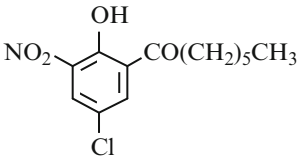
Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-fluorophenyl enanthate with aluminium chloride at 130–140° for 3 h (90 %) [1550].
$b.p._{.0.5}$ 140° [1550].

2,4-Dinitrophenylhydrazone [1814-29-5] $C_{19}H_{20}ClFN_4O_5$ mol. wt. 438.84

m.p. 132° [1550].

1-(5-Chloro-2-hydroxy-3-nitrophenyl)-1-heptanone

[85052-25-1] $C_{13}H_{16}ClNO_4$ mol. wt. 285.73

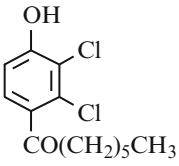


Synthesis
-Preparation by treatment of 5-chloro-2-hydroxyheptanophenone with concentrated nitric acid (60 %) in acetic acid in the presence of one drop of concentrated sulfuric acid for 25 min at r.t. (92 %) [2105].

^{1}H NMR [2105], MS [2105].

1-(2,3-Dichloro-4-hydroxyphenyl)-1-heptanone

[55507-84-1] $C_{13}H_{16}Cl_2O_2$ mol. wt. 275.17

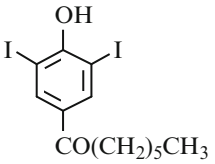


Syntheses
-Refer to: [733, 739].
m.p. 82–84° [739].

USE: Preparation and etherification of, with bromoacetate [733].

1-(4-Hydroxy-3,5-diiodophenyl)-1-heptanone

$C_{13}H_{16}I_2O_2$ mol. wt. 458.08



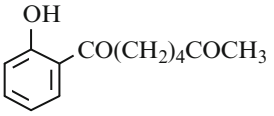
Synthesis

-Obtained by reaction of iodine with 4-hydroxyenanthophenone in ethanol in the presence of yellow mercuric oxide [516].

colourless needles [516]; m.p. 50° [516].

1-(2-Hydroxyphenyl)-1,6-heptanedione

[1237740-92-9] $C_{13}H_{16}O_3$ mol. wt. 220.27



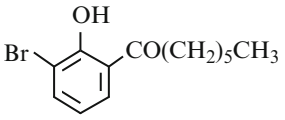
Synthesis

-Refer to: [498].

^{1}H NMR [498], ^{13}C NMR [498], IR [498], MS [498].

1-(3-Bromo-2-hydroxyphenyl)-1-heptanone

$C_{13}H_{17}BrO_2$ mol. wt. 285.18



Synthesis

-Refer to: [3036].

Methyl ether [952103-47-8]

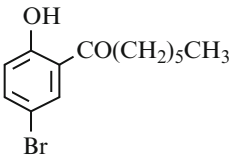
$C_{14}H_{19}BrO_2$ mol. wt. 299.21

-Refer to: [2214, 3036].

USE: Preparation of optically active-4-phenylthiazole derivs. [3036]; Preparation of thrombopoietin receptor agonist by yeast [2214].

1-(5-Bromo-2-hydroxyphenyl)-1-heptanone

$C_{13}H_{17}BrO_2$ mol. wt. 285.18



Synthesis

-Obtained by Fries rearrangement of 4-bromophenyl heptanoate with aluminium chloride [2797].

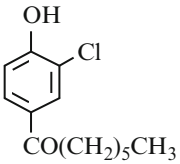
2,4-Dinitrophenylhydrazone

$C_{19}H_{21}BrN_4O_5$ mol. wt. 465.30

m.p. 189° [2798].

1-(3-Chloro-4-hydroxyphenyl)-1-heptanone

$C_{13}H_{17}ClO_2$ mol. wt. 240.73



Synthesis
-Refer to: [789].

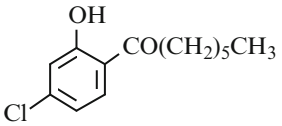
Methyl ether [250686-92-1]
$C_{14}H_{19}ClO_2$ mol. wt. 254.76

m.p. 24° [1160].

USE: News nematics with negative dielectric anisotropy [789].

1-(4-Chloro-2-hydroxyphenyl)-1-heptanone

$C_{13}H_{17}ClO_2$ mol. wt. 240.73



Syntheses
-Preparation by Fries rearrangement of 3-chlorophenyl heptoate with aluminium chloride,
*without solvent at 130° for 2 h (83 %) [2802];
*in nitrobenzene at 25° for 6 h (83 %) [2802].

$b.p._{.30}$ 200° [2802].

2,4-Dinitrophenylhydrazone $C_{19}H_{21}ClN_4O_5$ mol. wt. 420.85

m.p. 189° [2797].

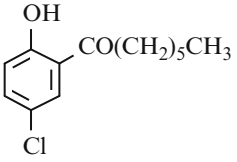
Methyl ether $C_{14}H_{19}ClO_2$ mol. wt. 254.76

-Obtained by methylation of the above ketone in the usual way (90 %) [2802].

$b.p._{.36}$ 180° [2802].

1-(5-Chloro-2-hydroxyphenyl)-1-heptanone

[85052-18-2] $C_{13}H_{17}ClO_2$ mol. wt. 240.73

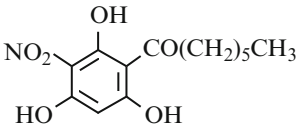


Syntheses
-Obtained by Fries rearrangement of 4-chlorophenyl enanthate with titanium tetrachloride at 100° for 18 h (72 %) [2105].
-Also refer to: [1702].

$b.p._{.5}$ 140–144° [1702]; m.p. 43.5° [1702];
^{1}H NMR [2105]; MS [2105].

1-(2,4,6-Trihydroxy-3-nitrophenyl)-1-heptanone

[119691-97-3] $C_{13}H_{17}NO_6$ mol. wt. 283.28



Syntheses

-Obtained by adding hexane, then a mixture of concentrated sulfuric acid and fuming nitric acid at 0° to a solution of 1-(2,4,6-trihydroxyphenyl)-1-heptanone in concentrated sulfuric acid below 0° (70–80 %) [3414].

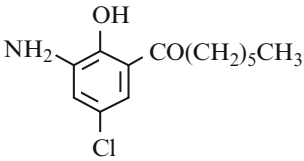
-Also refer to: [3406].

Amorphous [3414]; ^{1}H NMR [3414], IR [3414], MS [3414].

BIOLOGICAL ACTIVITY: Germination inhibitory activity [3414]; PET inhibitory activity [3414].

1-(3-Amino-5-chloro-2-hydroxyphenyl)-1-heptanone

[85052-73-9] $C_{13}H_{18}ClNO_2$ mol. wt. 255.74



Synthesis

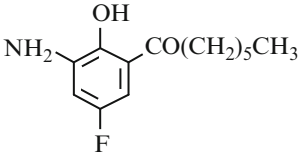
-Obtained by reduction of 1-(5-chloro-2-hydroxy-3-nitro-phenyl)-1-heptanone with titanium trichloride [2105].

Hydrochloride [85052-45-5]

$C_{13}H_{18}ClNO_2$, HCl mol. wt. 292.20

1-(3-Amino-5-fluoro-2-hydroxyphenyl)-1-heptanone

$C_{13}H_{18}FNO_2$ mol. wt. 239.29

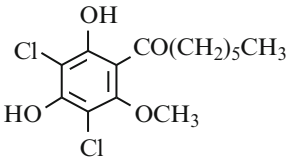


Synthesis

-Refer to: [2105].

1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-heptanone

[118191-32-5] $C_{14}H_{18}Cl_2O_4$ mol. wt. 321.20



Synthesis

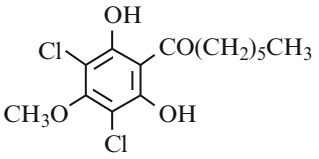
-Obtained by reaction of chlorine with 2,4-dihydroxy-6-methoxyheptanophenone in water [2012].

^{1}H NMR [2012], MS [2012].

BIOLOGICAL ACTIVITY: Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-heptanone
(DIF-1) (+1)

[118191-33-6] $C_{14}H_{18}Cl_2O_4$ mol. wt. 321.20



Syntheses

-Preparation by adding a solution of sulfuryl chloride (1.5 equiv.) in ethanol to a solution of 2,6-dihydroxy-4-methoxyheptanophenone in chloroform at r.t.; then, the solution was stirred at r.t. [1129].

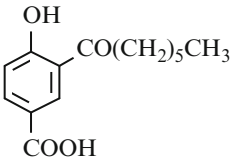
-Also obtained by reaction of chlorine with 2,4-dihydroxy-6-methoxyheptanophenone in water [2012].
-Also refer to: [1772, 1773, 2341].

yellow amorphous solid [1129]; ^{1}H NMR [2012], MS [1129, 2012].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129]; Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

3-Heptanoyl-4-hydroxybenzoic acid

$C_{14}H_{18}O_4$ mol. wt. 250.29



Synthesis

-Obtained by hydrolysis of its ethyl ester [967].
m.p. 183° [967].

Acetate $C_{16}H_{20}O_5$ mol. wt. 292.33

-Obtained by acetylation of 3-heptanoyl-4-hydroxybenzoic acid [967].

m.p. 101° [967].

Methyl ether $C_{15}H_{20}O_4$ mol. wt. 264.32

-Obtained by methylation of 3-heptanoyl-4-hydroxybenzoic acid [967].

m.p. 163° [967].

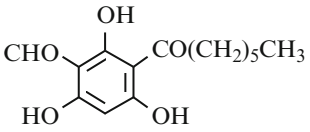
Ethyl ester $C_{16}H_{22}O_4$ mol. wt. 278.35

-Obtained by reaction of heptanoyl chloride with ethyl 4-hydroxybenzoate in the presence of aluminium chloride in tetrachloroethane, then the reaction mixture was heated at 120° for 3–4 h [967].

b.p.$_{22}$ 210° [967]; $n_D^{35.5} = 1.5115$ [967].

2,4,6-Trihydroxy-3-(1-oxoheptyl)benzaldehyde

[96573-33-0] $C_{14}H_{18}O_5$ mol. wt. 266.29



Syntheses

-Obtained by reaction of ethyl orthoformate with 2,4,6-trihydroxyenantophenone in the presence of aluminium chloride in methylene chloride with cooling in an ice bath for 30 min (70 %) [421].

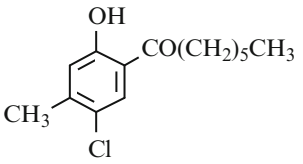
-Also refer to: [3406].

m.p. 103–105° [421]; ^{1}H NMR [421], IR [421], MS [421].

BIOLOGICAL ACTIVITY: As photosynthetic electron transport (PET) [3405].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-heptanone

$C_{14}H_{19}ClO_2$ mol. wt. 254.76



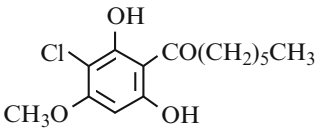
Synthesis

-Refer to: [3138].

Fluorescence [3138].

1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-1-heptanone
(DIF-3) (+1)

[861889-89-6] $C_{14}H_{19}ClO_4$ mol. wt. 286.76



Syntheses

-Obtained by reaction of sulfuryl chloride (1.5 equiv.) with 2,6-dihydroxy-4-methoxyheptanophenone in a chloroform/ethanol mixture at r.t. [1129].

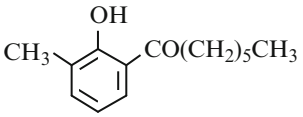
-Also refer to: [1772].

colourless amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2-Hydroxy-3-methylphenyl)-1-heptanone

[1000598-85-5] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses
-Obtained by acylation of organometallic reagents (53 %) [1627].
-Also refer to: [2270].

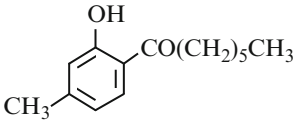
colourless oil [1627]; $b.p._{14–15}$ 161–162° [2270];
^{1}H NMR [1627], ^{13}C NMR [1627], MS [1627].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 151–152° [2270].

1-(2-Hydroxy-4-methylphenyl)-1-heptanone

$C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses
-Preparation by Fries reaction of m-tolyl enanthate with aluminium chloride,
*without solvent at 160° for 2 h (84 %) [726], at 140–150° [906] or at 120–140° for 10–20 min (67 %) [243];

*in nitrobenzene at 25° for 24 h (73 %) [243] or at 25–30° for 66 h (82 %) [244].

$b.p._1$ 123–124° [906], $b.p._4$ 148° [243], $b.p._{15}$ 172–174° [726];
m.p. 18° [726].

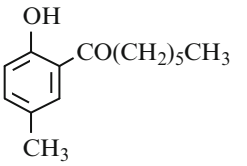
Phenylhydrazone $C_{20}H_{26}N_2O$ mol. wt. 310.44

-Refer to: [243].

m.p. 82–83° [243].

1-(2-Hydroxy-5-methylphenyl)-1-heptanone

[74604-13-0] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses
-Preparation by Fries rearrangement of p-cresyl enanthate with aluminium chloride,
*for 10 min at 120° (86 %) [2647];
*in tetrachloroethane at 120° [2520];
*without solvent at 130–150° [2520].

-Also refer to: [244, 1437, 1438, 2647].

$b.p._{0.1}$ 113° [2520], $b.p._8$ 158° [244], $b.p._{10}$ 168° [2647];
^{1}H NMR [1437], IR [1437, 2520], UV [2520], MS [1437].

Oxime [74604-06-1] $C_{14}H_{21}NO_2$ mol. wt. 235.33

m.p. 88° [2520]; IR [2520], UV [2520].

USE: Solvent extraction of copper (II) [2520].

Phenylhydrazone $C_{20}H_{26}N_2O$ mol. wt. 310.44

m.p. 107–108° [244].

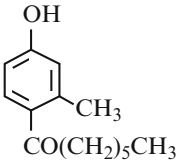
Methyl ether [194359-57-4] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Refer to: [1437, 1438].

^{1}H NMR [1437].

1-(4-Hydroxy-2-methylphenyl)-1-heptanone

$C_{14}H_{20}O_2$ mol. wt. 220.31



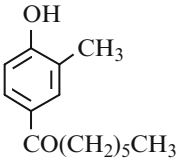
Synthesis

-Obtained by Fries reaction of m-tolyl enanthate with aluminium chloride in nitrobenzene at 25–30° for 66 h (10 %) [244].

m.p. 67–67.5° [244].

1-(4-Hydroxy-3-methylphenyl)-1-heptanone

[95102-27-5] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses

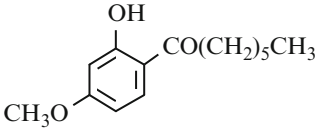
-Obtained by Friedel-Crafts acylation of o-cresol with n-enantoyl chloride in the presence of aluminium chloride in nitrobenzene at 30° for 24 h (92 %) [2704].

-Also refer to: [1595].

USE: Colour developer, for thermal recording materials [1595].

1-(2-Hydroxy-4-methoxyphenyl)-1-heptanone

[143286-89-9] $C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses

-Obtained by reaction of methyl bromide with 2,4-dihydroxyenanthophenone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

-Also obtained by reaction of dimethyl sulfate with 2,4-dihydroxyenanthophenone in the presence of potassium carbonate in refluxing acetone for 4–6 h (85–90 %) [2501].

m.p. 24° [284].

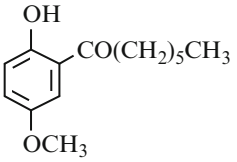
Oxime [143286-58-2] $C_{14}H_{21}NO_3$ mol. wt. 251.33

-Obtained by reaction of hydroxylamine hydrochloride with 1-(2-hydroxy-4-methoxyphenyl)-1-heptanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 76° [284]; ^{1}H NMR [284].

1-(2-Hydroxy-5-methoxyphenyl)-1-heptanone

[100864-00-4] $C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses

-Obtained by reaction of enanthyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in refluxing carbon disulfide for 8 h [550].

-Also refer to: [161, 1515].

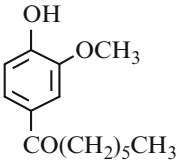
yellow crystals [550];
m.p. 43–44° [1515], 34° [550], 33–33.5° [161];
^{1}H NMR [1515].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_6$ mol. wt. 416.43

m.p. 145° [550].

1-(4-Hydroxy-3-methoxyphenyl)-1-heptanone

[114515-52-5] $C_{14}H_{20}O_3$ mol. wt. 236.31



Synthesis

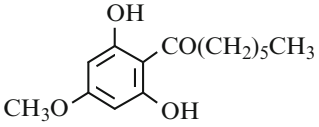
-Obtained by adding DDQ to 1-(4-hydroxy-3-methoxy-phenyl)-1-heptanol in benzene and the reaction mixture stirred for 4 h at r.t. [2989].

m.p. 49° [2989]; ^{1}H NMR [2989].

BIOLOGICAL ACTIVITY: Chloleretic [2989].

1-(2,6-Dihydroxy-4-methoxyphenyl)-1-heptanone

[861889-76-1] $C_{14}H_{20}O_4$ mol. wt. 252.31



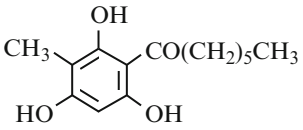
Synthesis

-Obtained by reaction of heptanoyl chloride with 5-methoxyresorcinol in the presence of aluminium chloride in methylene chloride at r.t. [1129].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2,4,6-Trihydroxy-3-methylphenyl)-1-heptanone

$C_{14}H_{20}O_4$ mol. wt. 252.31

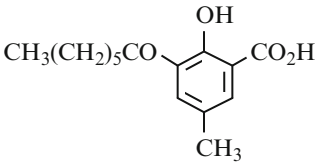


Synthesis
-Obtained by reaction of enanthic nitrile with 3-methyl-phloroglucinol (Hoesch reaction) [1608].

m.p. 143–144° [1608].

3-Heptanoyl-2-hydroxy-5-methylbenzoic acid

$C_{15}H_{20}O_4$ mol. wt. 264.32



Synthesis
-Obtained by saponification of its methyl ester below with 50 % potassium hydroxide in methanol (70 %) [3235].
m.p. 131° [3235].

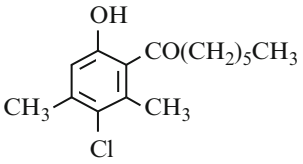
Methyl ester $C_{16}H_{22}O_4$ mol. wt. 278.35

-Preparation by Fries rearrangement of methyl 2-(heptanoyloxy)-5-methylbenzoate with aluminium chloride in carbon disulfide for 2 h at 60° (90 %) [3235].

$b.p._{.0.2}$ 204–210° [3235]; m.p. 51–52° [3235].

1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-heptanone

[102003-68-9] $C_{15}H_{21}ClO_2$ mol. wt. 268.78



Synthesis
-Preparation by Fries rearrangement of 4-chloro-3,5-dimethylphenyl heptanoate with aluminium chloride in carbon disulfide at 80° for 2 h, then at 110° for 2 h after solvent elimination (69 %) [3114].

m.p. 80° [3114].

Semicarbazone [107151-50-8] $C_{16}H_{24}ClN_3O_2$ mol. wt. 325.84

m.p. 154° [3114].

Allyl ether [101892-45-9] $C_{18}H_{25}ClO_2$ mol. wt. 308.85

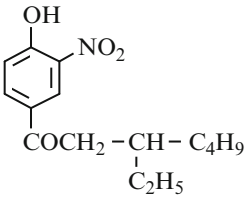
-Obtained by reaction of allyl bromide with the title ketone in the presence of potassium carbonate in refluxing acetone for 6 h (87 %) [3114].

$b.p._{.2}$ 187° [3114].

USE: Insecticide [3114].

3-Ethyl-1-(4-hydroxy-3-nitrophenyl)-1-heptanone

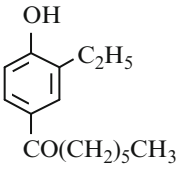
[214058-35-2] $C_{15}H_{21}NO_4$ mol. wt. 279.33



Synthesis
-Refer to: [1315].

1-(3-Ethyl-4-hydroxyphenyl)-1-heptanone

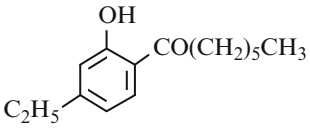
[95185-66-3] $C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis
-Refer to: [2704].

1-(4-Ethyl-2-hydroxyphenyl)-1-heptanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Obtained by Fries rearrangement of 3-ethylphenyl enanthate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (91 %) [2801];
*in the presence of aluminium chloride (2.8 M),

first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (88 %) [2801].

b.p.$_4$ 176° [2801].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 143° [2801].

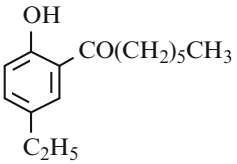
Methyl ether $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by reaction of dimethyl sulfate with 1-(4-ethyl-2-hydroxyphenyl)-1-heptanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (90 %) [2801].

b.p.$_{40}$ 195° [2801].

1-(5-Ethyl-2-hydroxyphenyl)-1-heptanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



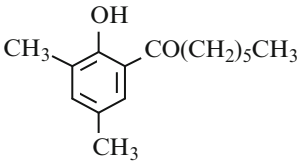
Synthesis
-Obtained by Fries rearrangement of 4-ethylphenyl heptanoate with aluminium chloride at 100° for 2 h (80 %) [2800].
b.p.$_9$ 178° [2800].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 129° [2800].

1-(2-hydroxy-3,5-dimethylphenyl)-1-heptanone

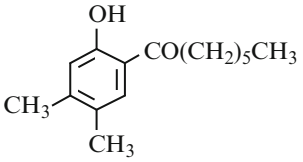
$C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis
-Obtained by Fries rearrangement of 2,4-dimethylphenyl heptanoate (b.p.$_{16}$ 180–182°) with aluminium chloride (74 %) [184].
pale yellow; b.p.$_{16}$ 186–190° [184].

1-(2-hydroxy-4,5-dimethylphenyl)-1-heptanone

[50342-14-8] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Obtained by Fries rearrangement of 3,4-dimethylphenyl enanthate with aluminium chloride at 110° without solvent (83 %) [3117].
-Refer to: [2665].

b.p.$_9$ 220° [3117].

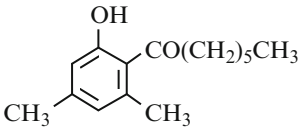
USE: Cyclization of, with chloroacetal [2665].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 211° [3117].

1-(2-Hydroxy-4,6-dimethylphenyl)-1-heptanone

[855899-90-0] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses

-Obtained by Fries rearrangement of 3,5-dimethylphenyl enanthate (1 equiv.),

*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (73 %) [2801];

*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (63 %) [2801].

b.p.$_{.5}$ 160° [2801].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 165° [2801].

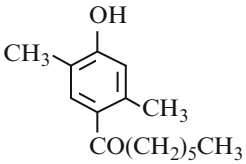
Methyl ether $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxy-4,6-dimethylphenyl)-1-heptanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (61 %) [2801].

b.p.$_{.36}$ 205° [2801].

1-(4-Hydroxy-2,5-dimethylphenyl)-1-heptanone

[95102-39-9] $C_{15}H_{22}O_2$ mol. wt. 234.34



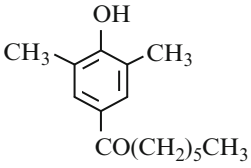
Syntheses

-Refer to: [1595, 2704].

USE: Colour developer, for thermal recording materials [2704].

1-(4-hydroxy-3,5-dimethylphenyl)-1-heptanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



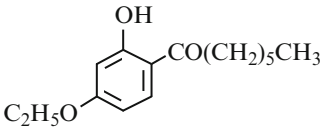
Synthesis

-Obtained by Fries rearrangement of 2,6-dimethylphenyl heptanoate (*vic-m-Xylenyl heptoate*) (b.p.$_{12}$ 162–164°) in the presence of aluminium chloride (65 %) [184].

pale yellow [184]; b.p.$_{12}$ 220–230° [184]; m.p. 92–93° [184].

1-(4-Ethoxy-2-hydroxyphenyl)-1-heptanone

[14683-92-2] $C_{15}H_{22}O_3$ mol. wt. 250.34

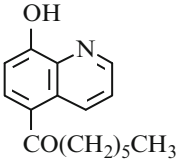


Synthesis
-Obtained by reaction of ethyl bromide with enanthoylresorcinol in the presence of ethanolic potassium hydroxyde solution for 2 h (74 %) [3474].

b.p.$_1$ 162–163° [3474]; m.p. 33–34° [3474].

1-(8-Hydroxy-5-quinolinyl)-1-heptanone

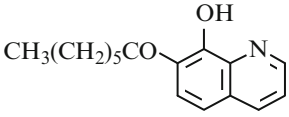
[62189-88-2] $C_{16}H_{19}NO_2$ mol. wt. 257.33



Synthesis
-Refer to: [2360].
m.p. 69–70° [2360]; ^{1}H NMR [2360], IR [2360].

1-(8-Hydroxy-7-quinolinyl)-1-heptanone

[60697-65-6] $C_{16}H_{19}NO_2$ mol. wt. 257.33



Syntheses
-Obtained by acylation of 8-quinolinol with n-heptanoyl chloride in the presence of aluminium chloride (20 %) [2361].
-Refer to: [2360, 2362].

m.p. 75–76° [2362]; ^{1}H NMR [2362], IR [2362].

Copper complex [62153-16-6]

-Refer to: [2360].

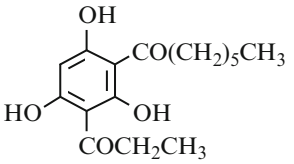
Ethyl ether [62189-86-0] $C_{18}H_{23}NO_2$ mol. wt. 285.38

-Obtained by ethylation of 7-heptanoyl-8-quinolinol with ethyl sulfide (71 %) [2360].

b.p.$_2$ 188–194° [2360]; ^{1}H NMR [2360], IR [2360];
$n_D^{20} = 1.5614$ [2360].

1-[2,4,6-Trihydroxy-3-(1-oxopropyl)phenyl]-1-heptanone

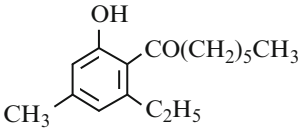
[129227-94-7] $C_{16}H_{22}O_5$ mol. wt. 294.35



Synthesis
-Obtained from 2,4,6-trihydroxy-3-(1-oxoheptyl)-benzaldehyde [3406].

1-(2-Ethyl-6-hydroxy-4-methylphenyl)-1-heptanone

$C_{16}H_{24}O_2$ mol. wt. 248.37



Syntheses
-Preparation by Fries rearrangement of 3-ethyl-5-methylphenyl enanthate with aluminium chloride,
*without solvent at 130° for 2 h (80 %) [2802];
*in nitrobenzene at 25° for 6 h (84 %) [2802].

b.p.$_2$ 200° [2802].

Methyl ether $C_{17}H_{26}O_2$ mol. wt. 262.39

-Obtained by methylation of the above ketone in the usual way (76 %) [2802].

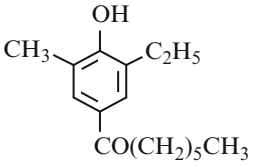
b.p.$_{35}$ 220° [2802].

2,4-Dinitrophenylhydrazone $C_{22}H_{28}N_4O_5$ mol. wt. 428.49

m.p. 184° [2802].

1-(3-Ethyl-4-hydroxy-5-methylphenyl)-1-heptanone

$C_{16}H_{24}O_2$ mol. wt. 248.37

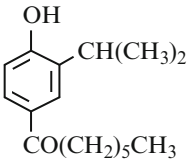


Synthesis
-Obtained by Fries rearrangement of 2-ethyl-6-methylphenyl n-heptanoate (b.p.$_{12}$ 172–174°) in the presence of aluminium chloride (70 %) [184].

b.p.$_{12}$ 230–240° [184]; m.p. 56–57.5° [184].

1-(4-Hydroxy-3-(1-methylethyl)phenyl)-1-heptanone

[95102-18-4] $C_{16}H_{24}O_2$ mol. wt. 248.37

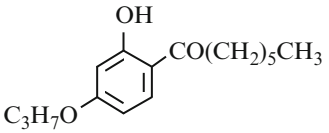


Syntheses
-Refer to: [1595, 2704] (Japanese patents).
m.p. 85° [2704].

USE: As colour developer [2704]; In preparation of thermographic recording material [1595].

1-(2-Hydroxy-4-propoxyphenyl)-1-heptanone

[14683-93-3] $C_{16}H_{24}O_3$ mol. wt. 264.37

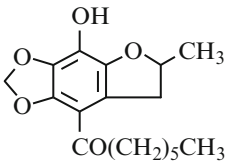


Synthesis
-Obtained by reaction of n-propyl bromide with enanthoylresorcinol in the presence of ethanolic potassium hydroxyde solution for 2 h (72 %) [3474].

b.p.$_1$ 164–165° [3474]; m.p. 44° [3474].

1-(6,7-Dihydro-4-hydroxy-6-methylfuro[2,3-f]-1,3-benzodioxol-8-yl)-1-heptanone

$C_{17}H_{22}O_5$ mol. wt. 306.36



Synthesis
-Refer to: [2179].
Methyl ether [82652-35-5]
(Heptanoyl furapiole)
$C_{18}H_{24}O_5$ mol. wt. 320.39

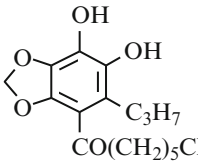
-Obtained by reaction of heptanoyl chloride with furapiole in the presence of fused zinc chloride in methylene chloride for 3–4 h in an ice bath (70 %) [2179].

colourless plates; m.p. 58° [2179]; ^{1}H NMR [2179], IR [2179].

USE: Synergistic insecticidal activity of, with pyrethrum [2179].

1-(6,7-Dihydroxy-5-propyl-1,3-benzodioxol-4-yl)-1-heptanone

$C_{17}H_{24}O_5$ mol. wt. 308.37



Synthesis
-Refer to: [2179].

Dimethyl ether [82652-27-5]
(Heptanoyl dihydrodillapiole)
$C_{19}H_{28}O_5$ mol. wt. 336.43

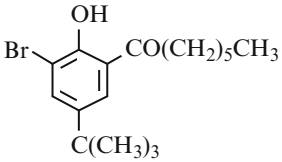
-Obtained by reaction of heptanoyl chloride with dihydrodillapiole in the presence of fused zinc chloride in methylene chloride for 3–4 h in an ice bath (70 %) [2179].

colourless solid [2179]; ^{1}H NMR [2179], IR [2179].

USE: Synergistic insecticidal activity of, with pyrethrum [2179].

1-[3-Bromo-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-heptanone

[101577-83-7] $C_{17}H_{25}BrO_2$ mol. wt. 341.29



Synthesis
-Preparation by Fries rearrangement of 2-bromo-4-tert-butylphenyl heptanoate in the presence of aluminium chloride at 110° for 2 h (65 %) [3113].
b.p.$_2$ 200° [3113].

2,4-Dinitrophenylhydrazone $C_{23}H_{29}BrN_4O_5$ mol. wt. 521.41

m.p. 140–141° [3113].

Allyl ether [102465-47-4] $C_{20}H_{29}BrO_2$ mol. wt. 381.35

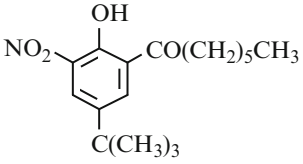
-Obtained by reaction of allyl bromide with the title ketone in the presence of potassium carbonate in refluxing acetone for 8 h (68 %) [3113].

b.p.$_1$ 164° [3113].

USE: Insecticide [3113].

1-[5-(1,1-Dimethylethyl)-2-hydroxy-3-nitrophenyl]-1-heptanone

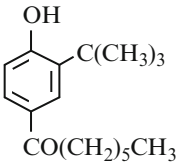
[85052-35-3] $C_{17}H_{25}NO_4$ mol. wt. 307.39



Synthesis
-Obtained by nitration of 5-tert-butyl-2-hydroxyheptanophenone (65 %) [2105] according to the process [1475].
^{1}H NMR [2105].

1-[3-(1,1-Dimethylethyl)-4-hydroxyphenyl]-1-heptanone

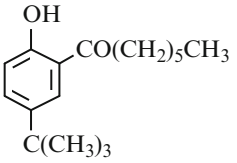
[95185-65-2] $C_{17}H_{26}O_2$ mol. wt. 262.39



Synthesis
-Refer to: [2704].

1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-heptanone

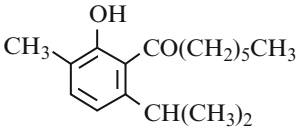
[85052-34-2] $C_{17}H_{26}O_2$ mol. wt. 262.39



Synthesis
-Refer to: [2105].

1-[2-Hydroxy-3-methyl-6-(1-methylethyl)phenyl]-1-heptanone

$C_{17}H_{26}O_2$ mol. wt. 262.39



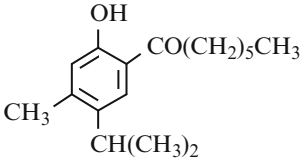
Synthesis
-Obtained by Fries rearrangement of carvacryl heptanoate with aluminium chloride at 120° (73 %) [2798].
b.p.$_3$ 176° [2798].

2,4-Dinitrophenylhydrazone $C_{23}H_{30}N_4O_5$ mol. wt. 442.52

m.p. 122° [2798].

1-[2-Hydroxy-4-methyl-5-(1-methylethyl)phenyl]-1-heptanone

[129375-11-7] $C_{17}H_{26}O_2$ mol. wt. 262.39

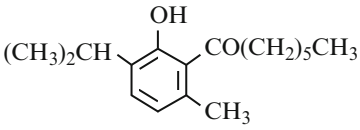


Synthesis
-Preparation by Fries rearrangement of 3-methyl-4-(1-methylethyl)phenyl heptanoate (**20**) with titanium tetrachloride in nitromethane at 20° for 170 h (95 %) (**26**) [1997].

pale yellow crystals [1997]; m.p. 38° (Sadtler standard N° 79765K) [1997];
^{1}H NMR (Sadtler standard N° 52708M) [1997],
IR (Sadtler standard N° 79765K) [1997], UV [1997], MS [1997].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-heptanone

[855956-24-0] $C_{17}H_{26}O_2$ mol. wt. 262.39



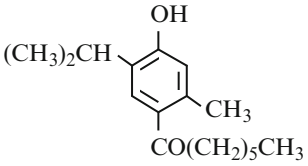
Synthesis
-Obtained by Fries rearrangement of thymyl heptanoate with aluminium chloride at 120° (84 %) [2803].
b.p.$_2$ 173° [2803].

2,4-Dinitrophenylhydrazone $C_{23}H_{30}N_4O_5$ mol. wt. 442.52

m.p. 174° [2803].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-heptanone

$C_{17}H_{26}O_2$ mol. wt. 262.39



Synthesis
-Obtained by treatment of its methyl ether (**VIII**) with boiling pyridinium chloride (205–215°) for 4 h (20 %) (**XXVII**) [2660].
b.p.$_{20}$ 240–245° [2660]; m.p. 95° [2660].

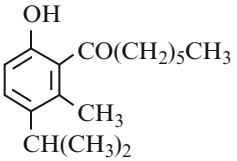
Methyl ether (**VIII**) $C_{18}H_{28}O_2$ mol. wt. 276.42

-Obtained by reaction of enanthyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (52 %) [2660].

b.p.$_{18}$ 209–211° [2660]; $n_D^{23} = 1.5185$ [2660].

1-[6-Hydroxy-2-methyl-3-(1-methylethyl)phenyl]-1-heptanone

[129375-15-1] $C_{17}H_{26}O_2$ mol. wt. 262.39

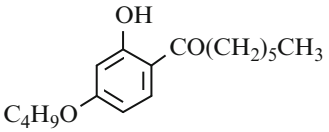


Synthesis
-Preparation by treatment of 1-[3-(1,1-dimethylethyl)-2-hydroxy-6-methyl-5-(1-methylethyl)phenyl]-1-heptanone (**29**) with aluminium chloride in nitromethane at 20° for 24 h (82 %) (**32**) [1997].

m.p. 65° (Sadtler standard N° 79805K) [1997];
^{1}H NMR (Sadtler standard N° 52746M) [1997],
IR (Sadtler standard N° 79805K) [1997], UV [1997], MS [1997].

1-(4-Butoxy-2-hydroxyphenyl)-1-heptanone

[14683-94-4] $C_{17}H_{26}O_3$ mol. wt. 278.39



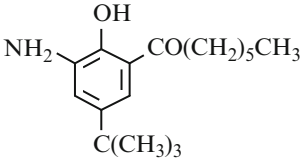
Synthesis

-Obtained by reaction of n-butyl bromide with enanthoylresorcinol in the presence of ethanolic potassium hydroxyde solution for 2 h (69 %) [3474].

b.p.$_4$ 190–195° [3474]; IR [3474].

1-[3-Amino-5-(1,1-methylethyl)-2-hydroxyphenyl]-1-heptanone

$C_{17}H_{27}NO_2$ mol. wt. 277.41



Synthesis

-Refer to: [2105].

Hydrochloride

$C_{17}H_{27}NO_2$, HCl mol. wt. 313.87

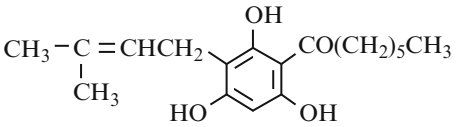
-Obtained from the 5-tert-butyl-2-hydroxy-3-nitroheptanophenone (52 %) [2105].

m.p. 125–126° [2105];
^{1}H NMR [2105], IR [2105], MS [2105]; TLC [2105].

1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-heptanone

2-Heptanoyl-4-(3-methylbuten-2-yl)phloroglucinol (**12**) [1026].

[69916-11-6] $C_{18}H_{26}O_4$ mol. wt. 306.40



Syntheses

-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and prenyl bromide to a solution of phloroheptanophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

-Also prepared by adding prenyl bromide to a suspension of the sodium salt of phloroheptanophenone in benzene, then the mixture obtained was kept overnight at 0° [2110] or refluxed for 3 h [1026].

-Also obtained by reaction of prenyl chloride with phloroheptanophenone in an alkaline two-phase (aqueous-ether) system and catalyzed by CuCl [838, 3193].

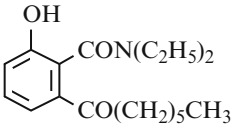
-Also prepared by adding at 5° a solution of sodium methoxide in methanol, followed by isopentenyl bromide in ethyl ether to a solution of phloroheptanophenone in benzene and ethyl ether; then the mixture was stirred at r.t. for 6 h (15 %) [2113].

m.p. 157° [2113], 136–138° [3193].
N.B.: One of the reported melting point is obviously wrong.
^{13}C NMR [1026, 3193], IR [1026].

BIOLOGICAL ACTIVITY: Antifungal against *Trichophyton* species [2113]; Bactericidal and fungicidal [1026, 3193].

N,N-Diethyl-2-heptanoyl-6-hydroxybenzamide

$C_{18}H_{27}NO_3$ mol. wt. 305.40



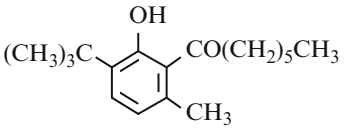
Synthesis
-Refer to: [2321].
Methyl ether [334698-83-8]
$C_{19}H_{29}NO_3$ mol. wt. 319.44

-Obtained by adding a solution of N,N-diethyl-2-(1-hydroxyheptyl)-6-methoxybenzamide in methylene chloride to a suspension of PDC in the same solvent under an argon atmosphere at r.t. and the mixture stirred for 15 h (89 %) [2321].

colourless oil [2321];
^{1}H NMR [2321], ^{13}C NMR [2321], IR [2321].

1-[3-(1,1-Dimethylethyl)-2-hydroxy-6-methylphenyl]-1-heptanone

$C_{18}H_{28}O_2$ mol. wt. 276.42



Syntheses
-Obtained by Fries rearrangement of 2-tert-butyl-5-methylphenyl enanthate,
*in the presence of aluminium chloride (1.5 equiv.) in nitrobenzene at 25° for 6 h (76 %) [3118];

*in the presence of aluminium chloride (3 equiv.) at 110° for 2 h (72 %) [3118].

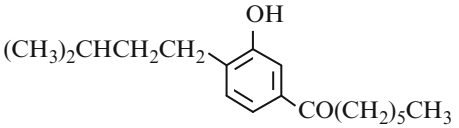
b.p.$_{12}$ 155° [3118].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 187° [3117, 3118].

1-[3-Hydroxy-4-(3-methylbutyl)phenyl]-1-heptanone

[101873-72-7] $C_{18}H_{28}O_2$ mol. wt. 276.42



Synthesis
-Obtained by diazotization of 3-amino-4-iso-amylheptanophenone [551].

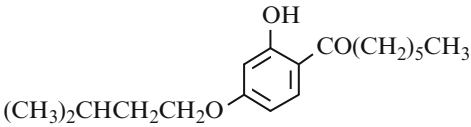
m.p. 98–98.5° [551].

2,4-Dinitrophenylhydrazone [113927-77-8] $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 165° [551].

1-[2-Hydroxy-4-(3-methylbutoxy)phenyl]-1-heptanone

[14683-95-5] $C_{18}H_{28}O_3$ mol. wt. 292.42



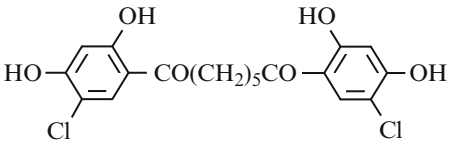
Synthesis

-Obtained by reaction of isoamyl bromide with enanthoylresorcinol in the presence of ethanolic potassium hydroxyde solution for 2 h (45 %) [3474].

b.p.$_2$ 180–182° [3474].

1,7-Bis(5-chloro-2,4-dihydroxyphenyl)-1,7-heptanedione

[26086-80-6] $C_{19}H_{18}Cl_2O_6$ mol. wt. 413.25



Syntheses

-Obtained by reaction of pimelic acid dichloride with 4-chlororesorcinol in the presence of aluminium chloride [589, 591].

m.p. 203° [589, 591].

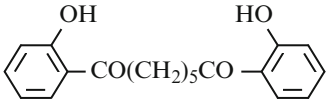
Tetramethyl ether [26086-83-9] $C_{23}H_{26}Cl_2O_6$ mol. wt. 469.36

-Obtained by reaction of pimelic acid dichloride with 4-chlororesorcinol dimethyl ether in the presence of aluminium chloride [589, 591].

m.p. 163° [589, 591]; IR [589].

1,7-Bis(2-hydroxyphenyl)-1,7-heptanedione

[10401-04-4] $C_{19}H_{20}O_4$ mol. wt. 312.36



Syntheses

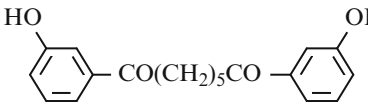
-Obtained by Fries rearrangement of phenyl pimelate with aluminium chloride (15–20 %) [1576].

-Also refer to: [1575].

m.p. 90° [1575, 1576].

1,7-Bis(3-hydroxyphenyl)-1,7-heptanedione

[10365-54-5] $C_{19}H_{20}O_4$ mol. wt. 312.36



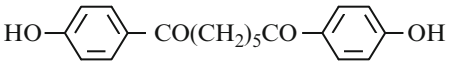
Syntheses
-Obtained by diazotization of 1,7-bis (3-aminophenyl)-1,7-heptanedione (40–50 %) [1576].

-Also refer to: [1575].

m.p. 136° [1575, 1576].

1,7-Bis(4-hydroxyphenyl)-1,7-heptanedione

[20837-38-1] $C_{19}H_{20}O_4$ mol. wt. 312.36



Syntheses
-Refer to: [584, 1148, 1576].

m.p. 187–189° [1148], 55° [584].
N.B.: One of the reported melting point is obviously wrong.

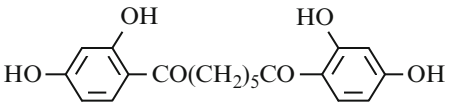
Dimethyl ether [10365-60-3] $C_{21}H_{24}O_4$ mol. wt. 340.42

-Obtained by reaction of pimelic acid dichloride with anisole in the presence of aluminium chloride (80–90 %) [1576].
-Also refer to: [584, 1148, 1575].

m.p. 100° [584, 1575, 1576], 95–97° [1148].

1,7-Bis(2,4-dihydroxyphenyl)-1,7-heptanedione

[7658-30-2] $C_{19}H_{20}O_6$ mol. wt. 344.36



Syntheses
-Obtained by adding resorcinol into the dinitrile of pimelic acid and hydrogen chloride in ethyl ether in the presence of zinc chloride.

Then, the diketimine dihydrochloride obtained was hydrolyzed by boiling water (76 %) [2674].
-Also obtained by reaction of pimelic acid dichloride with resorcinol in the presence of aluminium chloride [591].
-Also refer to: [589, 1735, 2504].

m.p. 166° (d) [2504, 2674], 165° [589, 591];
UV [2504].

2,4-Dinitrophenylhydrazone [32354-10-2] $C_{31}H_{28}N_8O_{12}$ mol. wt. 704.61

m.p. 213° [589, 2674].

Tetramethyl ether [32246-62-1] $C_{23}H_{28}O_6$ mol. wt. 400.47

-Refer to: [589].

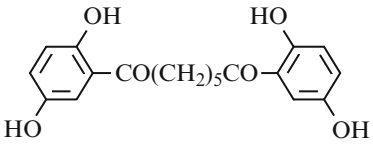
m.p. 123° [589].

Dioxime of the tetramethyl ether [32246-63-2] $C_{23}H_{30}N_2O_6$ mol. wt. 430.50

m.p. 164° [589].

1,7-Bis(2,5-dihydroxyphenyl)-1,7-heptanedione

$C_{19}H_{20}O_6$ mol. wt. 344.36



Synthesis

-Refer to: [1575].

Tetramethyl ether [10365-24-9]

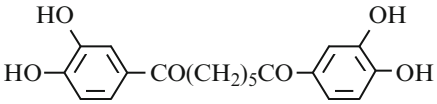
$C_{23}H_{28}O_6$ mol. wt. 400.47

-Obtained by reaction of pimelic acid dichloride (1 mol) with hydroquinone dimethyl ether (2.5 mol) in the presence of aluminium chloride (1 mol) (58 %) [1575].

m.p. 76° [1575].

1,7-Bis(3,4-dihydroxyphenyl)-1,7-heptanedione

$C_{19}H_{20}O_6$ mol. wt. 344.36



Synthesis

-Refer to: [1014].

Tetramethyl ether [32246-69-8]

$C_{23}H_{28}O_6$ mol. wt. 400.47

-Obtained by reaction of pimelic acid dichloride with pyrocatechol dimethyl ether in the presence of aluminium chloride [591].

-Also obtained by hydrogenating of its oxime in acetic acid in the presence of 10 % Pd/C in a Parr apparatus at r.t. and 45–50 psig for 12–36 h (68 %) [1014].

-Also refer to: [589, 1012, 2342].

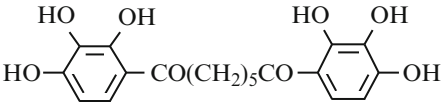
m.p. 95° [589, 591], 94–95° [1012], 91–93° [1014];
^{1}H NMR [2342], ^{13}C NMR [2342].

Dioxime of the tetramethyl ether [50766-29-5] $C_{23}H_{30}N_2O_6$ mol. wt. 430.50

m.p. 115–117° [1014].

1,7-Bis(2,3,4-trihydroxyphenyl)-1,7-heptanedione

$C_{19}H_{20}O_8$ mol. wt. 376.36



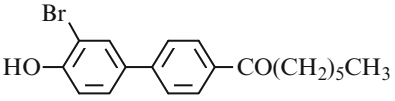
Synthesis
-Refer to: [1575].
Hexamethyl ether [10475-17-9]
$C_{25}H_{32}O_8$ mol. wt. 460.52

-Obtained by reaction of pimelic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride [591].
-Also obtained by reaction of dimethyl sulfate with 1,7-bis(2-hydroxy-3,4-dimethoxyphenyl)-1,7-heptanedione the presence of 30 % sodium hydroxide (65–90 %) [1574].
-Also refer to: [1575] (Japanese paper).

m.p. 114° [591], m.p. 60° [1574, 1575].
N.B.: One the reported melting point is obviously wrong.

1-(3′-Bromo-4′-hydroxy[1,1′-biphenyl]-4-yl)-1-heptanone

$C_{19}H_{21}BrO_2$ mol. wt. 361.27

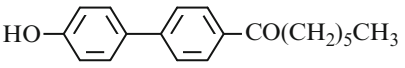


Synthesis
-Refer to: [2992].
Methyl ether [77007-22-8]
$C_{20}H_{23}BrO_2$ mol. wt. 375.30

-Obtained by acylation of 2-bromo-4-phenylanisole with nonanoyl chloride (64 %) [2992].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-heptanone

[390358-13-1] $C_{19}H_{22}O_2$ mol. wt. 282.38



Syntheses
-Obtained by Fries rearrangement of 4-heptanoyl-oxybiphenyl with aluminium chloride in nitrobenzene, first at 20° for 12 h, then at 60° for 1 h [522].

-Also refer to: [1518].

USE: For preparation of biphenylyl sulfamates as steroid sulfatase inhibitors for estrogen-dependent diseases [1518].

Acetate [126516-15-2] $C_{21}H_{24}O_3$ mol. wt. 324.42

-Refer to: [847, 2080].

Various ethers (11)

-Preparations and liquid crystalline properties of, [847].

Methyl ether [56116-79-1] $C_{20}H_{24}O_2$ mol. wt. 296.41

-Obtained from heptanoyl chloride and 4-methoxybiphenyl [522].
-Also refer to: [514, 847].

smooth spangles [522]; b.p.$_{12}$ 250–252° [514, 522]; m.p. 118° [514, 522].

Ethyl ether [56116-88-2] $C_{21}H_{26}O_2$ mol. wt. 310.44

-Refer to: [847].

Propyl ether [56116-96-2] $C_{22}H_{28}O_2$ mol. wt. 324.46

-Refer to: [847].

Butyl ether [56117-04-5] $C_{23}H_{30}O_2$ mol. wt. 338.49

-Refer to: [847].

Pentyl ether [56117-13-6] $C_{24}H_{32}O_2$ mol. wt. 352.52

-Refer to: [847].

Hexyl ether [56117-22-7] $C_{25}H_{34}O_2$ mol. wt. 366.54

-Refer to: [847].

Heptyl ether [56117-31-8] $C_{26}H_{36}O_2$ mol. wt. 380.57

-Refer to: [847].

Octyl ether [56117-39-6] $C_{27}H_{38}O_2$ mol. wt. 394.60

-Refer to: [847].

Nonyl ether [56117-48-7] $C_{28}H_{40}O_2$ mol. wt. 408.62

-Refer to: [847].

Decyl ether [56117-57-8] $C_{29}H_{42}O_2$ mol. wt. 422.65

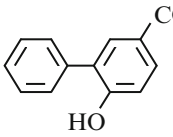
-Refer to: [847].

Dodecyl ether [56117-66-9] $C_{31}H_{46}O_2$ mol. wt. 450.71

-Refer to: [847].

1-(6-Hydroxy[1,1′-biphenyl]-3-yl)-1-heptanone

[95102-35-5] $C_{19}H_{22}O_2$ mol. wt. 282.38

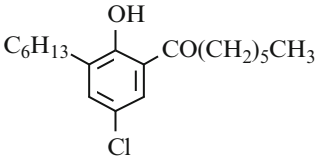


Syntheses
-Refer to: [1595, 2704].

USE: Colour developer, for thermal recording materials [2704].

1-(5-Chloro-3-hexyl-2-hydroxyphenyl)-1-heptanone

[855921-00-5] $C_{19}H_{29}ClO_2$ mol. wt. 324.89

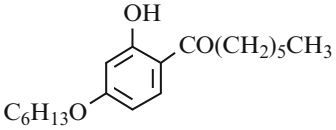


Synthesis
-Obtained by Fries rearrangement of 4-chloro-2-hexyl-phenyl enanthate with aluminium chloride at 120° for 1 h (44 %) [3235].

oil [3235]; b.p.$_{0.2}$ 198–205° [3235].

1-[4-(Hexyloxy)-2-hydroxyphenyl]-1-heptanone

[143286-90-2] $C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Obtained by reaction of hexyl bromide with 2,4-dihydroxyheptanophenone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 27.5–28.5° [284].

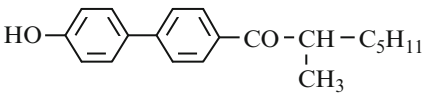
Oxime [143286-59-3] $C_{19}H_{31}NO_3$ mol. wt. 321.46

-Obtained by reaction of hydroxylamine hydrochloride with 1-[4-(hexyloxy)-2-hydroxyphenyl]-1-heptanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 45–48° [284]; ^{1}H NMR [284].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-2-methyl-1-heptanone

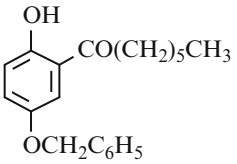
[186041-43-0] $C_{20}H_{24}O_2$ mol. wt. 296.41
[186041-40-6] (S)



Synthesis
-Refer to: [2278].

1-[2-Hydroxy-5-(phenylmethoxy)phenyl]-1-heptanone

[719315-64-7] $C_{20}H_{24}O_3$ mol. wt. 312.40

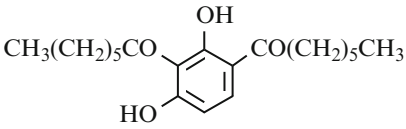


Syntheses
-Refer to: [3460–3462].

USE: Electroluminescent devices employing complex fluorene-containing compounds [3461].

1,1′-(2,4-Dihydroxy-1,3-phenylene)bis-1-heptanone

$C_{20}H_{30}O_4$ mol. wt. 334.46



Synthesis
-Also obtained by Fries rearrangement of resorcinol dilenanthate with aluminium chloride in nitrobenzene for 8 h at 40–50° (25 %) [379].

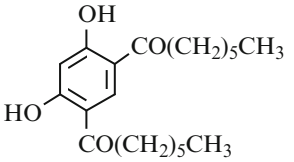
m.p. 48–49° [379].

2,4-Dinitrophenylhydrazone $C_{26}H_{34}N_4O_7$ mol. wt. 514.57

m.p. 196° [379].

1,1′-(4,6-Dihydroxy-1,3-phenylene)bis-1-heptanone

$C_{20}H_{30}O_4$ mol. wt. 334.46



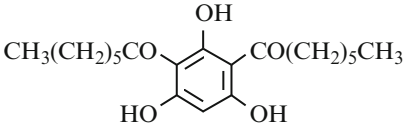
Synthesis
-Also obtained by Fries rearrangement of resorcinol dilenanthate with aluminium chloride in nitrobenzene for 8 h at 40–50° (25 %) [379].
m.p. 48–49° [379].

2,4-Dinitrophenylhydrazone $C_{26}H_{34}N_4O_7$ mol. wt. 514.57

m.p. 196° [379].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-heptanone

[3118-36-3] $C_{20}H_{30}O_5$ mol. wt. 350.46



Syntheses
-Obtained by reaction of heptanoyl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene for 3 days at r.t. (5–10 %) [421].

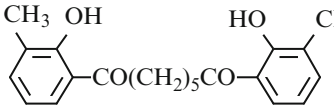
-Also obtained by reaction of heptanoic anhydride with phloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].
-Also refer to: [457, 600, 644, 2911, 3033].

m.p. 98–99° [421], 96–98° [457, 2911];
^{1}H NMR [421], IR [421], MS [421].

BIOLOGICAL ACTIVITY: Inhibitory effects of treatment with this acylphenol on TPA Induced EBV-EA Activation [3033]; Antiviral activity towards the replication of vesicular stomatitis virus in HEL cell cultures [644]; Germination inhibition in cress (*Lepidium sativum*) seeds [421]; For treatment of immune dysfunction associated with human immuno deficiency virus infection [600]; Anthelmintic [457].

1,7-Bis(2-hydroxy-3-methylphenyl)-1,7-heptanedione

[10365-66-9] $C_{21}H_{24}O_4$ mol. wt. 340.42



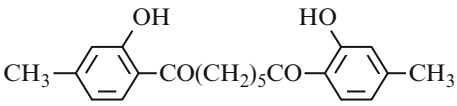
Syntheses
-Obtained by Fries rearrangement of o-cresol pimelate with aluminium chloride (15–20 %) [1576].

-Also refer to: [1575].

m.p. 76° [1575, 1576].

1,7-Bis(2-hydroxy-4-methylphenyl)-1,7-heptanedione

[13221-24-4] $C_{21}H_{24}O_4$ mol. wt. 340.42



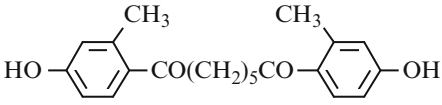
Syntheses
-Obtained by Fries rearrangement of m-cresol pimelate with aluminium chloride (70–80 %) [1576].

-Also refer to: [1575].

m.p. 127° [1575, 1576].

1,7-Bis(4-hydroxy-2-methylphenyl)-1,7-heptanedione

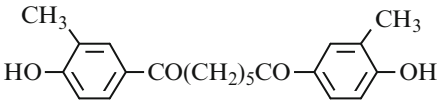
[22860-00-0] $C_{21}H_{24}O_4$ mol. wt. 340.42



Synthesis
-Refer to: [584].
m.p. 100° [584].

1,7-Bis(4-hydroxy-3-methylphenyl)-1,7-heptanedione

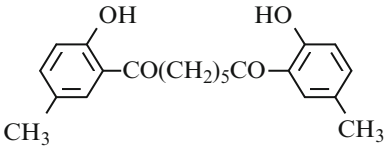
[22859-96-7] $C_{21}H_{24}O_4$ mol. wt. 340.42



Synthesis
-Refer to: [584].
m.p. 110° [584].

1,7-Bis(2-hydroxy-5-methylphenyl)-1,7-heptanedione

[111162-35-7] $C_{21}H_{24}O_4$ mol. wt. 340.42



Syntheses

-Obtained by Fries rearrangement of di (4-methyl-phenyl) pimelate with aluminium chloride in refluxing chlorobenzene for 6 h (59.5 %) [3107].

-Also refer to: [584].

m.p. 140° [584], 100–101° [3107].
N.B.: One of the reported melting points is obviously wrong.
IR [3107].

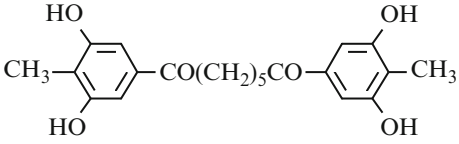
Dimethyl ether [10400-50-7] $C_{23}H_{28}O_4$ mol. wt. 368.47

-Obtained by reaction of pimelic acid dichloride with p-cresol methyl ether in the presence of aluminium chloride (50–70 %) [1576].
-Also refer to: [1575].

m.p. 82° [1575, 1576].

1,7-Bis(3,5-dihydroxy-4-methylphenyl)-1,7-heptanedione

$C_{21}H_{24}O_6$ mol. wt. 372.42



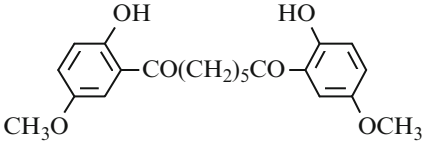
Synthesis

-Refer to: [1316].

m.p. 207° [1316].

1,7-Bis(2-hydroxy-5-methoxyphenyl)-1,7-heptanedione

[10365-29-4] $C_{21}H_{24}O_6$ mol. wt. 372.42



Synthesis

-Obtained by reaction of pimelic acid dichloride with p-dimethoxybenzene in the presence of aluminium chloride [1575].

m.p. 107° [1575].

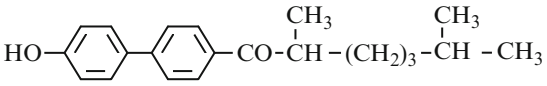
Diacetate [10365-34-1] $C_{25}H_{28}O_8$ mol. wt. 456.49

-Obtained by reaction of acetic anhydride (4 vol) with the title ketone in the presence of 1–2 drops concentrated sulfuric acid, the mixture warmed 5 min [1575].

m.p. 92° [1575].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-2,6-dimethyl-1-heptanone

[117693-02-4] $C_{21}H_{26}O_2$ mol. wt. 310.44



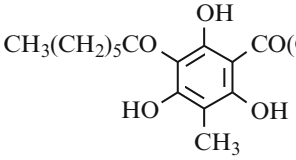
Synthesis
-Refer to: [2095].

Benzyl ether [117693-01-3] $C_{28}H_{32}O_2$ mol. wt. 400.56

-Refer to: [2095].

1,1-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-heptanone

[3118-39-6] $C_{21}H_{32}O_5$ mol. wt. 364.48



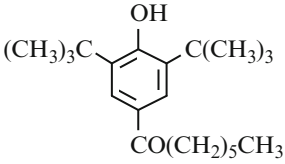
Syntheses
-Obtained by reaction of heptanoic anhydride with 2-methylphloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].
-Also refer to: [457, 600, 2911].

m.p. 108–110° [457, 2911].

BIOLOGICAL ACTIVITY: For treatment of immune dysfunction associated with human immuno deficiency virus infection [600]; Anthelmintic [457].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-heptanone

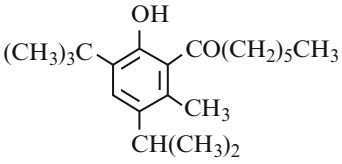
$C_{21}H_{34}O_2$ mol. wt. 318.50



Syntheses
-Refer to: [3103, 3104].
m.p. 76–78° [3103, 3104];
^{1}H NMR [3103, 3104], ^{13}C NMR [3104], IR [3103, 3104].

1-[3-(1,1-Dimethylethyl)-2-hydroxy-6-methyl-5-(1-methylethyl)phenyl]-1-heptanone

[129375-14-0] $C_{21}H_{34}O_2$ mol. wt. 318.50

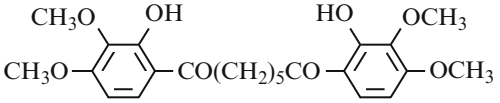


Synthesis
-Obtained by Fries rearrangement of 2-(1,1-dimethylethyl)-5-methyl-4-(1-methylethyl)phenyl heptanoate (**23**) with titanium tetrachloride in chlorobenzene at 100° for 2 h (67 %) (**29**) [1997].

pale yellow oil [1997]; b.p.$_{0.2}$ 156–157° [1997];
m.p. 29–30° (Sadtler standard N° 79804K) [1997];
^{1}H NMR (Sadtler standard N° 52745M) [1997],
IR (Sadtler standard N° 79804K) [1997], UV [1997], MS [1997].

1,7-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,7-heptanedione

[10351-91-4] $C_{23}H_{28}O_8$ mol. wt. 432.47



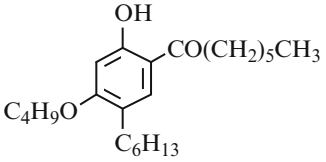
Syntheses
-Obtained by reaction of pimelic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride in tetrachloroethane [1574].

-Also refer to: [589, 1575].

m.p. 116° [1574, 1575], 114° [589].

1-(4-Butoxy-5-hexyl-2-hydroxyphenyl)-1-heptanone

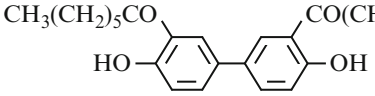
[143287-07-4] $C_{23}H_{38}O_3$ mol. wt. 362.55



Synthesis
-Obtained (**12b**) by reaction of 1-bromobutane with 1-(2,4-dihydroxy-5-hexylphenyl)-1-heptanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].
m.p. 32–33° [284].

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-heptanone

[104098-36-4] $C_{26}H_{34}O_4$ mol. wt. 410.55



Syntheses
-Preparation by Fries rearrangement of 4,4′-biphenyl dienanthate with aluminium chloride,

*in the presence of sodium chloride at 140° (85 %) [2091];
*in refluxing chlorobenzene for 24 h (52 %) [2377].

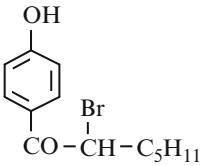
m.p. 93–94° [2377]; IR [2377].

2 Aromatic Hydroxyketones Derived from Various Halogenoheptanoic Acids

2.1 Unsubstituted Hydroxyketones

2-Bromo-1-(4-hydroxyphenyl)-1-heptanone

$C_{13}H_{17}BrO_2$ mol. wt. 285.18



Synthesis

-Refer to: [1140].

Tert-butyl ether [97744-27-9]

2-Bromo-1-[4-(1,1-dimethylethoxy)phenyl]-1-heptanone

$C_{17}H_{25}BrO_2$ mol. wt. 341.29

-Refer to: [1140].

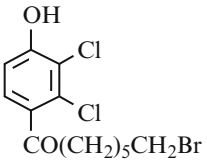
Methyl ether [1033774-79-6] $C_{14}H_{19}BrO_2$ mol. wt. 299.21

-Refer to: [2987].

2.2 Substituted Hydroxyketones

7-Bromo-1-(2,3-dichloro-4-hydroxyphenyl)-1-heptanone

$C_{13}H_{15}BrCl_2O_2$ mol. wt. 354.07



Synthesis

-Refer to: [3333].

Methyl ether [53107-72-5]

$C_{14}H_{17}BrCl_2O_2$ mol. wt. 368.10

-Obtained by reaction of 7-bromoheptanoyl chloride with 2,3-dichloroanisole in the presence of aluminium chloride (58 %) [3333].

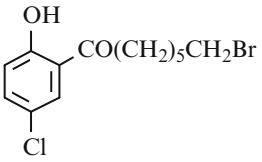
-Also refer to: [740, 2051–2053].

m.p. 57° [2051, 2052, 3333].

USE: Preparation and cyclization of, [2053]; Preparation and reaction of, with formaldehyde [2052].

7-Bromo-1-(5-chloro-2-hydroxyphenyl)-1-heptanone

[206051-19-6] $C_{13}H_{16}BrClO_2$ mol. wt. 319.63

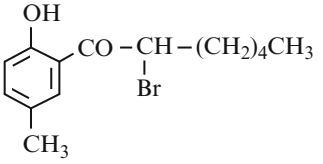


Synthesis
-Refer to: [3284].

Methyl ether [187396-82-3]
$C_{14}H_{18}BrClO_2$ mol. wt. 333.65
-Refer to: [308, 3284].

2-Bromo-1-(2-hydroxy-5-methylphenyl)-1-heptanone

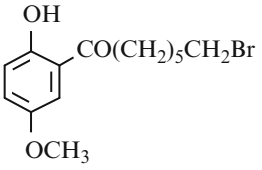
$C_{14}H_{19}BrO_2$ mol. wt. 299.21



Synthesis
-Refer to: [181].
Fluorescence [181].

7-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-heptanone

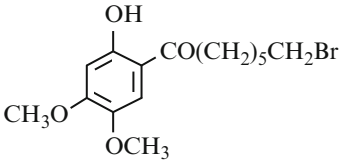
[173055-36-2] $C_{14}H_{19}BrO_3$ mol. wt. 315.20



Synthesis
-Refer to: [2623].

7-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-heptanone

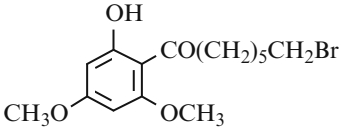
[173055-42-0] $C_{15}H_{21}BrO_4$ mol. wt. 345.23



Synthesis
-Refer to: [2623].

7-Bromo-1-(2-hydroxy-4,6-dimethoxyphenyl)-1-heptanone

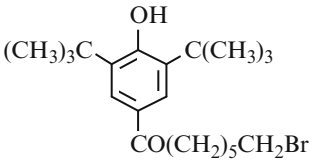
[173055-48-6] $C_{15}H_{21}BrO_4$ mol. wt. 345.23



Synthesis
-Refer to: [2623].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-7-bromo-1-heptanone

[158869-48-8] $C_{21}H_{33}BrO_2$ mol. wt. 397.39



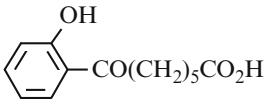
Synthesis
-Refer to: [1689].

3 Aromatic Hydroxyketones Derived from 7-Oxoheptanoic Acids

3.1 Unsubstituted Hydroxyketones

7-(2-Hydroxyphenyl)-7-oxo-1-heptanoic acid

[57262-58-5] $C_{13}H_{16}O_4$ mol. wt. 236.27



Syntheses
-Obtained by treatment of tetrahydroxanthone (m.p. 104°) with 30 % KOH in refluxing ethanol for 1 h [1211].

-Also refer to: [1196].

colourless plates [1211]; m.p. 97–99° [1211], 94° [1196];
^{1}H NMR [1196], IR [1196], UV [1196].

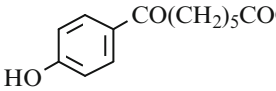
Methyl ester [133535-19-0] $C_{14}H_{18}O_4$ mol. wt. 250.29

-Refer to: [1211].

colourless plates [1211];
b.p.$_{.3}$ 182–184° [3370]; m.p. 40–42° [1211], 37.5–38.5° [3370].

7-(4-Hydroxyphenyl)-7-oxo-1-heptanoic acid

$C_{13}H_{16}O_4$ mol. wt. 236.27

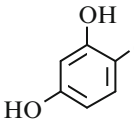


Syntheses
-Refer to: [445, 1196].
m.p. 140–141° [445]; IR [1196], UV [1196].

7-(2,4-Dihydroxyphenyl)-7-oxo-1-heptanoic acid

4-(6-Carboxyhexanoyl)resorcinol [2184]

[30414-64-3] $C_{13}H_{16}O_5$ mol. wt. 252.27



Syntheses

-Obtained by reaction of pimelic acid with resorcinol in the presence of zinc chloride at 140° for 5 h (50 %) [445].

-Also obtained by passing rapidly for 3 h hydrogen chloride into a mixture of resorcinol, methyl 6-cyanohexanoate, anhydrous zinc chloride and ether at 0°. The mixture was kept at 0° overnight and the resulting red oil was boiled with water for 30 min (20.4 %) [2184].

plates [2184];
m.p. 131–131.5° [2184], 126–127° [2606], 126° [589], 124–126° [445];
IR [2184], UV [2184].

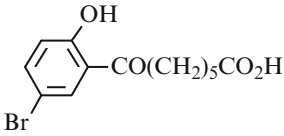
Methyl ester $C_{14}H_{18}O_5$ mol. wt. 266.29

$b.p._{.0.4}$ 250–255° [445].

3.2 Substituted Hydroxyketones

7-(5-Bromo-2-hydroxyphenyl)-7-oxo-1-heptanoic acid

$C_{13}H_{15}BrO_4$ mol. wt. 315.16



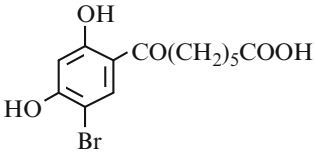
Synthesis

-Obtained by treatment of 7-bromotetrahydroxanthone (m.p. 151°) with 30 % KOH in refluxing dilute ethanol for 1 h [1211].

colourless plates [1211]; m.p. 120° [1211].

7-(5-Bromo-2,4-dihydroxyphenyl)-7-oxo-1-heptanoic acid

[32246-72-3] $C_{13}H_{15}BrO_5$ mol. wt. 331.16



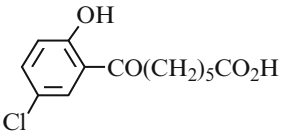
Synthesis

-Refer to: [589].

m.p. 140° [589].

7-(5-Chloro-2-hydroxyphenyl)-7-oxo-1-heptanoic acid

[22994-79-2] $C_{13}H_{15}ClO_4$ mol. wt. 270.71

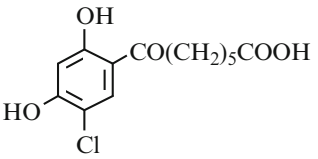


Syntheses
-Obtained by treatment of 7-chlorotetrahydroxanthone (m.p. 154°) with 30 % KOH in refluxing dilute ethanol for 1 h [1211].
-Also refer to: [584].

colourless plates [1211]; m.p. 122° [1211], 119° [584].

7-(5-Chloro-2,4-dihydroxyphenyl)-7-oxo-1-heptanoic acid

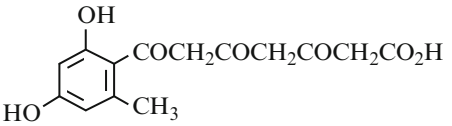
[32340-75-3] $C_{13}H_{15}ClO_5$ mol. wt. 286.71



Synthesis
-Refer to: [589].
m.p. 147–148° [589].

7-(2,4-Dihydroxy-6-methylphenyl)-3,5,7-trioxo-1-heptanoic acid

$C_{14}H_{14}O_7$ mol. wt. 294.26



Syntheses
-Obtained from 3,5,7,9,11,13-hexaoxotetradecanoic acid [1253].
-Also refer to: [1259, 1287].

USE: Precursor of 2,2′,4,4′,6-pentahydroxy-6′-methylbenzophenone in the biosynthesis of griseofulvin [1253].

Dimethyl ether [62643-23-6] $C_{16}H_{18}O_7$ mol. wt. 322.31

-Obtained by adding 1-(2,4-dimethoxy-6-methylphenyl)-1,3,5-hexanetrione to lithium diisopropylamide in THF at 0° under nitrogen. After 10 min, CO_2 was bubbled into the red-brown reaction mixture for 5 min. The solvent was evaporated in vacuo and the residue was acidified with cold, dilute HCl (19 %) [1259].

m.p. 84–85.5° [1259]; ^{1}H NMR [1259], IR [1259], UV [1259].

Methyl ester of the dimethyl ether [38071-49-7] $C_{17}H_{20}O_7$ mol. wt. 336.34

-Obtained by treatment of methyl 7-(2-hydroxy-4-methoxy-6-methylphenyl)-3,5,7-trioxoheptanoate with diazomethane in ethyl ether for 30 s (95 %) [1259, 1287].

yellow oil [1259]; ^{1}H NMR [1259], IR [1259], UV [1259].

Dibenzyl ether [38071-43-1] $C_{28}H_{26}O_7$ mol. wt. 474.51

-Refer to: [1259].

Methyl ester of the dibenzyl ether [38071-44-2] $C_{29}H_{28}O_7$ mol. wt. 488.54

-Refer to: [1259, 1287].

IR [1259], UV [1259].

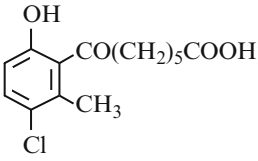
Methyl ester [38071-45-3] $C_{15}H_{16}O_7$ mol. wt. 308.29

-Refer to: [1259].

-Obtained by hydrogenolysis of methyl ester of dibenzyl ether [1287].

7-(5-Chloro-2-hydroxy-6-methylphenyl)-7-oxo-1-heptanoic acid

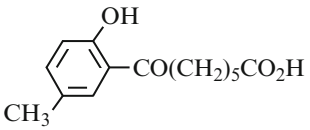
$C_{14}H_{17}ClO_4$ mol. wt. 284.74



Synthesis
-Refer to: [584].
m.p. 148° [584]

7-(2-hydroxy-5-methylphenyl)-7-oxo-1-heptanoic acid

$C_{14}H_{18}O_4$ mol. wt. 250.29

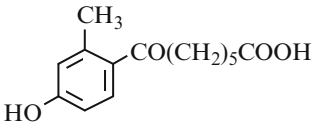


Synthesis
-Obtained by treatment of 7-methyltetrahydroxanthone (m.p. 102–103°) with 30 % KOH in refluxing dilute ethanol for 1 h [1211].

colourless plates [1211]; m.p. 87° [1211].

7-(4-Hydroxy-2-methylphenyl)-7-oxo-1-heptanoic acid

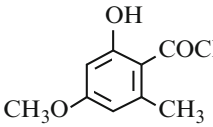
[22811-84-3] $C_{14}H_{18}O_4$ mol. wt. 250.29



Synthesis
-Refer to: [584].
m.p. 105° [584].

7-(2-Hydroxy-4-methoxy-6-methylphenyl)-3,5,7-trioxo-1-heptanoic acid

$C_{15}H_{16}O_7$ mol. wt. 308.29



Synthesis
-Refer to: [1259].

Methyl ester

$C_{16}H_{18}O_7$ mol. wt. 322.31

-Obtained by hydrogenolysis of its benzyl ether (86 %) [1259].

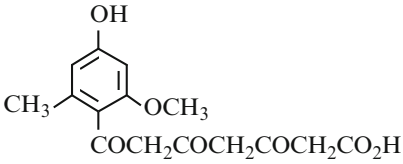
Benzyl ether of the methyl ester [62643-41-8] $C_{23}H_{24}O_7$ mol. wt. 412.44

-Obtained by treatment of 1-(2-benzyloxy-4-methoxy-6-methylphenyl)-1,3,5-hexanetrione with lithium diisopropylamide in THF for 15 min at 0° followed by gaseous CO_2 (28 %) [1259].

yellow oil [1259];
^{1}H NMR [1259], IR [1259], UV [1259], MS [1259].

7-(4-Hydroxy-2-methoxy-6-methylphenyl)-3,5,7-trioxo-1-heptanoic acid

$C_{15}H_{16}O_7$ mol. wt. 308.29

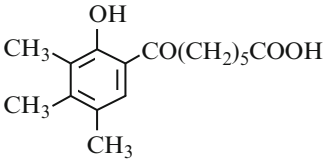


Synthesis
-Refer to: [1253].

USE: Precursor of griseophenone C in the biosynthesis of griseofulvin [1253].

7-(2-Hydroxy-3,4,5-trimethylphenyl)-7-oxo-1-heptanoic acid

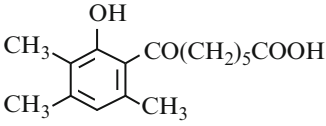
[84978-19-8] $C_{16}H_{22}O_4$ mol. wt. 278.35



Synthesis
-Refer to: [2325].
m.p. 105° [2325]; ^{1}H NMR [2325], IR [2325].

7-(2-Hydroxy-3,4,6-trimethylphenyl)-7-oxo-1-heptanoic acid

[58185-75-4] $C_{16}H_{22}O_4$ mol. wt. 278.35



Synthesis
-Refer to: [2149, 2325].
m.p. 119–125° [2149, 2325]; ^{1}H NMR [2149, 2325], IR [2149, 2325].

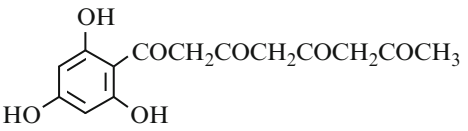
Chapter 6
Octanones

1 Aromatic Hydroxyketones Derived from Octanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2,4,6-Trihydroxyphenyl)-1,3,5,7-octanetetraone

[72327-96-9] $C_{14}H_{14}O_7$ mol. wt. 294.26



Syntheses
-Obtained from 3,5,7,9,11,13-hexaoxo-tetradecanoic acid [1253].
-Also refer to: [1259, 2699].

USE: Precursor of 2,2′,4,4′,6-pentahydroxy-6′-methylbenzophenone in the biosynthesis of griseofulvin [1253].

Trimethyl ether [76631-05-5] $C_{17}H_{20}O_7$ mol. wt. 336.34

-Preparation by acylation of dianion of 2,4-pentanedione with methyl 2,4,6-trimethoxyphenyl-3-oxopropanoate (42 %) [2699].
-Also obtained by acylation of trianion of 2,4,6-heptanetrione with methyl 2,4,6-trimethoxy-benzoate (65 %) [2699].

yellow crystals [2699]; m.p. 176–179° [2699];
^{1}H NMR [2699], IR [2699], MS [2699].

Tribenzyl ether [72327-93-6] $C_{35}H_{32}O_7$ mol. wt. 564.63

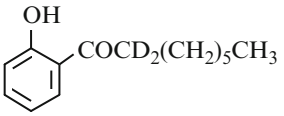
-Preparation by acylation of trianion of 2,4,6-heptanetrione with methyl 2,4,6-tribenzoxybenzoate (65 %) [2699].

orange-red oil [2699]; ^{1}H NMR [2699], IR [2699], MS [2699].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_6

1-(2-Hydroxyphenyl)-1-octanone-*2,2-d2*

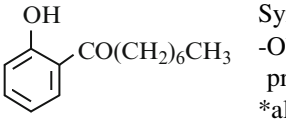
[956239-90-0] $C_{14}H_{18}D_2O_2$ mol. wt. 222.58



Synthesis
-Refer to: [173].
MS [173].

1-(2-Hydroxyphenyl)-1-octanone

[3226-27-5] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses
-Obtained by Fries rearrangement of phenyl caprylate in the presence of,
*aluminium chloride in nitrobenzene at 50° for 18 h (30 %) [775, 776] or in tetrachloroethane [3169] at 120° [2520] or at 80° for 12–15 h (37.7 %) [1585];
*titanium tetrachloride in tetrachloroethane at 70° for 6 h (22 %) [2552];
*ferric chloride in tetrachloroethane at 70° for 6 h (19 %) [2552];
*without solvent at 130–150° [2520] or at 140° for 45 min (41 %) [932].
-Also obtained by photo-Fries rearrangement of phenyl caprylate in cyclohexane, heptane, benzene or n-amyl alcohol in a sealed tube with an unfiltered Hanovia 450 w medium pressure lamp [2067].
-Also obtained by Friedel-Crafts reaction of caprylic chloride with phenol in the presence of aluminium chloride at 125–130° for 1 h (45 %) [2700],
*in nitrobenzene at 50° for 18 h (25 %) [775];
*in tetrachloroethane at 55° for 4 h (50 %) [2548], at 100° for 6 h (54 %) [2550], at 70° for 3 h (21 %) [2549], at 403–413 K for 6 h (36 %) [3348];
*in carbon disulfide at reflux (46°) (33 %) [2550];
*in skellysolve B at 65° (44 %) [2550].
-Also obtained by zeolite-catalyzed Friedel-Crafts reaction of anisole with octanoic acid [3266].
-Also refer to: [2658].

b.p.$_{.1}$ 97–99° [2548], b.p.$_{0.1}$ 104° [932], b.p.$_{0.01}$ 110.5–114° [1585], b.p.$_{0.02}$ 112° [2520],
b.p.$_{.1}$ 115–120° [2549, 2550], b.p.$_{0.4}$ 123.5–124.5° [3169], b.p.$_{11}$ 169–170° [2700];
m.p. 22.3° [2700], 22° [2520];
^{1}H NMR [2067], IR [2067, 2520], UV [1996, 2067, 2520], MS [2067];
n_D^{25} = 1.5151 [1585], $n_D^{25.5}$ = 1.5169 [2700];
X-ray data [3348]; TLC [1994]; GLC [2067]; GC [2067].

USE: In a process for the preparation of 2-hydroxy-3-(C6-10 n-alkyl) benzaldoximes for use in the solvent extraction and recovery of copper from mineral and other wastes [3162].

2,4-Dinitrophenylhydrazone [17744-54-6] $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 145° [3169], 144.5–145° [2549], 140–141° [2548], 140° [932].

Oxime [57835-34-4] $C_{14}H_{21}NO_2$ mol. wt. 235.33

-Refer to: [1142, 1585, 2077, 2520].

m.p. 80° [2520], 76.5–77.5° [1585];
IR [2520], UV [2520].

USE: Blocking agent, binders containing blocked PAPI and phenolic resins for wood composites [2077]; Solvent extraction of copper (II) [2520]; For extn. of metals [1142].

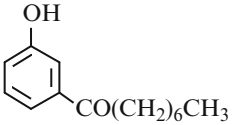
Methyl ether $C_{15}H_{22}O_2$ mol. wt. 234.34

-Obtained by oxidation of 1-(2-methoxyphenyl)-1-octanol with CrO_3 (0.05 equiv.) and t-BuOOH (3 equiv.) in methylene chloride at r.t. for 23 h (79 %) [2204].

oil [2204]; ^{1}H NMR [2204].

1-(3-Hydroxyphenyl)-1-octanone

[778630-63-0] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses
-Obtained by treatment of its methyl ether with aluminium chloride in benzene by heating on a water bath for 2 h (80 %) [966].
-Also refer to: [967].

m.p. 58° [966, 967].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 113° [967].

Methyl ether [136116-43-3] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Obtained by condensation of heptylmagnesium bromide with m-methoxybenzamide in ethyl ether. The reaction was carried out at 60° for 48 h under hydrogen atmosphere (60–70 %) [966].
-Also obtained by oxidation of 1-(3-methoxyphenyl)-1-octanol with CrO_3 (0.05 equiv.) and t-BuOOH (4 equiv.) in methylene chloride at r.t. for 23 h (95 %) [2204].
-Preparation by silyl chromate-catalyzed oxidation of allyl ether (96 %) [2203].
-Also refer to: [967].

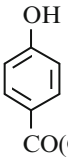
oil [2204]; b.p.$_{15}$ 160° [966, 967]; ^{1}H NMR [2204]; $n_D^{31.5} = 1.4700$ [967].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 90° [967].

1-(4-Hydroxyphenyl)-1-octanone

[2589-73-3] $C_{14}H_{20}O_2$ mol. wt. 220.31



Syntheses

-Preparation by Fries rearrangement of phenyl caprylate,

*with aluminium chloride in nitrobenzene [1585], (60 %) [2947], at 38° for 2 days (59 %) [414] at 50° for 18 h (55 %) [775, 776] or in tetrachloroethane [3169] at 80° for 12–15 h (42–44.6 %) [1585] or without solvent at 140° for 45 min (34 %) [932];

*in the presence of aluminium chloride in refluxing carbon disulfide for 5 h. Then, the mixture was kept at 80–90° for 2 h and at 140–150° for 1 h after solvent elimination [1222];

*with ferric chloride in tetrachloroethane at 70° for 6 h (52 %) [2552];

*with titanium tetrachloride in tetrachloroethane at 70° for 6 h (19 %) [2552];

*with boron trifluoride for 3 h at 75–80° (58.2 %) [1938].

-Also obtained by photo-Fries rearrangement of phenyl caprylate in cyclohexane, heptane, benzene or n-amyl alcohol in a sealed tube with an unfiltered Hanovia 450 w medium pressure lamp [2067].

-Also obtained by reaction of caprylyl chloride with phenol in the presence of aluminium chloride,

*without solvent at 125–130° for 1 h (38 %) [2700];

*in nitrobenzene at 50° for 18 h (67 %) [775] or at r.t. overnight (57 %) [1769];

*in methylene chloride for 1 h at 0°, then at r.t. overnight (100 %) [114] or for 14 h at r.t. (35 %) [1910];

*in tetrachloroethane at 70° for 3 h (49 %) [2549] at 55° for 4 h (12 %) [2548].

-Also obtained by reaction of caprylic acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3277].

-Also refer to: [61, 62, 113, 1087, 1116, 1395, 1536, 1892, 1977, 2658, 2692, 2704, 3371].

b.p.$_{.4}$ 178–181° [1769], b.p.$_1$ 183° [932, 1536], b.p.$_{.2.1}$ 210° [1938], b.p.$_{10}$ 218–221° [2947], b.p.$_{10}$ 224–225° [2700];

white solid [1910];

m.p. 72.9–73.2° [1910], 64.5° [2704], 63° [775, 776], 62.5–63.5° [2548], 62–63.5° [3277],

62–63° [2549], 62–62.5° [2550], 62° [2700], 61–62° [1769, 3169], 59.5–61° [1585], 59° [932, 1536], [1938] 58–60° [414];

^{1}H NMR [114, 1910, 1977, 2067], ^{13}C NMR [114, 1910, 1977], IR [1910, 2067], UV [1995, 2067], MS [1910, 2067];
TLC [1910, 1994]; GLC [2067]; GC [2067]; pKa [2590]; dipole moment [2590].

USE: In a process for the preparation of 2-hydroxy-3-(C6-10 n-alkyl) benzaldoximes for use in the solvent extraction and recovery of copper from mineral and other wastes [3162]; Activator for peroxygen bleach in laundry detergent for mud-soiled clothing [3371]; As colour developer [2704].

BIOLOGICAL ACTIVITY: Inhibition of 17-β hydroxysteroid dehydrogenase 3 [1910]; Estrogenic [2692].

Oxime [84498-21-5] $C_{14}H_{21}NO_2$ mol. wt. 235.33

-Refer to: [1142].

USE: For extn. of metals [1142].

2,4-Dinitrophenylhydrazone [17765-30-9] $C_{20}H_{24}N_4O_5$ mol. wt. 400.43

m.p. 178° [3169], 176–178° [2548], 171° [932].

Nicotinylhydrazone [102240-72-2] $C_{20}H_{25}N_3O_2$ mol. wt. 339.44

m.p. 148° [521, 520].

USE: In chemotherapy of leprosy [520, 521].

isoNicotinylhydrazone [102240-70-0] $C_{20}H_{25}N_3O_2$ mol. wt. 339.44

m.p. 206° [520, 521].

USE: In chemotherapy of leprosy [520, 521].

Phosphate (57 %) [114].

^{1}H NMR [114], ^{13}C NMR [114], ^{31}P NMR [114].

Sulfate [114]; ^{1}H NMR [114].

Methyl ether [62170-25-6] $C_{15}H_{22}O_2$ mol. wt. 234.34

-Surfactant-type iron complex-catalyzed mild oxidation of 4-octylanisole using aqueous TBHP as oxidant in water at 30° for 50 h (84 %) [2217].
-Also obtained by direct acylation of 4-bromoanisole with caprylic aldehyde by palladium catalysis (87 %) [2668].
-Also obtained by oxidation of 4-n-octylanisole at 30° in the presence of tert-butyl hydroperoxide and $Fe_2O(O_3SOC_{12}H_{25})_4$ [1714].

-Nickel-catalyzed cross-coupling of 4-iodo-1-(4-methoxyphenyl)-1-butanone with n-butylmagnesium chloride in DMA at −35° for 30 min (68 %) [3212].
-Also obtained by reaction of octanoic acid with anisole,
*over three large pore zeolites-beta (BEA) [282], faujasite (FAU) and mordenite (MOR) [3246];
*in the presence of $Cs_{2.5}H_{0.5}PW_{12}O_{40}$ at 110° for 5 h (33 %) [1636];
*on the solid surface of alumina in the presence of trifluoroacetic anhydride for 120 min at r.t. (94 %) [2563];
*over HZSM-5 catalyst for 48 h at 423° K (4 %) [3265];
*in the presence of an ultrastable Y zeolite (USY) catalyst [1941];
*in the presence of HY zeolite as catalyst [3264];
*in the presence of zeolite H-beta [1185].
-Also obtained by acylation of anisole with octanoyl chloride in the presence of strongly acidic mesoporous aluminosilicates prepared from zeolite seeds [2865].
-Also obtained by Friedel-Crafts acylation of anisole in the presence of zeolites [281].
-Also obtained by reaction of octanoic anhydride with anisole in the presence of Yb $(NTf_2)_3$ in nitromethane for 2 h at 25° (99 %) [2272].
-Also obtained by oxidation of 1-(4-methoxyphenyl)-1-octanol with CrO_3 (0.05 equiv.) and t-BuOOH (4 equiv.) in methylene chloride at r.t. for 17 h (94 %) [2204].
-Also obtained by zeolite-catalyzed Friedel-Crafts reaction of anisole with octanoic acid [3266].
-Also refer to: [279, 280, 698 (61 %), 929, 1009, 1120 (72 %), 1897, 2016].

white solid [1120];
m.p. 52.5–53° [2016], 48–49° [2204], 45.3–46.7° [1897], 44° [1120];
^{1}H NMR [698, 1120, 1864, 1897, 2204, 2217, 2272, 2563, 2668, 3212];
^{13}C NMR [698, 1120, 1864, 1897, 2204, 2217, 2668, 3212],
IR [698, 929, 1864, 2217, 2563, 2668], MS [698, 1864, 1897, 2668].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 140–140.5° [2016].

Benzoate $C_{21}H_{24}O_3$ mol. wt. 324.42

m.p. 107–108° [2700].

Caprylate [102946-00-9] $C_{22}H_{34}O_3$ mol. wt. 346.51

-Obtained by reaction of caprylic acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3277].
-Also obtained (by-product) by Fries rearrangement of phenyl octanoate,
*with titanium tetrachloride in tetrachloroethane for 6 h at 70° (10 %) [2552];
*with stannic chloride in tetrachloroethane for 7 h at 150° (5 %) [2552].

m.p. 56.5–57.5° [2551], 56–57° [3277].

Phenyl ether $C_{20}H_{24}O_2$ mol. wt. 296.41

-Obtained by treatment of diphenyl oxide with octanoyl chloride under Friedel-Crafts conditions [516].

m.p. 35° [516].

4-Octanoylphenyl ether [38051-39-7] $C_{28}H_{38}O_3$ mol. wt. 422.61

-Obtained by reaction of octanoyl chloride with diphenyl ether in the presence of aluminium chloride in refluxing carbon disulfide for 30 min (63 %) [463].

m.p. 103° [463]

Dioxime of the 4-octanoylphenyl ether $C_{28}H_{40}N_2O_3$ mol. wt. 452.64

-Preparation: A suspension of the diketone, 100 % excess of hydroxylamine hydrochloride, and powdered anhydrous sodium carbonate in butanol [463].

m.p. 102° [721], 76° [463]

Dihydrazone of the 4-octanoylphenyl ether $C_{28}H_{42}N_4O$ mol. wt. 450.67

$b.p._{0.02}$ 220–230° [721]; m.p. 76° [721].

N-Diethylaminoethyl ether [14392-78-0] $C_{20}H_{33}NO_2$ mol. wt. 319.49

-A solution of 4-hydroxyoctanophenone in ethanol was added to a solution of sodium in ethanol; the mixture was refluxed 1 h, cooled, and a solution of $ClCH_2CH_2N(C_2H_5)_2$ added (80 %) [414, 415].

$b.p._{0.005}$ 156–166° [414, 415]; $n_D^{21} = 1.51$ [414, 415].

Hydrochloride of the N-diethylaminoethyl ether

[102462-84-0] $C_{20}H_{33}NO_2$, HCl mol. wt. 355.95

m.p. 95° [2227].

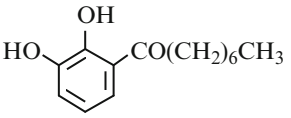
Fumarate of the N-diethylaminoethyl ether

[14392-93-9] $C_{20}H_{33}NO_2$, $C_4H_4O_4$ mol. wt. 435.56

m.p. 76–78° [415].

1-(2,3-Dihydroxyphenyl)-1-octanone

[862666-36-2] $C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses

-Obtained by deprotection of its dimethyl ether with boron tribromide in methylene chloride at 0°. Then, the mixture was stirred overnight at r.t. (71 %) [82].

-Also obtained (by-product) by Fries rearrangement of pyrocatechol dicaprylate with aluminium chloride in the presence of pyrocatechol for 4.5 h at 135–140° [2075].

brown solid [82]; b.p.$_4$ 210–220° [2075];
m.p. 87–88° [2075], 47° [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

USE: Reactant for preparation of lithium gallium/titanium ketone complexes [82].

Dimethyl ether [1854-64-4] $C_{16}H_{24}O_3$ mol. wt. 264.36

-Obtained by treatment of 1-(2,3-dimethoxyphenyl)-1-octanol in acetone with potassium dichromate in dilute sulfuric acid (Jones reagent) at r.t. for 3 h (49 %) [82].
-Also obtained by treatment of 2,3-dimethoxyphenylheptylcarbinol with potassium dichromate in dilute sulfuric acid at 30° (63 %) [3148].
-Also obtained from 2,3-dimethoxybenzoyl chloride by dialkylcadmium synthesis (41 %) [822].
-Also refer to: [2601].

colourless oil [82];
b.p.$_{0.1}$ 114–115° [822], b.p.$_{0.2}$ 128–129° [2601], b.p.$_{15}$ 198–201° [3148];
^{1}H NMR [82, 822], ^{13}C NMR [82], IR [82, 822], MS [82].

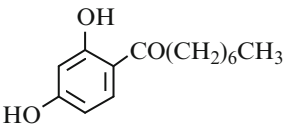
2,4-Dinitrophenylhydrazone of the dimethyl ether

[1854-63-3] $C_{22}H_{28}N_4O_6$ mol. wt. 444.49

m.p. 121° [3148].

1-(2,4-Dihydroxyphenyl)-1-octanone

[37622-68-7] $C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses

-Obtained by refluxing a mixture of caprylic acid, resorcinol and fused zinc chloride [2702] at 125–130° for 2 h (75 %) [3124].
-Also obtained by reaction of caprylic nitrile with resorcinol (Hoesch reaction) [1608].

-Also obtained by reaction of octanoyl chloride with resorcinol in the presence of aluminium chloride in 1,2-dichloroethane for 5 h at 65° [284].
-Also refer to: [651, 893, 1515, 2112, 2114, 2673, 2704, 2842, 3168, 3345].

b.p.$_{.4}$ 191–201° [3124], b.p.$_{.6–7}$ 214–216° [893, 2842];
m.p. 66° [2704], 62.5–64° [893, 2842], 62° [2673], 60–61° [3124], 58–59° [1608], 55–56° [1515];
^{1}H NMR [1515], ^{13}C NMR [1515], MS [1515].

USE: As colour developer [2704]; Wine preservation by, [3168].

BIOLOGICAL ACTIVITY: Antiseptic and germicidal product [2734]; Antifungal [651, 2112, 2114].

Hemihydrate $C_{14}H_{20}O_3$, 0.5 H_2O mol. wt. 245.32

m.p. 56–58° [1608].

2,4-Dinitrophenylhydrazone [94759-02-1] $C_{20}H_{24}N_4O_6$ mol. wt. 416.43

m.p. 202° [2673].

Dimethyl ether [6565-75-9] $C_{16}H_{24}O_3$ mol. wt. 264.36

-Obtained by reaction of octanoic acid with resorcinol dimethyl ether in the presence of polyphosphoric acid and heated on a water bath for 30 min (72 %) [2424].
-Also obtained by reaction of octanoyl chloride with resorcinol dimethyl ether in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].
-Also obtained by reaction of 2-chloro-1-(trimethylsilyl)-1-octanone with resorcinol dimethyl ether in the presence of titanium tetrachloride (84 %) [1354].

b.p.$_{.0.5}$ 140° [1354], b.p.$_{.2}$ 148–150° [2424];
^{1}H NMR [1354], ^{13}C NMR [1354], IR [1354].

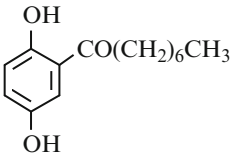
Azine $C_{28}H_{40}N_2O_4$ mol. wt. 468.64

-Refer to: [1793].

USE: Polyolefins stabilization [1793].

1-(2,5-Dihydroxyphenyl)-1-octanone

[4693-19-0] $C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses

-Obtained by reaction of caprylic acid with hydroquinone in the presence of a catalytic amount of trifluoromethanesulfonic acid [2985].

-Also obtained by reaction of caprylic acid with hydroquinone in the presence of boron trifluoride in 1,2-dichloroethane at 50–55°. The reaction mixture was allowed to stand overnight, then heated for 5–6 h on a steam bath (69 %) [142].

-Also obtained by treatment of 2-hydroxy-5-methoxyoctanophenone with aluminium bromide in refluxing benzene for 6 h (86 %) [770].

-Also obtained by treatment of 2-hydroxy-5-pentyloxyoctanophenone with aluminium chloride in carbon disulfide for 3 days at r.t. (77 %) [770].

-Also obtained by hydrolysis of 1-(2-hydroxy-5-octanoyloxyphenyl)-1-octanone with 10 % HCl in ethanol (quantitative yield) [2370].

-Preparation by reaction of octanoic acid with hydroquinone in the presence of boron trifluoride for 2 h at 125° [2063].

-Also refer to: [285], [3168, 3043, 3394] (Japanese patents).

yellow crystals [142]; yellow plates [2370];
m.p. 86–87° [2063, 2370], 86° [770], 84.5–86° [142];
IR [2370].

USE: Wine preservation by, [3168].

Oxime [140943-07-3] $C_{14}H_{21}NO_3$ mol. wt. 251.33

-Refer to: [285].

2,4-Dinitrophenylhydrazone $C_{20}H_{24}N_4O_6$ mol. wt. 416.43

m.p. 186° [770].

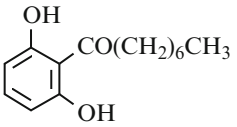
Dimethyl ether [132859-07-5] $C_{16}H_{24}O_3$ mol. wt. 264.36

-Obtained by reaction of octanoic acid chloride with hydroquinone dimethyl ether,
*in the presence of aluminium chloride [2859] in carbon disulfide first at 0°, kept overnight, heated to the boil [2874];
*in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].

m.p. 42–45° [2874]; ^{1}H NMR [2859], MS [2859].

1-(2,6-Dihydroxyphenyl)-1-octanone

[13936-91-9] $C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses

-Preparation by treating resorcinol-4,6-dicarboxylic acid dimethyl ester with caprylyl chloride in the presence of aluminium chloride, followed by hydrolysis and decarboxylation of the compound obtained (30 %) [862].

-Also refer to: [2672].

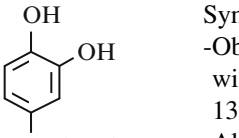
m.p. 77.5–78° [2672], 58–59° [862].
N.B.: One of the reported melting point is obviously wrong.

Dimethyl ether $C_{16}H_{24}O_3$ mol. wt. 264.36

b.p.$_{1.5}$ 163–165° [2672].

1-(3,4-Dihydroxyphenyl)-1-octanone

[37622-78-9] $C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses

-Obtained by Fries rearrangement of pyrocatechol dicaprylate with aluminium chloride in the presence of pyrocatechol at 135–140° for 4.5 h (50 %) [2075] or for 5 h (20 %) [283].

-Also obtained by reaction of octanoyl chloride with pyrocatechol in the presence of aluminium chloride in nitrobenzene, first at 5–7° for 2 h, then at r.t. for 2–3 days (54 %) [1726].

-Also refer to: [3056, 3110].

b.p.$_{2}$ 210–215° [283], b.p.$_{4}$ 210–220° [3056], b.p.$_{5}$ 225° [2075];
m.p. 95.5–96.5° [283, 2075]; ^{1}H NMR [283, 1726].

Diethyl ether [810661-49-5] $C_{18}H_{28}O_3$ mol. wt. 292.42

-Preparation by direct acylation of pyrocatechol diethyl ether with octanoic acid, in the presence of 6 mol% of $AlPW_{12}O_{40}$ (aluminium dodecatungstophosphate) as catalyst in the presence of trifluoroacetic anhydride (TFAA) for 1.5 h (94 %) [1009].

light yellow solid [1009]; m.p. 43° [1009];
^{1}H NMR [1009], ^{13}C NMR [1009], IR [1009], MS [1009]; TLC [1009]; GC [1009].

Dimethyl ether [93157-10-9] $C_{16}H_{24}O_3$ mol. wt. 264.36

-Obtained by reaction of octanoyl chloride with veratrole in the presence of zinc chloride in refluxing carbon disulfide,
*for 6 h and then left overnight (49 %) [2420];
*for 4 h and then left overnight (59 %) [2836].
-Also obtained by reaction of octanoyl chloride with veratrole in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].
-Also refer to: [3364].

silky white flakes [2836];
b.p.$_{.4}$ 165–168° [2420], b.p.$_{.6}$ 180–183° [2836];
m.p. 50° [2836]; IR [3364].

2,4-Dinitrophenylhydrazone of the dimethyl ether

[102758-82-7] $C_{22}H_{28}N_4O_6$ mol. wt. 444.49

red needles; m.p. 130–131° [2420].

Semicarbazone of the dimethyl ether [107778-10-9] $C_{17}H_{27}N_3O_3$ mol. wt. 321.42

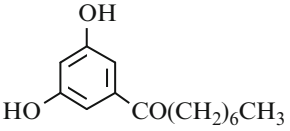
white needles [2836]; m.p. 133° [2836].

Dibenzyl ether $C_{28}H_{32}O_3$ mol. wt. 416.56

-Refer to: [2657]; m.p. 53° [2657].

1-(3,5-Dihydroxyphenyl)-1-octanone

[1257228-28-6] $C_{14}H_{20}O_3$ mol. wt. 236.31



Syntheses
-Refer to: [25, 1893].

BIOLOGICAL ACTIVITY: Receptor binding affinity [1893].

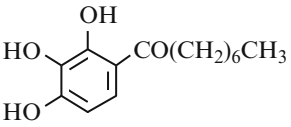
Dimethyl ether $C_{16}H_{24}O_3$ mol. wt. 264.36

-Preparation in the usual way: [25 (60 %), 2990].
-Also refer to: [29].

b.p.$_{0.5}$ 155° [25], b.p.$_2$ 180° [29]; m.p. 36–37° [29].

1-(2,3,4-Trihydroxyphenyl)-1-octanone
4-Octanoylpyrogallol

[43043-28-3] $C_{14}H_{20}O_4$ mol. wt. 252.31



Syntheses
-Obtained by reaction of octanoic acid with pyrogallol in the presence of zinc chloride (Nencki reaction) at 135–140° for 2 h (40 %) [1283].

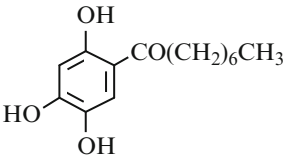
-Also obtained by reaction of octanoyl chloride with pyrogallol in the presence of aluminium chloride in nitrobenzene, first at 5–7° for 2 h, then at r.t. for 2–3 days (57 %) [1726].
-Also refer to: [1660, 2511, 3168].

m.p. 73–74° [1283]; ^{1}H NMR [1726].

USE: Wine preservation by, [3168].

1-(2,4,5-Trihydroxyphenyl)-1-octanone

[107821-60-3] $C_{14}H_{20}O_4$ mol. wt. 252.31



Syntheses
-Preparation by Friedel-Crafts-type catalysts or Fries rearrangement of 1,2,4-trioctanoyloxybenzene with aluminium chloride in nitrobenzene [291].
-Also obtained by reaction of octanoyl chloride with 2,4-trihydroxybenzene in the presence of aluminium chloride in nitrobenzene,

*at r.t. several hrs, and heated 0.5 h at 65° [290];
*first at 25°, then at 60° for 45 min [292].
-Also refer to: [1708].

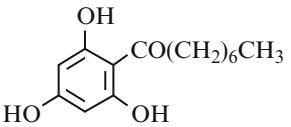
m.p. 113–114° [290–292].

USE: Antioxidant [1708]; Antioxidant for fats and oils [290, 291]; Antioxidant for fats, oils and paraffin waxes [292].

BIOLOGICAL ACTIVITY: Toxicity [1708].

1-(2,4,6-Trihydroxyphenyl)-1-octanone

[43043-32-9] $C_{14}H_{20}O_4$ mol. wt. 252.31



Syntheses
-Obtained by reaction of caprylic nitrile with phloroglucinol (Hoesch reaction) [1441, 1608].
-Also obtained by reaction of octanoyl chloride with phloroglucinol in the presence,

*of boron trifluoride etherate, first at 0°, then at r.t. for 48 h under nitrogen [2786];
*of aluminium chloride in nitrobenzene first between 5 and 10°, then at r.t. overnight (40 %) [2276].
-Also obtained by reaction of octanoyl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene and carbon disulfide mixture (60 %) [2113], (45 %) [2620].
-Also refer to: [1026, 1065, 1441, 2111, 3168].

m.p. 128–129° [2276], 128° [2620], 125° [1441, 2113], 124° [1608].
IR [2276], MS [2276].

USE: Wine preservation by, [3168].

BIOLOGICAL ACTIVITY: Antifungal [2111, 2113].

Monohydrate $C_{14}H_{20}O_4, H_2O$ mol. wt. 270.39

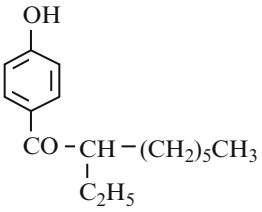
m.p. 106° [1608], 105–106° [1441].

Trimethyl ether [441353-19-1] $C_{17}H_{26}O_4$ mol. wt. 294.39

-Refer to: [1065].

2-Ethyl-1-(4-hydroxyphenyl)-1-octanone (+)

[120837-04-9] (+) $C_{16}H_{24}O_2$ mol. wt. 248.37

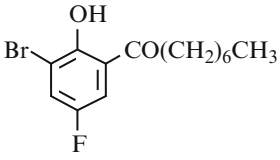


Syntheses
-Refer to: [1318, 1321].

1.2 Substituted Hydroxyketones

1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-octanone

[2262-19-3] $C_{14}H_{18}BrFO_2$ mol. wt. 317.20



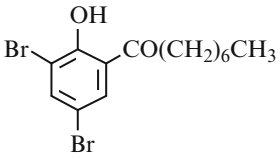
Synthesis
-Obtained by Fries rearrangement of 2-bromo-4-fluoro-phenyl caprylate with aluminium chloride at 130–140° for 3 h (85 %) [1550].
b.p.$_{0.2–0.3}$ 150° [1550].

2,4-Dinitrophenylhydrazone [2414-79-1] $C_{20}H_{22}BrFN_4O_5$ mol. wt. 497.32

m.p. 150° [1550].

1-(3,5-Dibromo-2-hydroxyphenyl)-1-octanone

$C_{14}H_{18}Br_2O_2$ mol. wt. 378.10

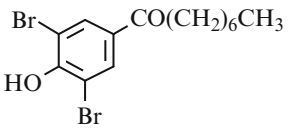


Synthesis
-Refer to: [1039].
Oxime [74832-96-5]
$C_{14}H_{19}Br_2NO_2$ mol. wt. 393.12

USE: Extn. properties with respect to Cu and Mo were detd [1039].

1-(3,5-Dibromo-4-hydroxyphenyl)-1-octanone

[20683-51-6] $C_{14}H_{18}Br_2O_2$ mol. wt. 378.10

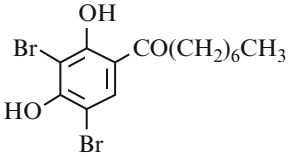


Synthesis
-Obtained by bromination in acetic acid: [2339].

BIOLOGICAL ACTIVITY: Inhibition of enzyme activity [2339].

1-(3,5-Dibromo-2,4-dihydroxyphenyl)-1-octanone

[76092-85-8] $C_{14}H_{18}Br_2O_3$ mol. wt. 394.10

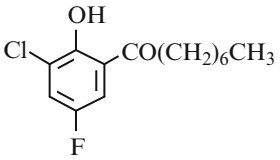


Synthesis
-Refer to: [2112].

BIOLOGICAL ACTIVITY: Antifungal compns. contg., [2112].

1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-octanone

[2262-21-7] $C_{14}H_{18}ClFO_2$ mol. wt. 272.75



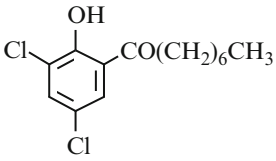
Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-fluorophenyl caprylate with aluminium chloride at 130–140° for 3 h (70 %) [1550].
b.p.$_{2.5–3}$ 160° [1550].

2,4-Dinitrophenylhydrazone [2194-77-6] $C_{20}H_{22}ClFN_4O_5$ mol. wt. 452.87

m.p. 120° [1550].

1-(3,5-Dichloro-2-hydroxyphenyl)-1-octanone

[131427-29-7] $C_{14}H_{18}Cl_2O_2$ mol. wt. 289.20



Syntheses
-Refer to: [433, 1372].

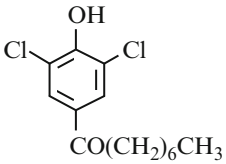
USE: Light stabilizer for vinylidene chloride polymers [1372].

Oxime [74832-95-4] $C_{14}H_{19}Cl_2NO_2$ mol. wt. 304.22

USE: Extn. properties with respect to Cu and Mo were detd. [1039].

1-(3,5-Dichloro-4-hydroxyphenyl)-1-octanone

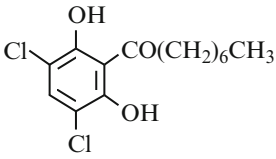
[131427-27-5] $C_{14}H_{18}Cl_2O_2$ mol. wt. 289.20



Synthesis
-Refer to: [433].

1-(3,5-Dichloro-2,6-dihydroxyphenyl)-1-octanone

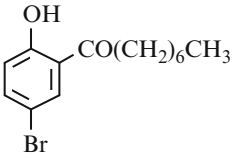
[910457-86-2] $C_{14}H_{18}Cl_2O_3$ mol. wt. 305.20



Synthesis
-Refer to: [2373] (Japanese patent).

1-(5-Bromo-2-hydroxyphenyl)-1-octanone

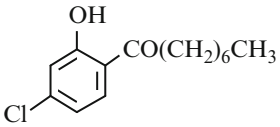
[105465-02-9] $C_{14}H_{19}BrO_2$ mol. wt. 299.21



Syntheses
-Obtained by Fries rearrangement of 4-bromophenyl caprylate with aluminium chloride (77 %) [1640].
-Also refer to: [3404].
b.p.$_{0.65}$ 190–195° [1640]; IR [1640].

1-(4-Chloro-2-hydroxyphenyl)-1-octanone

$C_{14}H_{19}ClO_2$ mol. wt. 254.76



Syntheses
-Preparation by Fries rearrangement of 3-chlorophenyl caprylate with aluminium chloride,
*without solvent at 130° for 2 h (64 %) [2802];
*in nitrobenzene at 25° for 6 h (75 %) [2802].

b.p.$_{18}$ 188° [2802].

Methyl ether $C_{15}H_{21}ClO_2$ mol. wt. 268.78

-Obtained by methylation of the above ketone in the usual way (90 %) [2802].

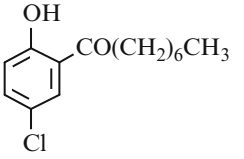
b.p.$_{19}$ 110° [2802].

2,4-Dinitrophenylhydrazone $C_{20}H_{23}ClN_4O_5$ mol. wt. 434.88

m.p. 175° [2802].

1-(5-Chloro-2-hydroxyphenyl)-1-octanone

[52196-48-2] $C_{14}H_{19}ClO_2$ mol. wt. 254.76



Syntheses
-Obtained by Fries rearrangement of 4-chlorophenyl caprylate with aluminium chloride [3170], (56.4 %) [1640].
-Also obtained by reaction of octanoyl chloride with 4-chlorophenol in the presence of aluminium chloride (50.8 %) [2680].

-Also refer to: [1702, 1798].

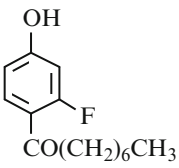
b.p.$_{0.65}$ 152–154° [1640], b.p.$_{2}$ 145–147° [2680];
m.p. 64–65° [2680], 64° [3170], 63° [1702];
IR [1640], UV [3170].

BIOLOGICAL ACTIVITY: Nematocide [1798].

USE: Ionization of, in methylpyrrolidinone [1763].

1-(2-Fluoro-4-hydroxyphenyl)-1-octanone

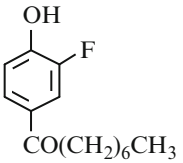
[136964-18-6] $C_{14}H_{19}FO_2$ mol. wt. 238.30



Syntheses
-Refer to: [2363, 3041].

1-(3-Fluoro-4-hydroxyphenyl)-1-octanone

$C_{14}H_{19}FO_2$ mol. wt. 238.30

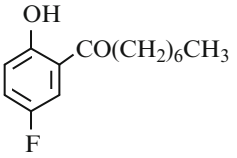


Synthesis
-Refer to: [1549].

Methyl ether [137866-03-6]
$C_{15}H_{21}FO_2$ mol. wt. 252.33
-Refer to: [3041].

1-(5-Fluoro-2-hydroxyphenyl)-1-octanone

[784-64-5] $C_{14}H_{19}FO_2$ mol. wt. 238.30



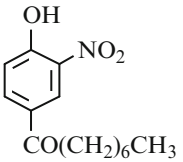
Synthesis
-Preparation by Fries rearrangement of 4-fluorophenyl caprylate [1641] with aluminium chloride at 130° for 2 h (95 %) [1549].
m.p. 47° [1549].

2,4-Dinitrophenylhydrazone [2728-92-9] $C_{20}H_{23}FN_4O_5$ mol. wt. 418.42

m.p. 141° [1549].

1-(4-Hydroxy-3-nitrophenyl)-1-octanone

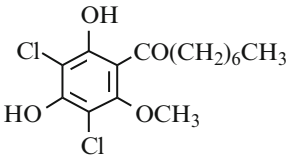
[70079-26-4] $C_{14}H_{19}NO_4$ mol. wt. 265.31



Synthesis
-Obtained by treatment of 4-octanoylphenol with concentrated nitric acid in concentrated sulfuric acid at 0° for 1 h 15 min [1222].
m.p. 51–52° [1222].

1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-octanone

[118222-72-3] $C_{15}H_{20}Cl_2O_4$ mol. wt. 335.23

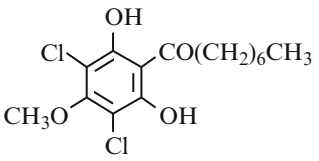


Synthesis
-Obtained by reaction of chlorine with 2,4-dihydroxy-6-methoxyoctanophenone in water [2012].
^{1}H NMR [2012], MS [2012].

BIOLOGICAL ACTIVITY: Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-octanone
(DIF-1) (+2)

[118191-34-7] $C_{15}H_{20}Cl_2O_4$ mol. wt. 335.23



Syntheses
-Preparation by adding a solution of sulfuryl chloride (1.5 equiv.) in ethanol to a solution of 2,6-dihydroxy-4-methoxyoctanophenone in chloroform at r.t.; then, the solution was stirred for 1 h at r.t. [1129].
-Also obtained by reaction of chlorine with 2,6-dihydroxy-4-methoxyoctanophenone in water [2012].

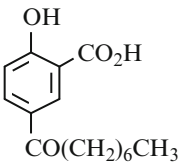
-Also refer to: [1772, 1773, 2341].

yellow amorphous solid [1129]; ^{1}H NMR [2012], MS [1129, 2012].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129]; Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

2-Hydroxy-5-octanoylbenzoic acid

[78418-01-6] $C_{15}H_{20}O_4$ mol. wt. 264.32



Syntheses
-Obtained by saponification of the methyl ester (93 %) [689].
-Also refer to: [80, 174, 196, 320, 974, 1844, 1855, 2439, 2582].

m.p. 117° [921], 113–114° [689]; ^{1}H NMR [921], IR [921], MS [921].

BIOLOGICAL ACTIVITY: Antibacterial [1855]; Deodorant [1855].

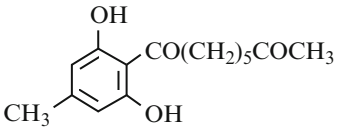
Methyl ester [78417-96-6] $C_{16}H_{22}O_4$ mol. wt. 278.35

-Obtained by reaction of octanoyl chloride with methyl salicylate in the presence of aluminium chloride in carbon disulfide first at 5–10°, then at r.t. for 12 h (85 %) [689].

m.p. 57–58° [689].

1-(2,6-Dihydroxy-4-methylphenyl)-1,7-octanedione
3,5-Dihydroxy-4-(7-oxo-octanoyl)toluene

[30414-67-6] $C_{15}H_{20}O_4$ mol. wt. 264.32



Synthesis
-Obtained by reaction of 7-oxooctanoic acid with 3,5-dihydroxytoluene in the presence of polyphosphoric acid at 60° for 2 h (17.5 %) [2184].

pale yellow needles [2184]; m.p. 139.5–140.5° [2184];
^{1}H NMR [2184], IR [2184], UV [2184].

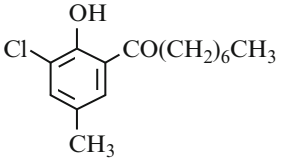
Dimethyl ether [30414-68-7] $C_{17}H_{24}O_4$ mol. wt. 292.37

-Obtained by reaction of dimethyl sulfate with the title ketone in the presence of potassium carbonate in refluxing acetone for 3 h (98 %) [2184].

oil [2184]; b.p. 100° (bath)/ 10^{-3} Torr [2184];
^{1}H NMR [2184], IR [2184], UV [2184].

1-(3-Chloro-2-hydroxy-5-methylphenyl)-1-octanone

[74604-16-3] $C_{15}H_{21}ClO_2$ mol. wt. 268.78



Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-methyl-phenyl octanoate (b.p.$_{0.03}$ 112°) [2520].
pale yellow-brown prisms [2520];
m.p. 35° [2520]; IR [2520], UV [2520].

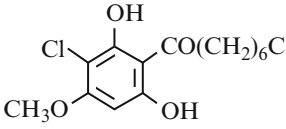
Oxime [74604-08-3] $C_{15}H_{22}ClNO_2$ mol. wt. 283.80

m.p. 101° [2520]; IR [2520], UV [2520].

USE: Solvent extraction of copper (II) [2520].

1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-1-octanone
(DIF-3) (+2)

[861889-90-9] $C_{15}H_{21}ClO_4$ mol. wt. 300.78



Syntheses
-Preparation by adding a solution of sulfuryl chloride (1.5 equiv.) in ethanol to a solution of 2,6-dihydroxy-4-methoxyoctanophenone in chloroform at r.t.; then, the solution was stirred for 1 h at r.t. [1129].

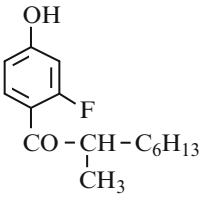
-Also refer to: [1772].

colourless amorphous solid [1129]; MS [1129].

BIOLOGICAL ACTIVITY: Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-(2-Fluoro-4-hydroxyphenyl)-2-methyl-1-octanone

[127928-54-5] $C_{15}H_{21}FO_2$ mol. wt. 252.33

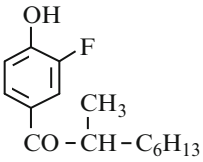


Synthesis
-Refer to: [1322].

Methyl ether (+) [127928-64-7]
$C_{16}H_{23}FO_2$ mol. wt. 266.36
-Refer to: [1322].

1-(3-Fluoro-4-hydroxyphenyl)-2-methyl-1-octanone

[127928-53-4] (+) $C_{15}H_{21}FO_2$ mol. wt. 252.33

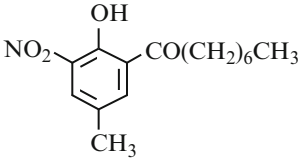


Synthesis
-Refer to: [1322].

Methyl ether (+) [127928-56-7]
$C_{16}H_{23}FO_2$ mol. wt. 266.36
-Refer to: [1322].

1-(2-Hydroxy-5-methyl-3-nitrophenyl)-1-octanone

[74604-14-1] $C_{15}H_{21}NO_4$ mol. wt. 279.33



Synthesis
-Obtained by treatment of 1-(2-hydroxy-5-methylphenyl)-1-octanone with concentrated nitric acid in acetic acid at 65° [2520].
m.p. 68° [2520]; IR [2520], UV [2520].

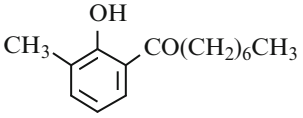
Oxime [74604-07-2] $C_{15}H_{22}N_2O_4$ mol. wt. 294.35

m.p. 105° [2520]; IR [2520], UV [2520].

USE: Solvent extraction of copper (II) [2520].

1-(2-Hydroxy-3-methylphenyl)-1-octanone

[108667-53-4] $C_{15}H_{22}O_2$ mol. wt. 234.34

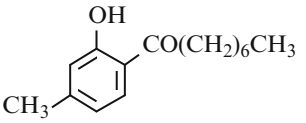


Synthesis
-Obtained by Fries rearrangement of o-cresyl caprylate with aluminium chloride at 160–180° for 30 min (44 %) [1644].

$b.p._{13}$ 176–182° [1644].

1-(2-Hydroxy-4-methylphenyl)-1-octanone

[108666-97-3] $C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis
-Obtained by Fries rearrangement of m-cresyl caprylate with aluminium chloride at 140–150° [906] or at 120–148° for 30 min (76 %) [1644].

b.p.$_1$ 129–131° [906], b.p.$_9$ 173–175° [1644].

Phenylhydrazone [112744-63-5] $C_{21}H_{28}N_2O$ mol. wt. 324.47

m.p. 64–66° [1644].

Oxime [84498-20-4] $C_{15}H_{23}NO_2$ mol. wt. 249.35

-Extn. by, of copper from aq. soln. [1143].
-Prepn. of, for extn. of metals [1142].

Oxime (*E*) [113962-76-8] $C_{15}H_{23}NO_2$ mol. wt. 249.35

-Extn. by, of cupric cation [230].

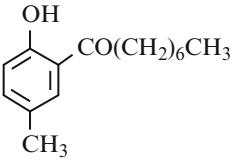
Oxime, **nickel complex** [108111-23-5]

-Refer to: [2284].

USE: Photog. magenta dye image stabilizer [2284].

1-(2-Hydroxy-5-methylphenyl)-1-octanone

[36946-07-3] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Obtained by Fries rearrangement of p-cresyl caprylate with aluminium chloride,
*at 120° for 10 min (70 %) [1644];
*in tetrachloroethane at 120° [2520];
*without solvent at 130–150° [2520].
-Also obtained by reaction of octanoyl chloride with p-cresol in the presence of aluminium chloride in ethylene chloride at 110–120° for 8 h (58 %) [1769].

-Also refer to: [1763, 2647].
N.B.: Changes of volatiles in soy sauce-stewed pork during cold storage and reheating [1895].

m.p. 36° [1644, 2647], 35.5° [2520], 34–34.5° [1769];
IR [2520], UV [2520].

USE: Detn. of, by potentiometric titration in methylpyrrolidinone [1763].

Oxime [51528-14-4] $C_{15}H_{23}NO_2$ mol. wt. 249.35

-Refer to: [2520, 3445].

m.p. 88.5–89.5° [888], 86° [2520]; IR [2520], UV [2520].

USE: Extraction of copper, kinetics and mechanism of, [2521, 3198, 3199]; Solvent extraction of copper (II) [1769, 2520].

Oxime (*E*) [103582-39-4] $C_{15}H_{23}NO_2$ mol. wt. 249.35

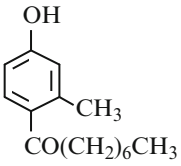
85–86° [1769];
^{1}H NMR [1769], ^{13}C NMR [1769], IR [1769],
UV [1769], MS [1921].

2,4-Dinitrophenylhydrazone [127699-72-3] $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 146–147° [1769].

1-(4-Hydroxy-2-methylphenyl)-1-octanone

$C_{15}H_{22}O_2$ mol. wt. 234.34



Synthesis
-Refer to: [2503].

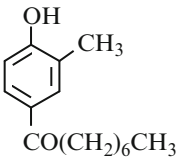
Phenyl ether [791615-79-7]
$C_{21}H_{26}O_2$ mol. wt. 310.44

-Obtained by adding a mixture of m-phenoxytoluene and octanoyl chloride to a suspension of aluminium chloride in methylene chloride at 0°, then the mixture stirred for 1.5–2 h at 3–5° (59 %) [2503].

b.p.$_3$ 228–229° [2503]; ^{1}H NMR [2503], IR [2503], MS [2503].

1-(4-Hydroxy-3-methylphenyl)-1-octanone

[95102-41-3] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Obtained by Fries rearrangement of o-cresyl caprylate with aluminium chloride at 160–180° for 30 min (15 %) [1644].
-Also refer to: [1595, 2704].
m.p. 91° [2704], 70–73° [1644].

USE: As colour developer [2704]; Colour developer, for thermal recording materials [1595].

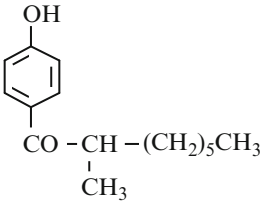
Methyl ether [810661-48-4] $C_{16}H_{24}O_2$ mol. wt. 248.37

-Preparation by direct acylation of 2-methylanisole with octanoic acid in the presence of 6 mol% of $AlPW_{12}O_{40}$ (aluminium dodecatungstophosphate) as catalyst,
*at 120° for 4 h (85 %) [1009];
*in the presence of trifluoroacetic anhydride (TFAA) for 0.34 h (93 %) [1009].

colourless viscous oil [1009]; b.p.$_{32}$ 218° [1009];
^{1}H NMR [1009], ^{13}C NMR [1009], IR [1009], MS [1009];
TLC [1009]; GC [1009].

1-(4-Hydroxyphenyl)-2-methyl-1-octanone

[120837-00-5] (*S*) $C_{15}H_{22}O_2$ mol. wt. 234.34
[131033-26-6] (+)



Syntheses
-Refer to: [1062, 1319 (S), 1321 (+), 1324 (+), 1416, 1418, 1419, 1716, 1719–1721, 3025].
^{1}H NMR [1062], IR [1062], MS [1062].

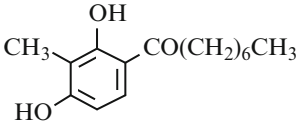
USE: In preparation of polymeric ferroelectric liquid crystals [3025]; Liquid crystal siloxanes and liquid crystal compn. [1419].

Methyl ether (+) [120837-13-0] $C_{16}H_{24}O_2$ mol. wt. 248.37

-Refer to: [1320–1322, 1324].

1-(2,4-Dihydroxy-3-methylphenyl)-1-octanone

[95149-08-9] $C_{15}H_{22}O_3$ mol. wt. 250.34

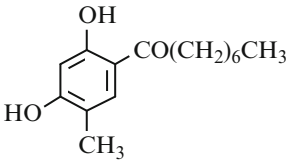


Syntheses
-Refer to: [1515, 1595, 2704].
m.p. 81° [2704], 75.8–77° [1515];
^{1}H NMR [1515], ^{13}C NMR [1515], MS [1515].

USE: As colour developer [2704]; Colour developer, for thermal recording materials [1595].

1-(2,4-Dihydroxy-5-methylphenyl)-1-octanone

[95185-58-3] $C_{15}H_{22}O_3$ mol. wt. 250.34

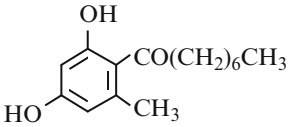


Synthesis
-Refer to: [2704] (Japanese patent).
m.p. 93.5° [2704].

USE: As colour developer [2704].

1-(2,4-Dihydroxy-6-methylphenyl)-1-octanone

[30414-65-5] $C_{15}H_{22}O_3$ mol. wt. 250.34



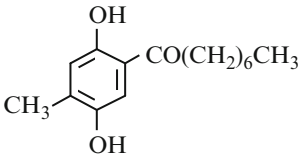
Synthesis
-Obtained by reaction of octanoyl chloride with orcinol in the presence of aluminium chloride in nitrobenzene at 0°, followed by hydrolysis next day (26.5 %) [2184].

This compound being heated at 106° (bath)/6 x 10^{-5} Torr gave a waxy sublimate [2184].

plates [2184]; m.p. 90–91° [2184];
^{1}H NMR [2184], IR [2184], UV [2184].

1-(2,5-Dihydroxy-4-methylphenyl)-1-octanone

[21182-61-6] $C_{15}H_{22}O_3$ mol. wt. 250.34

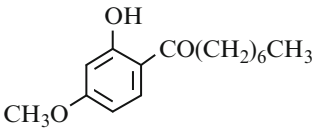


Synthesis
-Obtained by treatment of 2-hydroxy-5-methoxy-4-methyl-octanophenone with aluminium chloride in boiling carbon disulfide for 34 h (63 %) [2370].

yellow plates [2370]; m.p. 103–104° [2370]; IR [2370].

1-(2-Hydroxy-4-methoxyphenyl)-1-octanone

[143286-91-3] $C_{15}H_{22}O_3$ mol. wt. 250.34



Syntheses
-Obtained by reaction of methyl bromide with 1-(2,4-dihydroxyphenyl)-1-octanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

-Also refer to: [1787].

m.p. 30–34° [284].

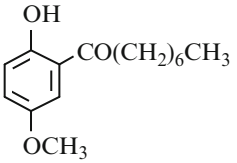
Oxime [143286-60-6] $C_{15}H_{23}NO_3$ mol. wt. 265.35

-Obtained by reaction of hydroxylamine hydrochloride with 1-(2-hydroxy-4-methoxyphenyl)-1-octanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 49–53° [284].

1-(2-Hydroxy-5-methoxyphenyl)-1-octanone

[21182-57-0] $C_{15}H_{22}O_3$ mol. wt. 250.34



Syntheses

-Obtained by reaction of caprylic acid with p-methoxyphenol in the presence of boron trifluoride in tetrachloroethane for 4 h. The reaction mixture was allowed to stand overnight at r.t. and was then heated on a steam bath for about 3 h (55 %) [142].

-Also obtained by Fries rearrangement of 4-methoxyphenyl caprylate (b.p.$_1$ 137–140°) with boron trifluoride in *sym*-tetrachloroethane for 6 h, following 5 h of heating on a steam bath (33 %) [142].
-Also obtained by action of octanoyl chloride with quinol dimethyl ether in the presence of aluminium chloride in carbon disulfide for 2 h, then at r.t. for 1 h and refluxed 10 h on the steam bath (83 %) [770], (58 %) [2370].
-Also refer to: [1907, 2541].

yellow plates [2370]; b.p.$_{2–4}$ 188–189° [2541];
m.p. 45° [770, 2541], 44–45° [2370], 42.5–44° [142, 1907];
IR [2370].

Oxime [140943-14-2] $C_{15}H_{23}NO_3$ mol. wt. 265.35

-Refer to: [285].

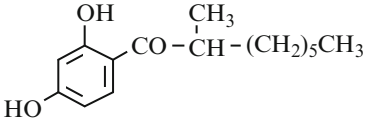
BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_6$ mol. wt. 430.46

m.p. 134° [770].

1-(2,4-Dihydroxyphenyl)-2-methyl-1-octanone

[134925-05-6] $C_{15}H_{22}O_3$ mol. wt. 250.34



Synthesis

-Refer to: [3025].

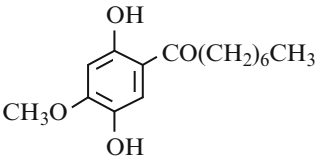
Isomer (S) $C_{15}H_{22}O_3$ mol. wt. 250.34

-Obtained by reaction of (S)-(+)-2-methyloctanoic acid with resorcinol in the presence of zinc chloride at 150° for 30 min (46.2 %) [1715].
-Refer to: [1715, 1716, 1719–1721].

orange viscous liquid [1715];
$(\alpha)_D^{20} = 15.2°$ (chloroform) [1715]; ^{1}H NMR [1715], IR [1715].

1-(2,5-Dihydroxy-4-methoxyphenyl)-1-octanone

[133831-11-5] $C_{15}H_{22}O_4$ mol. wt. 266.34

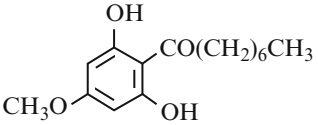


Synthesis
-Refer to: [3276].

USE: Gradation and background whiteness-improved colour photographic material [3276].

1-(2,6-Dihydroxy-4-methoxyphenyl)-1-octanone

[861889-77-2] $C_{15}H_{22}O_4$ mol. wt. 266.34

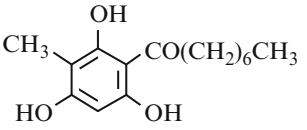


Synthesis
-Preparation by reaction of octanoyl chloride with phloroglucinol monomethyl ether in the presence of aluminium chloride in methylene chloride at r.t. [1129].

BIOLOGICAL ACTIVITY: DIF-1 derivs. for treating diabetes and obesity [1773]; Structural requirements of Dictyostelium differentiation-inducing factors for their stalk-cell-inducing activity in Dictyostelium cells and antiproliferative activity in K562 human leukemic cells [1129].

1-[2,4,6-Trihydroxy-3-methylphenyl]-1-octanone

[74478-10-7] $C_{15}H_{22}O_4$ mol. wt. 266.34



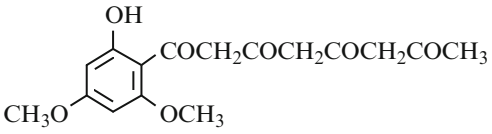
Syntheses
-Obtained by reaction of caprylic nitrile with 3-methyl-phloroglucinol (Hoesch reaction) [1608].
-Also refer to: [2111].

m.p. 135° [1608].

BIOLOGICAL ACTIVITY: Fungicidal [2111].

1-(2,4-Dimethoxy-6-hydroxyphenyl)-1,3,5,7-octanetetraone

[76631-04-4] $C_{16}H_{18}O_7$ mol. wt. 322.31

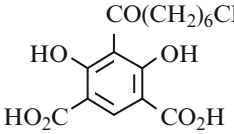


Synthesis
-Preparation by acylation of trianion of 2,4,6-heptanetrione with methyl 2,4-dimethoxy-6-hydroxybenzoate (48 %) [2699].

orange-yellow crystals [2699]; m.p. 59–64° [2699];
^{1}H NMR [2699], MS [2699].

[4,6-Dihydroxy-5-(1-oxooctyl)phenyl]-1,3-dicarboxylic acid

$C_{16}H_{20}O_7$ mol. wt. 324.33



Synthesis
-Refer to: [862].

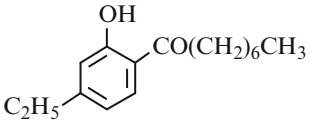
Dimethyl ester [13937-26-3]
$C_{18}H_{24}O_7$ mol. wt. 352.38

-Preparation by treating resorcinol-4,6-dicarboxylic acid dimethyl ester with caprylyl chloride in the presence of aluminium chloride (75 %) [862].

m.p. 63–65° [862].

1-(4-Ethyl-2-hydroxyphenyl)-1-octanone

$C_{16}H_{24}O_2$ mol. wt. 248.37



Syntheses
-Obtained by Fries rearrangement of 3-ethylphenyl n-caprylate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (84 %) [2801];
*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (84 %) [2801].

b.p.$_{28}$ 200° [2801].

Methyl ether $C_{17}H_{26}O_2$ mol. wt. 262.39

-Obtained by reaction of dimethyl sulfate with 1-(4-ethyl-2-hydroxyphenyl)-1-octanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (79 %) [2801].

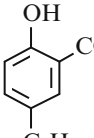
b.p.$_{35}$ 182° [2801].

2,4-Dinitrophenylhydrazone $C_{22}H_{28}N_4O_5$ mol. wt. 428.49

m.p. 136° [2801].

1-(5-Ethyl-2-hydroxyphenyl)-1-octanone

$C_{16}H_{24}O_2$ mol. wt. 248.37



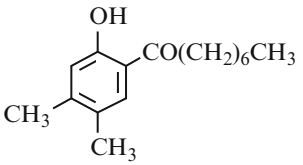
Synthesis
-Obtained by Fries rearrangement of 4-ethylphenyl caprylate with aluminium chloride at 100° for 2 h (80 %) [2800].
$b.p._{11}$ 184° [2800].

2,4-Dinitrophenylhydrazone $C_{22}H_{28}N_4O_5$ mol. wt. 428.49

m.p. 122° [2800].

1-(2-Hydroxy-4,5-dimethylphenyl)-1-octanone

[778637-79-9] $C_{16}H_{24}O_2$ mol. wt. 248.37



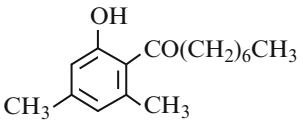
Synthesis
-Obtained by Fries rearrangement of 3,4-dimethylphenyl caprylate with aluminium chloride at 110° without solvent (75 %) [3117].
$b.p._8$ 236° [3117].

2,4-Dinitrophenylhydrazone $C_{22}H_{28}N_4O_5$ mol. wt. 428.49

m.p. 169° [3117].

1-(2-Hydroxy-4,6-dimethylphenyl)-1-octanone

[101271-65-2] $C_{16}H_{24}O_2$ mol. wt. 248.37



Syntheses
-Obtained by Fries rearrangement of 3,5-dimethylphenyl caprylate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (82 %) [2801];
*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (80 %) [2801].
-Also obtained by reaction of caprylic acid with 3,5-xylenol in the presence of boron trifluoride at 70° for 2 h (91 %) [1685].

$b.p._3$ 180° [2801], $b.p._{15}$ 199–199.5° [1685]; m.p. 22° [1685].

2,4-Dinitrophenylhydrazone $C_{22}H_{28}N_4O_5$ mol. wt. 428.49

m.p. 180° [2801].

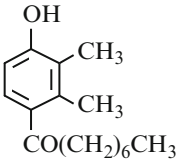
Methyl ether $C_{17}H_{26}O_2$ mol. wt. 262.39

-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxy-4,6-dimethylphenyl)-1-octanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (73 %) [2801].

$b.p._{.40}$ 200° [2801].

1-(4-Hydroxy-2,3-dimethylphenyl)-1-octanone

[95102-20-8] $C_{16}H_{24}O_2$ mol. wt. 248.37

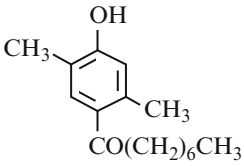


Syntheses
-Refer to: [1595, 2704].
m.p. 80° [2704].

USE: As colour developer [2704]; In preparation of thermographic recording material [1595].

1-(4-Hydroxy-2,5-dimethylphenyl)-1-octanone

[95185-67-4] $C_{16}H_{24}O_2$ mol. wt. 248.37

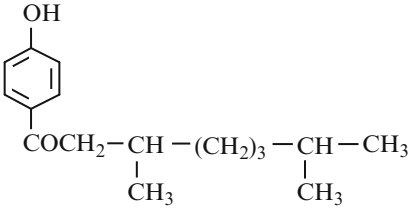


Synthesis
-Refer to: [2704] (Japanese patent).
m.p. 100° [2704].

USE: As colour developer [2704].

1-(4-Hydroxyphenyl)-3,7-dimethyl-1-octanone

[14392-73-5] $C_{16}H_{24}O_2$ mol. wt. 248.37



Syntheses
-Obtained by Fries rearrangement of phenyl 3,7-dimethyloctanoate with aluminium chloride in nitrobenzene at 38° for 2 days (48 %) [414, 415].
m.p. 80° [415], 79–80° [414].

N-Diethylaminoethyl ether [14392-80-4] $C_{22}H_{37}NO_2$ mol. wt. 347.54

-A solution of 1-(4-hydroxyphenyl)-3,7-dimethyl-1-octanone in ethanol was added to a solution of sodium in ethanol; the mixture was refluxed 1 h, cooled, and a solution of $ClCH_2CH_2N(C_2H_5)_2$ added (80 %) [414, 415].

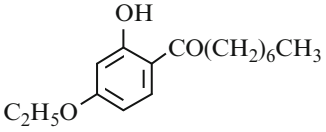
b.p.$_{0.005}$ 156–166° [414, 415]; $n_D^{21} = 1.5058$ [414, 415].

Fumarate of the N-diethylaminoethyl ether $C_{22}H_{37}NO_2$, $C_4H_4O_4$ mol. wt. 463.61

m.p. 76–78° [414, 415].

1-(4-Ethoxy-2-hydroxyphenyl)-1-octanone

[22198-47-6] $C_{16}H_{24}O_3$ mol. wt. 264.36



Syntheses

-Obtained by reaction of octanoyl chloride with m-diethoxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°.

The temperature was then raised to 80° and stirring was continued at that temperature for 5 h (64.5 %) [1194].

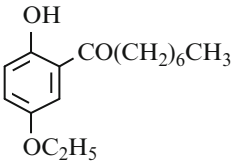
-Also refer to: [3469].

m.p. 54.5° [1194, 3469]; UV [1194, 3469].

USE: UV absorber [1194]; Light-stabilizer of polymeric materials [1194].

1-(5-Ethoxy-2-hydroxyphenyl)-1-octanone

[140943-33-5] $C_{16}H_{24}O_3$ mol. wt. 264.36



Synthesis

-Refer to: [285].

Oxime [140943-20-0]

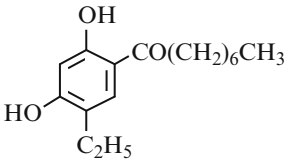
$C_{16}H_{25}NO_3$ mol. wt. 279.38

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-(5-Ethyl-2,4-dihydroxyphenyl)-1-octanone

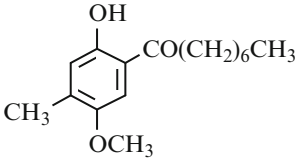
[95185-59-4] $C_{16}H_{24}O_3$ mol. wt. 264.36



Synthesis
-Refer to: [2704].

1-(2-Hydroxy-5-methoxy-4-methylphenyl)-1-octanone

[21182-60-5] $C_{16}H_{24}O_3$ mol. wt. 264.36

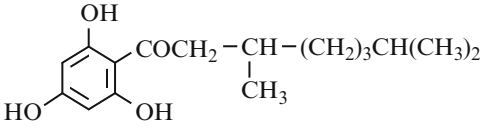


Synthesis
-Obtained by action of octanoyl chloride with 2,5-dimethoxytoluene in the presence of aluminium chloride in refluxing carbon disulfide for 10 h on the steam bath (94 %) [2370].

pale yellow needles [2370]; m.p. 57–59° [2370]; IR [2370].

3,7-Dimethyl-1-(2,4,6-trihydroxyphenyl)-1-octanone

[198878-73-8] $C_{16}H_{24}O_4$ mol. wt. 280.36



Syntheses
-Obtained by reaction of 3,7-dimethyl-octanoyl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene for 24 h at r.t. [3166].

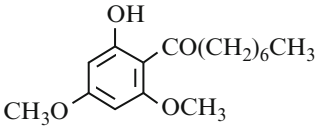
-Also refer to: [2683, 2685].

pale yellow oil [3166]; ^{1}H NMR [2683], MS [2683]; TLC [3166].

BIOLOGICAL ACTIVITY: As preventive and therapeutic agent for bone and cartilage diseases [2685].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-octanone

[1142936-18-2] $C_{16}H_{24}O_4$ mol. wt. 280.36

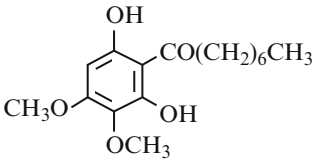


Synthesis
-Obtained by reaction of dimethyl sulfate with 1-(2,4,6-trihydroxyphenyl)-1-octanone in the presence of potassium carbonate in acetone at 50–60° for 1.5 h under nitrogen (34 %) [2786].

m.p. 73–74° [2786];
^{1}H NMR [2786], ^{13}C NMR [2786], MS [2786].

1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-octanone

[134081-95-1] $C_{16}H_{24}O_5$ mol. wt. 296.36

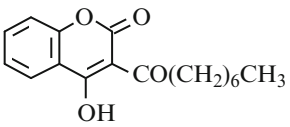


Synthesis
-Preparation by treatment of 1-[6-hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy) phenyl]-1-octanone with potassium carbonate in refluxing methanol for 1–3 h (82 %) [1353].

m.p. 93–94.5° [1353]; ^{1}H NMR [1353].

4-Hydroxy-3-(1-oxooctyl)-2*H*-1-benzopyran-2-one

[36953-90-9] $C_{17}H_{20}O_4$ mol. wt. 288.34



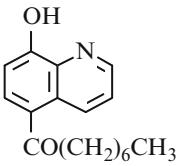
Syntheses
-Obtained by reaction of octanoyl chloride with 4-hydroxy-coumarin in pyridine containing one drop of piperidine for 12 h on a water bath (68 %) [3174].

-Also refer to: [3144].

m.p. 104–105° [3174].

1-(8-Hydroxy-5-quinolinyl)-1-octanone

[110593-82-3] $C_{17}H_{21}NO_2$ mol. wt. 271.36



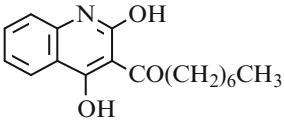
Synthesis
-Obtained by reaction of octanoyl chloride with 8-hydroxy-quinoline in the presence of aluminium chloride in nitrobenzene at 80–85° for 15–16 h (39 %) [1725].

m.p. 63.5–64.2° [1725]; ^{1}H NMR [1725], IR [1725].

USE: Ion flotation with, of gallium [1725].

1-(2,4-Dihydroxy-3-quinolinyl)-1-octanone

[107276-31-3] $C_{17}H_{21}NO_3$ mol. wt. 287.36



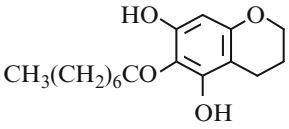
Synthesis
-Obtained by reaction of octanoyl chloride with 2,4-dihydroxyquinoline in the presence of aluminium chloride in nitrobenzene on the steam bath for 3 h (17 %) [3123].

m.p. 168–169° [3123]; UV [3123].

BIOLOGICAL ACTIVITY: Antibacterial properties (Staphylococcus aureus and Escherichia coli) [3123].

1-(3,4-Dihydro-5,7-dihydroxy-2*H*-1-benzopyran-6-yl)-1-octanone

[85602-40-0] $C_{17}H_{24}O_4$ mol. wt. 292.37

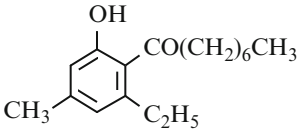


Synthesis
-Refer to: [1026].

BIOLOGICAL ACTIVITY: Bactericidal and fungicidal [1026].

1-(2-Ethyl-6-hydroxy-4-methylphenyl)-1-octanone

$C_{17}H_{26}O_2$ mol. wt. 262.39



Syntheses
-Preparation by Fries rearrangement of 3-ethyl-5-methyl-phenyl caprylate with aluminium chloride,
*without solvent at 130° for 2 h (77 %) [2802];
*in nitrobenzene at 25° for 6 h (79 %) [2802].

b.p.$_6$ 220° [2802].

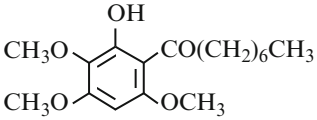
Methyl ether $C_{18}H_{28}O_2$ mol. wt. 276.42

-Obtained by methylation of the above ketone in the usual way (76 %) [2802].

b.p.$_{30}$ 205° [2802].

1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-octanone

[134081-64-4] $C_{17}H_{26}O_5$ mol. wt. 310.39



Syntheses
-Obtained by partial selective demethylation of crude 2,3,4,6-tetramethoxyoctanophenone with aluminium chloride in acetonitrile at 50° for 1–2 h (82 %) [1353].
-Also refer to: [1351].

m.p. 49–50° [1353]; ^{1}H NMR [1353].

p-Toluenesulfonic ester [134081-79-1] $C_{24}H_{32}O_7S$ mol. wt. 464.58

-Obtained by reaction of p-toluenesulfonyl chloride with 2-hydroxy-3,4,6-trimethoxy-octanophenone in the presence of potassium carbonate in refluxing acetone for 6 to 14 h (93 %) [1353].

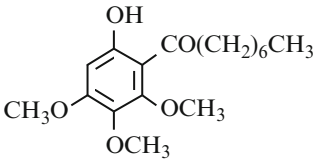
m.p. 83–85° [1353]; ^{1}H NMR [1353].

Methyl ether $C_{18}H_{28}O_5$ mol. wt. 324.42

-Obtained by reaction of octanoyl chloride with 1,2,3,5-tetramethoxybenzene in the presence of aluminium chloride in ethyl ether at 0° for 30 min [1353].

1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-octanone

[134081-71-3] $C_{17}H_{26}O_5$ mol. wt. 310.39



Syntheses

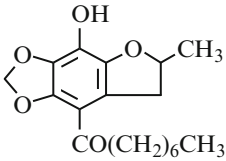
-Obtained by hydrogenation of (6-phenylmethoxy)-2,3,4-trimethoxyoctanophenone over 10 % palladium on charcoal in ethyl acetate/methanol (1:1) until the uptake of hydrogen ceased (88 %) [1353].

-Also refer to: [1351].

m.p. 40–42° [1353]; ^{1}H NMR [1353].

1-(6,7-Dihydro-4-hydroxy-6-methylfuro[2,3-f]-1,3-benzodioxol-8-yl)-1-octanone

$C_{18}H_{24}O_5$ mol. wt. 320.39



Synthesis

-Refer to: [2179].

Methyl ether Octanoyl furapiole

[82652-36-6]

$C_{19}H_{26}O_5$ mol. wt. 334.41

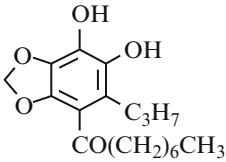
-Obtained by reaction of octanoyl chloride with furapiole in the presence of fused zinc chloride in methylene chloride for 3–4 h in an ice bath (70 %) [2179].

colourless plates; m.p. 55° [2179]; ^{1}H NMR [2179], IR [2179].

USE: Synergistic insecticidal activity of, with pyrethrum [2179].

1-(6,7-Dihydroxy-5-propyl-1,3-benzodioxol-4-yl)-1-octanone

$C_{18}H_{26}O_5$ mol. wt. 322.40



Synthesis

-Refer to: [2179].

Dimethyl ether octanoyl dihydrodillapiole

[82652-28-6]

$C_{20}H_{30}O_5$ mol. wt. 350.46

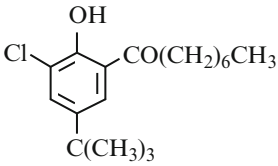
-Obtained by reaction of octanoyl chloride with dihydrodillapiole in the presence of fused zinc chloride in methylene chloride for 3–4 h in an ice bath (70 %) [2179].

colourless solid [2179]; ^{1}H NMR [2179], IR [2179].

USE: Synergistic insecticidal activity of, with pyrethrum [2179].

1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-octanone

[108300-00-1] $C_{18}H_{27}ClO_2$ mol. wt. 310.86



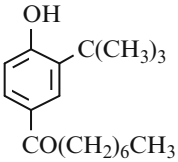
Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-tert-butyl-phenyl caprylate with aluminium chloride at 110° (72 %) [3119].
b.p.$_{10}$ 170° [3119].

2,4-Dinitrophenylhydrazone [102955-19-1] $C_{24}H_{31}ClN_4O_5$ mol. wt. 490.99

m.p. 127° [3119].

1-[3-(1,1-Dimethylethyl)-4-hydroxyphenyl]-1-octanone

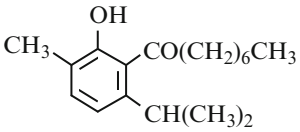
[95102-32-2] $C_{18}H_{28}O_2$ mol. wt. 276.42



Synthesis
-Refer to: [2704].

1-[2-Hydroxy-3-methyl-6-(1-methylethyl)phenyl]-1-octanone

$C_{18}H_{28}O_2$ mol. wt. 276.42



Synthesis
-Obtained by Fries rearrangement of carvacryl caprylate with aluminium chloride at 120° (60 %) [2798].

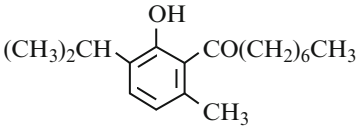
b.p.$_{10}$ 255° [2798].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 127° [2798].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-octanone

[778641-04-6] $C_{18}H_{28}O_2$ mol. wt. 276.42



Synthesis
-Obtained by Fries rearrangement of thymyl caprylate with aluminium chloride at 120° (81 %) [2803].

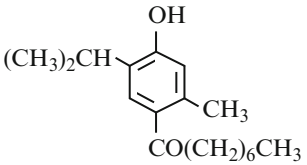
b.p.$_2$ 185° [2803].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 185° [2803].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-octanone

[95102-21-9] $C_{18}H_{28}O_2$ mol. wt. 276.42



Syntheses

-Obtained (**XXVIII**) by treatment of 4-methoxy-2-methyl-5-isopropyloctanophenone (**IX**) with boiling pyridinium chloride (205–215°) for 4.5 h (18 %) [2660].

-Also obtained by Fries rearrangement of thymyl caprylate with aluminium chloride in nitrobenzene for 16 h at 25° (84 %) [2647].

-Also refer to: [2704].

b.p.$_9$ 217–220° [2647], b.p.$_{14}$ 235° [2660];
m.p. 81–82° [2647], 80° [2660].

USE: Colour developer, for thermal recording materials [1595].

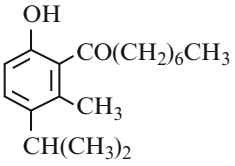
Methyl ether (**IX**) $C_{19}H_{30}O_2$ mol. wt. 290.45

-Obtained by reaction of caprylyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (61 %) [2660].

b.p.$_{13}$ 210° [2660]; $n_D^{23} = 1.5120$ [2660].

1-[6-Hydroxy-2-methyl-3-(1-methylethyl)phenyl]-1-octanone

$C_{18}H_{28}O_2$ mol. wt. 276.42



Synthesis

-Refer to: [2664].

Methyl ether [102020-37-1]

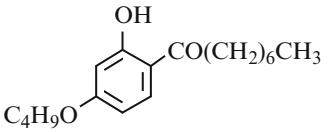
$C_{19}H_{30}O_2$ mol. wt. 290.45

-Obtained by reaction of octanoyl chloride with p-thymol in the presence of aluminium chloride in carbon disulfide for 24 h at r.t. (79 %) [2664].

pale yellow oil [2664]; b.p.$_{19}$ 212° [2664];
IR [2664]; $n_D^{24} = 1.5160$ [2664].

1-(4-Butoxy-2-hydroxyphenyl)-1-octanone

[24294-76-6] $C_{18}H_{28}O_3$ mol. wt. 292.42



Syntheses

-Obtained by reaction of octanoyl chloride with m-dibutoxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°.

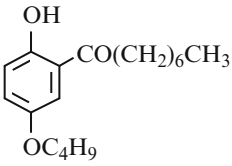
The temperature was then raised to 80° and stirring was continued at that temperature for 5 h (77 %) [1194, 1195].

m.p. 33.5–34° [1194, 1195]; UV [1194, 1195].

USE: UV absorber [1194]; Light-stabilizer of polymeric materials [1194].

1-(5-Butoxy-2-hydroxyphenyl)-1-octanone

[140943-38-0] $C_{18}H_{28}O_3$ mol. wt. 292.42



Synthesis

-Refer to: [285].

Oxime [140943-24-4]

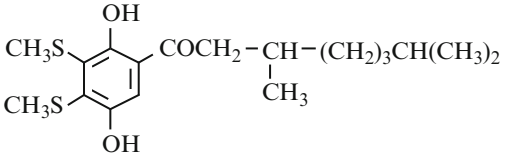
$C_{18}H_{29}NO_3$ mol. wt. 307.43

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-[2,5-Dihydroxy-3,4-bis(methylthio)phenyl]-3,7-dimethyl-1-octanone

$C_{18}H_{28}O_3S_2$ mol. wt. 356.55



Synthesis

-Refer to: [2352].

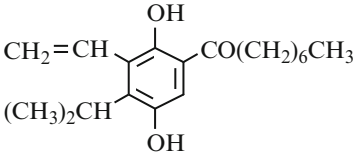
Dimethyl ether [357172-17-9]

$C_{20}H_{32}O_3S_2$ mol. wt. 384.60

-Refer to: [2352].

1-[2,5-Dihydroxy-3-(1-ethenyl)-4-(1-methylethyl)phenyl]-1-octanone

$C_{19}H_{28}O_3$ mol. wt. 304.43



Isolation from natural sources

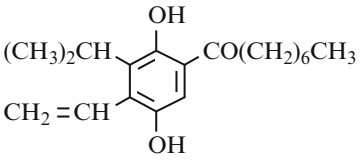
-From *Aspergillus echinulatus* Delacroix, Thom and Church [2539, 2541, 2542].

yellow crystals [2541];

m.p. 109–110° [2541].

1-[2,5-Dihydroxy-4-(1-ethenyl)-3-(1-methylethyl)phenyl]-1-octanone

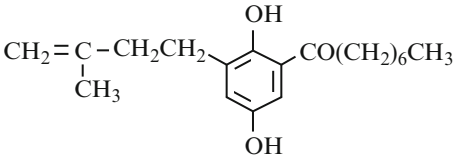
$C_{19}H_{28}O_3$ mol. wt. 304.43



Isolation from natural sources
-From *Aspergillus echinulatus* Delacroix, Thom and Church [2539, 2541, 2542].
yellow crystals [2541];
m.p. 109–110° [2541].

1-[2,5-Dihydroxy-3-(3-methyl-3-butenyl)phenyl]-1-octanone

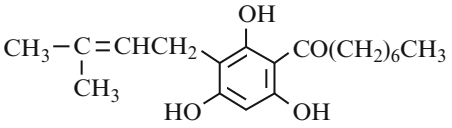
$C_{19}H_{28}O_3$ mol. wt. 304.43



Isolation from natural sources
-From *Aspergillus echinulatus* Delacroix, Thom and Church [2539, 2541, 2542].
yellow crystals [2541];
m.p. 109–110° [2541].

1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-octanone
2-octanoyl-4-(3-methylbuten-2-yl)phloroglucinol (**11**) [1026].

[85602-21-7] $C_{19}H_{28}O_4$ mol. wt. 320.43



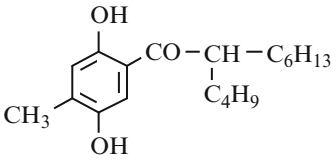
Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and prenyl bromide to a solution of phloro-octanophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].
-Also prepared by adding prenyl bromide to a suspension of the sodium salt of phlorooctanophenone in benzene, then the mixture obtained was refluxed for 3 h [1026].
-Also obtained by reaction of prenyl chloride with phlorooctanophenone in an alkaline two-phase (aqueous ether) system and catalyzed by CuCl [838, 3193].

m.p. 140–142° [3193]; ^{13}C NMR [1026, 3193], IR [1026].

BIOLOGICAL ACTIVITY: Bactericidal and fungicidal [1026, 3193]; Antimicrobial [3193].

2-Butyl-1-(2,5-dihydroxy-4-methylphenyl)-1-octanone

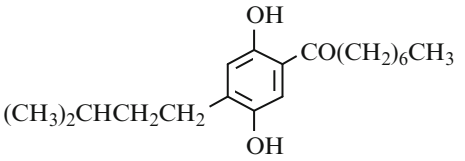
[357172-28-2] $C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Refer to: [2352].

1-[2,5-Dihydroxy-4-(3-methylbutyl)phenyl]-1-octanone

$C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Obtained by treatment of 2-hydroxy-5-methoxy-4-isoamyloctanophenone with aluminium bromide [161, 770].

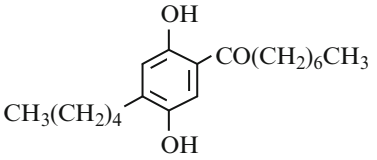
pale yellow solid [770]; m.p. 105–106° [161].

2,4-Dinitrophenylhydrazone $C_{25}H_{34}N_4O_6$ mol. wt. 486.57

m.p. 130–131° [161].

1-(2,5-Dihydroxy-4-pentylphenyl)-1-octanone

$C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Obtained by demethylation of 2-hydroxy-5-methoxy-4-amyloctophenone with aluminium bromide in benzene (almost quantitatively yield) [770].

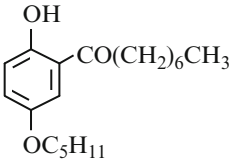
pale yellow needles [770]; m.p. 94° [770].

2,4-Dinitrophenylhydrazone $C_{25}H_{34}N_4O_6$ mol. wt. 486.57

purple needles [770]; m.p. 112° [770].

1-(2-Hydroxy-5-pentyloxyphenyl)-1-octanone

$C_{19}H_{30}O_3$ mol. wt. 306.45

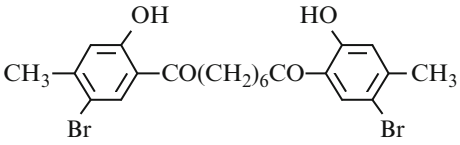


Synthesis
-Refer to: [770].
b.p.$_{1.5}$ 190–195° [770].
2,4-Dinitrophenylhydrazone
$C_{25}H_{34}N_4O_6$ mol. wt. 486.57

m.p. 121° [770].

1,8-Bis(5-bromo-2,4-dihydroxyphenyl)-1,8-octanedione

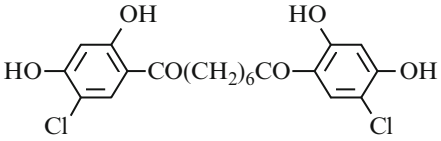
[32246-95-0] $C_{20}H_{20}Br_2O_6$ mol. wt. 516.18



Synthesis
-Obtained by reaction of suberic acid dichloride with 4-bromoresorcinol in the presence of aluminium chloride [589].
m.p. 226° [589].

1,8-Bis(5-chloro-2,4-dihydroxyphenyl)-1,8-octanedione

[26086-81-7] $C_{20}H_{20}Cl_2O_6$ mol. wt. 427.28



Syntheses
-Obtained by reaction of suberic acid dichloride with 4-chlororesorcinol in the presence of aluminium chloride [591].
-Also refer to: [589].

m.p. 227° [589, 591]; IR [589].

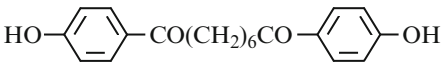
Tetramethyl ether [26086-84-0] $C_{24}H_{28}Cl_2O_6$ mol. wt. 483.39

-Obtained by reaction of suberic acid dichloride with 4-chlororesorcinol dimethyl ether in the presence of aluminium chloride [591].
-Also refer to: [589].

m.p. 186° [589, 591].

1,8-Bis(4-hydroxyphenyl)-1,8-octanedione

[22811-90-1] $C_{20}H_{22}O_4$ mol. wt. 326.39



Syntheses
-Refer to: [584, 1337, 2693].

m.p. 218–219° [1337], 200° [584].

Diacetate [102957-05-1] $C_{24}H_{26}O_6$ mol. wt. 410.47

m.p. 119–120° [1337].

Dimethyl ether [4280-50-6] $C_{22}H_{26}O_4$ mol. wt. 354.45

-Obtained by reaction of suberic acid dichloride with anisole in the presence of aluminium chloride without solvent at <40° (87 %) [905].
-Also refer to: [584, 2693 (70 %)].

m.p. 133° [584], 129–130° [905], 128.8–129.2° [2693].

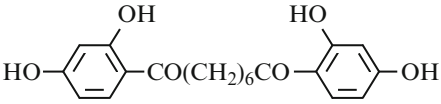
Di-2,4-dinitrophenylhydrazone of the dimethyl ether

[22811-95-6] $C_{34}H_{34}N_8O_{10}$ mol. wt. 714.69

m.p. 223.7–224.7° [2693], 200° [584].

1,8-Bis(2,4-dihydroxyphenyl)-1,8-octanedione

[26086-74-8] $C_{20}H_{22}O_6$ mol. wt. 358.39



Syntheses

-Obtained by reaction of suberic acid dichloride with resorcinol in the presence of aluminium chloride [591].

-Also obtained by reaction of suberic acid with resorcinol in the presence of zinc chloride at 140° for 5 h (55 %) [445].
-Also refer to: [445, 589, 2606].

m.p. 189° [589, 591], 187° [445], 186–187° [2606];
IR [589].

Tetramethyl ether [32246-82-5] $C_{24}H_{30}O_6$ mol. wt. 414.50

-Refer to: [589].

m.p. 140° [589]; IR [589].

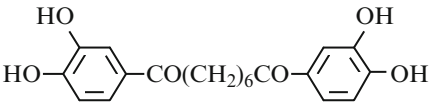
Tetraacetate $C_{28}H_{30}O_{10}$ mol. wt. 526.54

-Obtained by reaction of acetic anhydride with the titled diketone [445].

m.p. 135° [445].

1,8-Bis(3,4-dihydroxyphenyl)-1,8-octanedione

$C_{20}H_{22}O_6$ mol. wt. 358.39



Synthesis

-Refer to: [1014].

Tetramethyl ether [32435-18-0]
$C_{24}H_{30}O_6$ mol. wt. 414.50

-Obtained by reaction of suberic acid dichloride with pyrocatechol dimethyl ether in the presence of aluminium chloride [591].
-Also obtained by hydrogenating of its oxime in acetic acid in the presence of 10 % Pd/C in a Parr apparatus at r.t. and 45–50 psig for 12–36 h (63 %) [1014].
-Also refer to: [589].

m.p. 143° [589, 591], 141–143° [1014];
^{1}H NMR [2342], ^{13}C NMR [2342], IR [589].

Dioxime of the tetramethyl ether [50766-30-8] $C_{24}H_{32}N_2O_6$ mol. wt. 444.53

m.p. 140–143° [1014].

Di-2,4-dinitrophenylhydrazone of the tetramethyl ether

[32246-93-8] $C_{36}H_{38}N_8O_{12}$ mol. wt. 774.74

m.p. 230° [589].

Dimethylenedioxy $C_{22}H_{22}O_6$ mol. wt. 382.41

1,8-Bis(3,4-methylenedioxyphenyl)-1,8-octanedione

-Refer to: [2693 (36 %)].

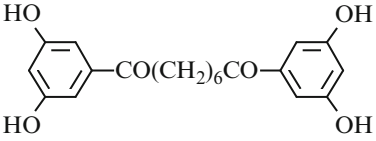
m.p. 180.3–181.3° [2693].

Di-2,4-dinitrophenylhydrazone of the dimethylenedioxy $C_{34}H_{30}N_8O_{12}$ mol. wt. 742.66

m.p. 280.4–281.4° [2693]

1,8-Bis(3,5-dihydroxyphenyl)-1,8-octanedione

$C_{20}H_{22}O_6$ mol. wt. 358.39



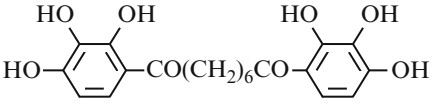
Synthesis

-Refer to: [1316].

m.p. 185–188° [1316].

1,8-Bis(2,3,4-trihydroxyphenyl)-1,8-octanedione

$C_{20}H_{22}O_8$ mol. wt. 390.39



Synthesis

-Refer to: [1575].

Hexamethyl ether [10373-32-7]

$C_{26}H_{34}O_8$ mol. wt. 474.55

-Obtained by reaction of suberic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride [591].

-Also obtained by reaction of dimethyl sulfate with 1,8-bis(2-hydroxy-3,4-dimethoxyphenyl)-1,8-octanedione the presence of 30 % sodium hydroxide (65–90 %) [1574].

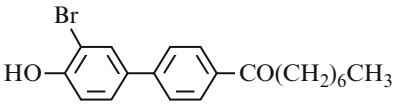
-Also refer to: [1575].

m.p. 160° [591], 101° [1574, 1575].

N.B.: One the reported melting point is obviously wrong.

1-(3′-Bromo-4′-hydroxy[1,1′-biphenyl]-4-yl)-1-octanone

$C_{20}H_{23}BrO_2$ mol. wt. 375.30



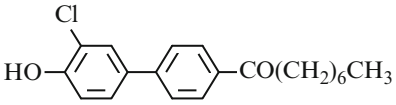
Synthesis
-Refer to: [2873].

Methyl ether [75058-74-1]
$C_{21}H_{25}BrO_2$ mol. wt. 389.33

-Refer to: [2873].

1-(3′-Chloro-4′-hydroxy[1,1′-biphenyl]-4-yl)-1-octanone

$C_{20}H_{23}ClO_2$ mol. wt. 330.85



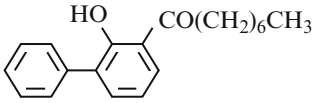
Syntheses
-Refer to: [2115, 2116].

Methyl ether [65687-21-0]
$C_{21}H_{25}ClO_2$ mol. wt. 344.88

-Refer to: [2115, 2116].

1-(2-Hydroxy[1,1′-biphenyl]-3-yl)-1-octanone

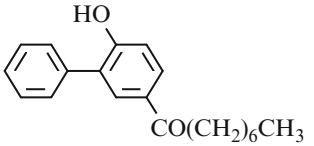
[51621-21-7] $C_{20}H_{24}O_2$ mol. wt. 296.41



Synthesis
-Refer to: [568].
b.p.$_{0.05}$ 167–168° [568].

1-(2-Hydroxy[1,1′-biphenyl]-5-yl)-1-octanone

[95102-22-0] $C_{20}H_{24}O_2$ mol. wt. 296.41

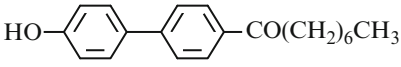


Syntheses
-Refer to: [2006, 2704] (Japanese patents).
m.p. 86° [2704].

USE: As colour developer [2006, 2704].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-octanone

[185555-11-7] $C_{20}H_{24}O_2$ mol. wt. 296.41



Syntheses
-Obtained by Fries rearrangement of 4-octanoyl-oxybiphenyl with aluminium chloride in nitrobenzene, first at 20° for 12 h, then at 60° for 1 h [522].

-Also refer to: [1568, 1923].

colourless silky needles [522]; m.p. 123° [522].

Methyl ether [56116-80-4] $C_{21}H_{26}O_2$ mol. wt. 310.44

-Obtained from octanoyl chloride and 4-methoxybiphenyl [522].
-Also refer to: [1923].

smooth spangles [522]; b.p.$_{15}$ 272–275° [522]; m.p. 120° [522].

Various ethers (10)

-Preparations and liquid crystalline properties of, [847].

Ethyl ether [56116-89-3] $C_{22}H_{28}O_2$ mol. wt. 324.46

Propyl ether [56116-97-3] $C_{23}H_{30}O_2$ mol. wt. 338.49

Butyl ether [56117-05-6] $C_{24}H_{32}O_2$ mol. wt. 352.52

Pentyl ether [56117-14-7] $C_{25}H_{34}O_2$ mol. wt. 366.54

Hexyl ether [56117-23-8] $C_{26}H_{36}O_2$ mol. wt. 380.57

Heptyl ether [56117-32-9] $C_{27}H_{38}O_2$ mol. wt. 394.60

Octyl ether [56117-40-9] $C_{28}H_{40}O_2$ mol. wt. 408.62

-Refer to: [1661].

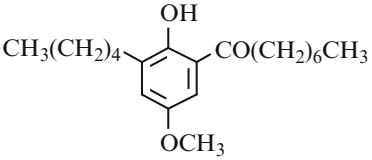
Nonyl ether [56117-49-8] $C_{29}H_{42}O_2$ mol. wt. 422.65

Decyl ether [56117-58-9] $C_{30}H_{44}O_2$ mol. wt. 436.68

Dodecyl ether [56117-67-0] $C_{32}H_{48}O_2$ mol. wt. 464.73

1-(2-Hydroxy-5-methoxy-3-pentylphenyl)-1-octanone

[873416-42-3] $C_{20}H_{32}O_3$ mol. wt. 320.47



Synthesis
-Obtained by Fries rearrangement of 4-methoxy-2-amylphenyloctanoate with aluminium chloride at 180° for 12 h under hydrogen (63 %) [770].

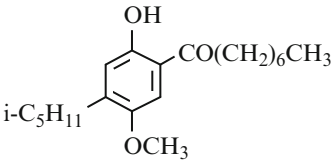
discoloured oil [770]; b.p.$_{0.1}$ 180–190° [770].

2,4-Dinitrophenylhydrazone $C_{26}H_{36}N_4O_6$ mol. wt. 500.60

m.p. 103° [770].

1-[2-Hydroxy-5-methoxy-4-(3-methylbutyl)phenyl]-1-octanone

[717103-49-6] $C_{20}H_{32}O_3$ mol. wt. 320.47



Synthesis
-Obtained by reaction of octanoyl chloride with 2,5-dimethoxyisoamylbenzene in the presence of aluminium chloride [161] in carbon disulfide (70 %) [770].

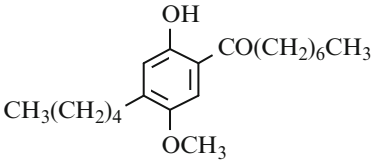
dark oil [770]; b.p.$_{0.4}$ 143–144° [161], b.p.$_{1-2}$ 170–174° [161].

2,4-Dinitrophenylhydrazone $C_{26}H_{36}N_4O_6$ mol. wt. 500.60

leaves [161]; m.p. 146° [770], 140–142° [161].

1-(2-Hydroxy-5-methoxy-4-pentylphenyl)-1-octanone

$C_{20}H_{32}O_3$ mol. wt. 320.47



Synthesis
-Obtained by reaction of octanoyl chloride with 2,5-dimethoxyamylbenzene in the presence of aluminium chloride in carbon disulfide for 2 h at 0°, then 1 h at r.t. and 8 h at reflux (87 %) [770].

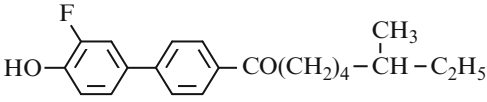
pale yellow needles [770]; m.p. 42° [770].

2,4-Dinitrophenylhydrazone $C_{26}H_{36}N_4O_6$ mol. wt. 500.60

m.p. 117° [770].

1-(3′-Fluoro-4′-hydroxy[1,1′-biphenyl]-4-yl)-6-methyl-1-octanone

$C_{21}H_{25}FO_2$ mol. wt. 328.43



Synthesis
-Refer to: [2107].

Decyl ether (S) [112780-64-0] $C_{31}H_{45}FO_2$ mol. wt. 468.70

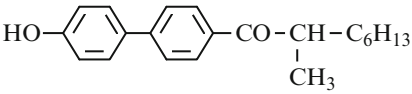
USE: Liq.-crystal compns. contg., for display devices [2107].

Dodecyl ether (S) [112780-65-1] $C_{33}H_{49}FO_2$ mol. wt. 496.75

USE: Liq.-crystal compns. contg., for display devices [2107].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-2-methyl-1-octanone

[120837-09-4] (+) $C_{21}H_{26}O_2$ mol. wt. 310.44
[127928-60-3] (S)



Syntheses
-Refer to: [1321 (+), 1323, 1324, 3278, 3403, 3420].

USE: For liquid crystal compns. for display devices [1323].

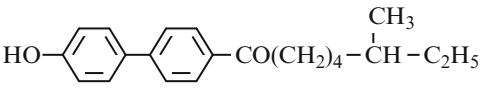
Methyl ether (+) [141681-77-8] $C_{22}H_{28}O_2$ mol. wt. 324.46

-Refer to: [3403].

IR [1457].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-6-methyl-1-octanone

$C_{21}H_{26}O_2$ mol. wt. 310.44



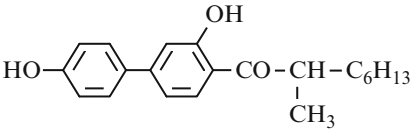
Synthesis
-Refer to: [2205].

Methyl ether [117235-07-1] $C_{22}H_{28}O_2$ mol. wt. 324.46

-Preparation from p-methoxybiphenyl and 6-methyloctanoyl chloride [2205].

1-(3,4′-Dihydroxy[1,1′-biphenyl]-4-yl)-2-methyl-1-octanone

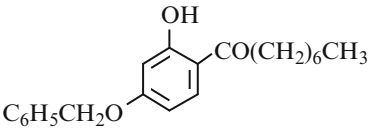
[133407-00-8] (S) $C_{21}H_{26}O_3$ mol. wt. 326.44



Synthesis
-Refer to: [1718].

1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-octanone

[143287-05-2] $C_{21}H_{26}O_3$ mol. wt. 326.44



Synthesis
-Obtained by reaction of benzyl chloride with 2,4-dihydroxycaprylylphenone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 60–64° [284].

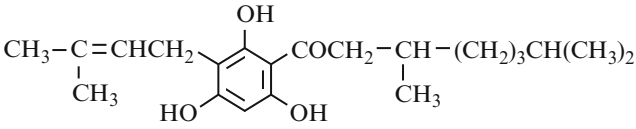
Oxime [143286-82-2] $C_{21}H_{27}NO_3$ mol. wt. 341.45

-Obtained by reaction of hydroxylamine hydrochloride with 1-[2-hydroxy-4-(phenylmethoxy)-phenyl]-1-octanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 62–66° [284]; ^{1}H NMR [284].

3,7-Dimethyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-octanone

[198878-80-7] $C_{21}H_{32}O_4$ mol. wt. 348.48

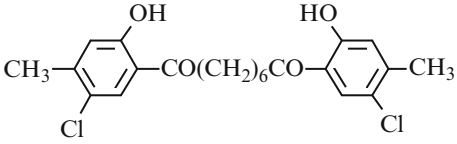


Synthesis
-Refer to: [2685].

BIOLOGICAL ACTIVITY: As preventive and therapeutic agent for bone and cartilage diseases [2685].

1,8-Bis(4-hydroxy-2-methylphenyl)-1,8-octanedione

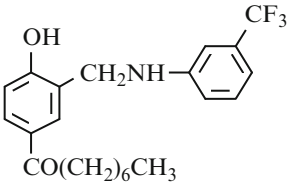
$C_{22}H_{24}Cl_2O_4$ mol. wt. 423.34



Synthesis
-Refer to: [584]
m.p. 115° [584].

1-[4-Hydroxy-3-[[[3-(trifluoromethyl)phenyl]amino]methyl]phenyl]-1-octanone

[107076-65-3] $C_{22}H_{26}F_3NO_2$ mol. wt. 393.45

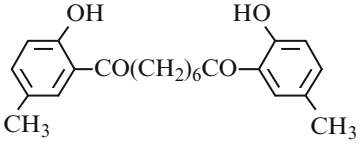


Synthesis
-Refer to: [1823].

USE: Antiplaque dentifrices contg. [1823].

1,8-Bis(2-hydroxy-5-methylphenyl)-1,8-octanedione

[13282-26-3] $C_{22}H_{26}O_4$ mol. wt. 354.45



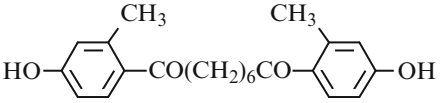
Syntheses
-Obtained by Fries rearrangement of di(4-methylphenyl) suberate with aluminium chloride,
*without solvent at 130° for 4 h (35 %) [3107];
*in refluxing chlorobenzene for 6 h (72 %) [3107].

-Also refer to: [584].

m.p. 136–137° [3107], 110° [584].
N.B.: One of the reported melting point is obviously wrong.
IR [3107].

1,8-Bis(4-hydroxy-2-methylphenyl)-1,8-octanedione

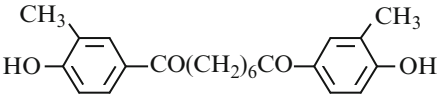
[22812-02-8] $C_{22}H_{26}O_4$ mol. wt. 354.45



Synthesis
-Refer to: [584]
m.p. 110° [584].

1,8-Bis(4-hydroxy-3-methylphenyl)-1,8-octanedione

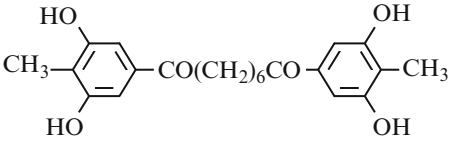
[22811-98-9] $C_{22}H_{26}O_4$ mol. wt. 354.45



Synthesis
-Refer to: [584]
m.p. 190° [584].

1,8-Bis(3,5-dihydroxy-4-methylphenyl)-1,8-octanedione

$C_{22}H_{26}O_6$ mol. wt. 386.45



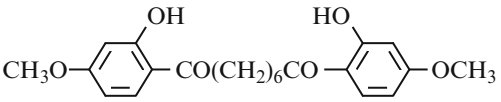
Synthesis
-Refer to: [3132].
Tetramethyl ether [196869-42-8]
$C_{26}H_{34}O_6$ mol. wt. 442.55

-Synthesis from 3,5-dimethoxy-4-methylbenzaldehyde (70 %) [3132].

Colourless solid [3132]; ^{1}H NMR [3132], ^{13}C NMR [3132].

1,8-Bis(2-hydroxy-4-methoxyphenyl)-1,8-octanedione

[26086-77-1] $C_{22}H_{26}O_6$ mol. wt. 386.45



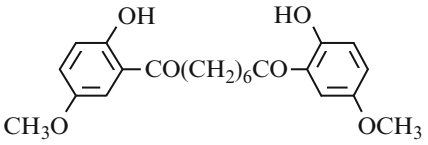
Syntheses
-Obtained by reaction of suberic acid dichloride with 3-methoxyphenol in the presence of aluminium chloride [591].

-Also refer to: [589].

m.p. 155° [589, 591].

1,8-Bis(2-hydroxy-5-methoxyphenyl)-1,8-octanedione

[10491-15-3] $C_{22}H_{26}O_6$ mol. wt. 386.45



Synthesis
-Obtained by reaction of suberic acid dichloride with p-dimethoxybenzene in the presence of aluminium chloride [1575].

m.p. 130° [1575].

Dimethyl ether [10491-14-2] $C_{24}H_{30}O_6$ mol. wt. 414.50

m.p. 116° [1575].

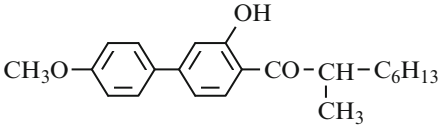
Diacetate [10365-35-2] $C_{26}H_{30}O_8$ mol. wt. 470.52

-Obtained by reaction of acetic anhydride (4 vol) with the title ketone in the presence of 1–2 drops concentrated sulfuric acid, the mixture warmed 5 min [1575].

m.p. 107° [1575].

1-(3-Hydroxy-4′-methoxy[1,1′-biphenyl]-4-yl)-2-methyl-1-octanone

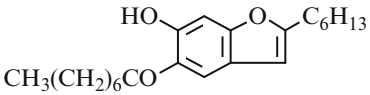
[133406-99-2] (S) $C_{22}H_{28}O_3$ mol. wt. 340.46



Synthesis
-Refer to: [1718].

1-(2-Hexyl-6-hydroxy-5-benzofuranyl)-1-octanone

$C_{22}H_{32}O_3$ mol. wt. 344.49

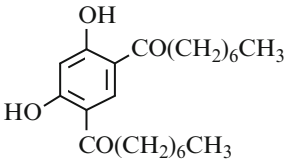


Synthesis
-Obtained by treatment of 2,4-bis(1-octynyl)-1,5-diacetoxybenzene with NaOH (6 equiv.) in THF/MeOH/H_2O at 80° (20 %) [1875].

^{1}H NMR [1875], ^{13}C NMR [1875], IR [1875], MS [1875].

1,1′-(4,6-Dihydroxy-1,3-phenylene)bis-1-octanone

[760989-23-9] $C_{22}H_{34}O_4$ mol. wt. 362.51



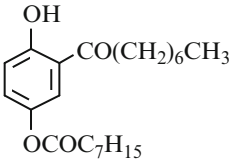
Synthesis

-Obtained by reaction of octanoic acid (2 mol) with resorcinol (1 mol) in the presence of a Lewis acid or a Bronsted acid catalyst [1077].

USE: For preparation of cosmetic active [1077].

1-(2-Hydroxy-5-octanoyloxyphenyl)-1-octanone

[21182-58-1] $C_{22}H_{34}O_4$ mol. wt. 362.51



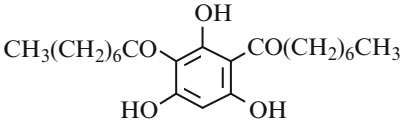
Synthesis

-Obtained by action of octanoyl chloride with quinol dimethyl ether in the presence of aluminium chloride in refluxing carbon disulfide for 10 h (6 %) [2370].

colourless needles [2370]; m.p. 58–59° [2370]; IR [2370].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-octanone

[3118-46-5] $C_{22}H_{34}O_5$ mol. wt. 378.51



Syntheses

-Obtained by reaction of caprylic acid with phloroglucinol in the presence of boron trifluoride etherate [3019], at 100° for 2 h (50–75 %) [338].

-Also obtained by reaction of octanoic anhydride with phloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].

-Also refer to: [457, 644, 2911].

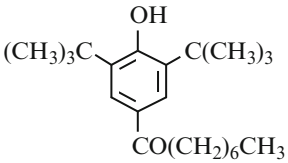
m.p. 93–95° [2911], 93–94° [457];

^{1}H NMR [3019], ^{13}C NMR [3019], IR [3019], UV [3019].

BIOLOGICAL ACTIVITY: As a new class of GPR40 (FFAR1) agonists [338]; Antagonist both thromboxane A_2 and Leukotriene D_4 [3019]; Antiviral activity towards the replication of vesicular stomatitis virus in HEL cell cultures [644]; Anthelmintic [457].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-octanone

[28441-00-1] $C_{22}H_{36}O_2$ mol. wt. 332.53



Syntheses
-Preparation by reaction of octanoyl chloride with 2,6-di-tert-butylphenol in the presence of aluminium chloride [2145], (65 %) [2810].
-Also refer to: [655, 951].
m.p. 90–91° [951, 2810]; IR [2810].

BIOLOGICAL ACTIVITY: High larvicidal activity in test on mosquito larvas [2810].

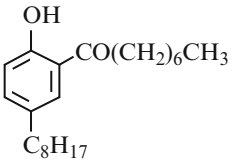
Acetate [30392-06-4] $C_{24}H_{38}O_3$ mol. wt. 374.56

-Obtained by acetylation of 3,5-di-tert-butyl-4-hydroxyoctanophenone [2145].
-Also refer to: [228].

$b.p._{.10}$ 234–236° [228]; ^1H NMR [2145], IR [2145].

1-(2-Hydroxy-5-octylphenyl)-1-octanone

[74604-21-0] $C_{22}H_{36}O_2$ mol. wt. 332.53



Synthesis
-Obtained by Fries rearrangement of 4-octylphenyl octanoate ($b.p._{.0.02}$ 168°) [2520].
$b.p._{.0.02}$ 170° [2520]; IR [2520], UV [2520].

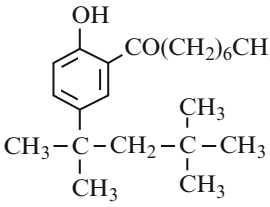
Oxime [74604-11-8] $C_{22}H_{37}NO_2$ mol. wt. 347.54

waxy needles [2520]; m.p. 59° [2520];
IR [2520], UV [2520].

USE: Solvent extraction of copper (II) [2520].

1-[2-Hydroxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-octanone

$C_{22}H_{36}O_2$ mol. wt. 332.53

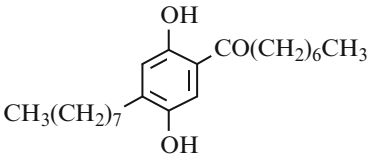


Syntheses
-Refer to: [3198, 3199].
Oxime [72782-46-8]
$C_{22}H_{37}NO_2$ mol. wt. 347.54
-Refer to: [3198, 3199].

USE: Extraction. by, of copper, kinetics and mechanism of, [3198, 3199].

1-(2,5-Dihydroxy-4-octylphenyl)-1-octanone

[63134-27-0] $C_{22}H_{36}O_3$ mol. wt. 348.53



Syntheses

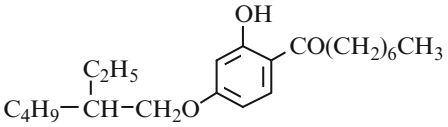
-Obtained by reaction of caprylic acid with 2-octylhydroquinone in the presence of boron trifluoride in 1,2-dichloroethane at 40–45° for 1.25 h. The mixture was allowed to stand overnight (70 %) [142].

-Also refer to: [1907].

m.p. 82–83° [142, 1907].

1-[4-[(2-Ethylhexyl)oxy]-2-hydroxyphenyl]-1-octanone

$C_{22}H_{36}O_3$ mol. wt. 348.53



Synthesis

-Refer to: [1050].

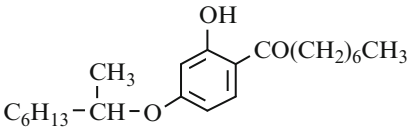
Oxime, **nickel complex**

[80848-72-2]

USE: Photog. stabilizer compns. contg. phenol derivs. and, for magenta images [1050].

1-[2-Hydroxy-4-[(1-methylheptyl)oxy]phenyl]-1-octanone

[127789-29-1] $C_{22}H_{36}O_3$ mol. wt. 348.53



Synthesis

-Refer to: [3345].

Oxime (*E*) [127789-31-5]

$C_{22}H_{37}NO_3$ mol. wt. 363.54

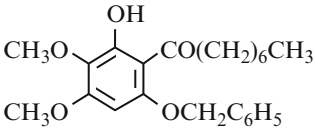
-Refer to: [3345].

Oxime (*Z*) [127789-34-8] $C_{22}H_{37}NO_3$ mol. wt. 363.54

-Refer to: [3345].

1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-octanone

[134082-03-4] $C_{23}H_{30}O_5$ mol. wt. 386.49



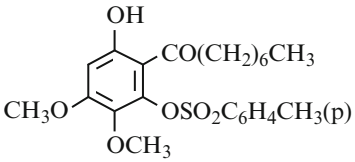
Synthesis

-Obtained by elimination of one phenylmethyl group in 2-position by treatment of 1-(2,6-dibenzyloxy-3,4-dimethoxyphenyl)-1-octanone with concentrated hydrochloric acid and acetic acid at r.t. for 2–3 h (84 %) [1353].

m.p. 85.5–86° [1353]; ^{1}H NMR [1353].

1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-octanone

[134081-87-1] $C_{23}H_{30}O_7S$ mol. wt. 450.55

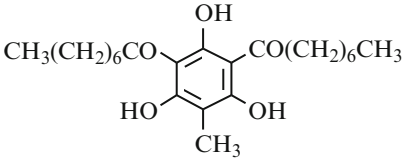


Synthesis
-Obtained by treatment of 1-(2-tosyloxy-3,4,6-trimethoxyphenyl)-1-octanone with 25 % aluminium bromide in acetonitrile at r.t. for 2–3 h (84 %) [1353].

m.p. 63–64.5° [1353]; ^{1}H NMR [1353].

1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-octanone

[3118-45-4] $C_{23}H_{36}O_5$ mol. wt. 392.54



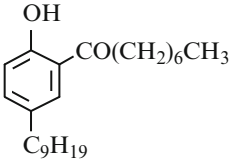
Syntheses
-Obtained by reaction of octanoic anhydride with 2-methylphloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].
-Also refer to: [457, 600, 2911].

m.p. 102–104° [457, 2911].

BIOLOGICAL ACTIVITY: For treatment of immune dysfunction associated with human immuno deficiency virus infection [600]; Anthelmintic [457].

1-(2-Hydroxy-5-nonylphenyl)-1-octanone

$C_{23}H_{38}O_2$ mol. wt. 346.55



Syntheses
-Obtained by Fries rearrangement of 4-nonylphenyl octanoate with aluminium chloride [3445].
-Also refer to: [1142, 1143, 1145, 1146, 1507].

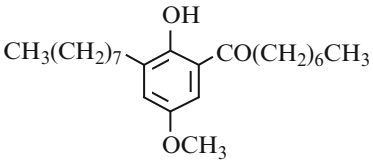
Oxime [51528-16-6] $C_{23}H_{39}NO_2$ mol. wt. 361.57

-Also refer to: [3445].

USE: Extn. by, of copper from aq. soln. [1143]; Prepn. of, for extn. of metals [1142]; Copper extn. by, [1146]; Extn. by, of copper, cobalt and nickel from sulfate solns [1507]; Extn. by, of non-ferrous metals [1145].

1-(2-Hydroxy-5-methoxy-3-octylphenyl)-1-octanone

[102898-66-8] $C_{23}H_{38}O_3$ mol. wt. 362.55



Syntheses

-Obtained by reaction of octanoic acid with 4-methoxy-2-octylphenol in the presence of boron trifluoride in tetrachloroethane for 6 h. The reaction mixture was allowed to stand overnight at r.t. and was then heated on a steam bath for about 5 h (43 %) [142].

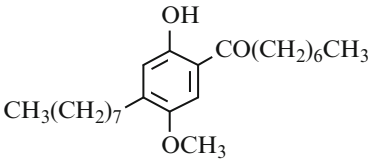
-Also obtained by Fries rearrangement of 4-methoxy-2-octylphenyl caprylate (b.p.$_1$ 170–180°) with boron trifluoride in *sym*-tetrachloroethane for 6 h, following 5 h of heating on a steam bath (59 %) [142].

-Also refer to: [1907].

b.p.$_1$ 195–205° [142, 1907]; m.p. 31–32° [142], 30–31° [1907].

1-(2-Hydroxy-5-methoxy-4-octylphenyl)-1-octanone

[21182-66-1] $C_{23}H_{38}O_3$ mol. wt. 362.55



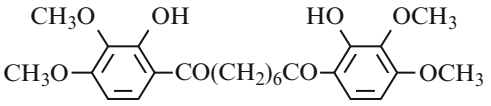
Synthesis

-Obtained by action of octanoyl chloride with 2-octylhydroquinone dimethyl ether in the presence of aluminium chloride in refluxing carbon disulfide for 10 h on the steam bath (68 %) [2370].

yellow plates [2370]; m.p. 53–54° [2370]; IR [2370].

1,8-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,8-octanedione

[10351-92-5] $C_{24}H_{30}O_8$ mol. wt. 446.50



Syntheses

-Obtained by reaction of suberic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride in tetrachloroethane [1574].

-Also refer to: [589, 1575].

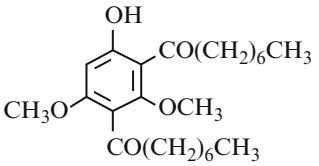
m.p. 163° [1574, 1575], 160° [589]; IR [589].

Dioxime [32246-91-6] $C_{24}H_{32}N_2O_8$ mol. wt. 476.53

m.p. 195° [589].

1,1′-(4-Hydroxy-2,6-dimethoxy-1,3-phenylene)bis-1-octanone

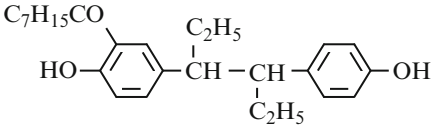
[1142936-30-8] $C_{24}H_{38}O_5$ mol. wt. 406.56



Synthesis
-Refer to: [2786].
^{1}H NMR [2786].

3-(4-Hydroxyphenyl)-4-[4-hydroxy-3-(1-oxooctyl)phenyl]hexane
(3-n-Butyrylhexestrol)

$C_{26}H_{36}O_3$ mol. wt. 396.57



Synthesis
-Obtained by treatment of its dimethyl ether by means of pyridinium chloride [510].

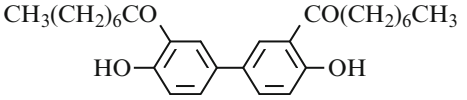
Dimethyl ether $C_{28}H_{40}O_3$ mol. wt. 424.62

-Obtained by reaction of octanoyl chloride with hexestrol dimethyl ether in the presence of aluminium chloride in nitrobenzene for 3 h at r.t. [510].

light colourless leaflets [510];
b.p.$_{15}$ about 300° [510]; m.p. 67° [510].

1-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-octanone

[104397-43-5] $C_{28}H_{38}O_4$ mol. wt. 438.61



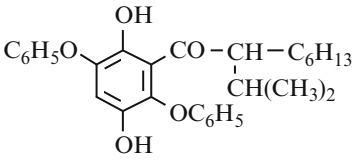
Syntheses
-Preparation by Fries rearrangement of 4,4′-biphenyl dicaprylate with aluminium chloride,

*in the presence of sodium chloride at 140°. The reaction is carried out by adding the ester to the melt, rapidly increasing the temperature to 200° and maintaining it there for 2 min before quick cooling [2091];
*in refluxing chlorobenzene for 24 h (88 %) [2377].

m.p. 88.5–90° [2377]; IR [2377].

1-(2,5-Dihydroxy-3,6-diphenoxyphenyl)-2-(1-methylethyl)-1-octanone

$C_{29}H_{34}O_5$ mol. wt. 462.59

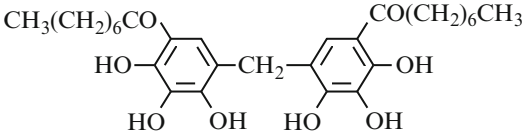


Synthesis
-Refer to: [2352].

Dimethyl ether [357172-44-2]
$C_{31}H_{38}O_5$ mol. wt. 490.59
-Refer to: [2352].

1,1′-[Methylenebis(4,5,6-trihydroxy-3,1-phenylene)]bis-1-octanone

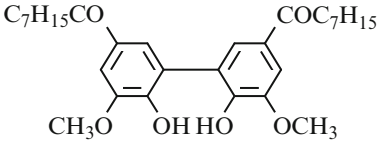
[145941-31-7] $C_{29}H_{40}O_8$ mol. wt. 516.63



Synthesis
-Refer to: [2511].

1,1′-(6,6′-Dihydroxy-5,5′-dimethoxy[1,1′-biphenyl]-3,3′-diyl)bis-1-octanone

[157687-62-2] $C_{30}H_{42}O_6$ mol. wt. 498.66



Synthesis
-Refer to: [1428].

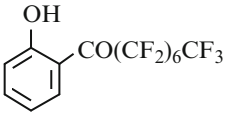
BIOLOGICAL ACTIVITY: As active oxygen scavenger, for therapeutic use [1428].

2 Aromatic Hydroxyketones Derived from Various Halogenooctanoic Acids

2.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-1-octanone

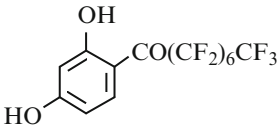
[176515-55-2] $C_{14}H_5F_{15}O_2$ mol. wt. 490.27



Synthesis
-Refer to: [3155].

1-(2-4-Dihydroxyphenyl)-2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-1-octanone

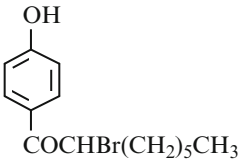
[105932-66-9] $C_{14}H_5F_{15}O_3$ mol. wt. 506.16



Synthesis
-Refer to: [2171].

2-Bromo-1-(4-hydroxyphenyl)-1-octanone

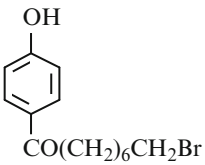
$C_{14}H_{19}BrO_2$ mol. wt. 299.21



Synthesis
-Refer to: [3472].
Methyl ether
$C_{15}H_{21}BrO_2$ mol. wt. 313.23
-Refer to: [3472].

8-Bromo-1-(4-hydroxyphenyl)-1-octanone

$C_{14}H_{19}BrO_2$ mol. wt. 299.21



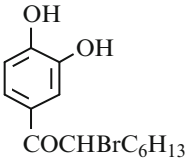
Synthesis
-Refer to: [572].
Methyl ether [224775-35-3]
$C_{15}H_{21}BrO_2$ mol. wt. 313.23

-Obtained by Friedel-Crafts acylation of anisole with 8-bromooctanoyl chloride in the presence of aluminium chloride in dichloromethane at −10° for 1–2 h under nitrogen (40 %) [572].

m.p. 45–48° [572]; ^{1}H NMR [572].

2-Bromo-1-(3,4-dihydroxyphenyl)-1-octanone

$C_{14}H_{19}BrO_3$ mol. wt. 315.20

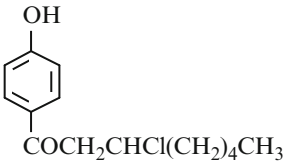


Synthesis
-Refer to: [2657].
Dibenzyl ether $C_{28}H_{31}BrO_3$ mol. wt. 495.46
-Obtained by reaction of N-bromosuccinimide with 3,4-(dibenzyloxy)caprylophenone in carbon tetrachloride in the presence of benzoyl peroxide at 50° (85–90 %) [2657].

m.p. 90° [2657].

3-Chloro-1-(4-hydroxyphenyl)-1-octanone

[848478-63-7] $C_{14}H_{19}ClO_2$ mol. wt. 254.76



Syntheses

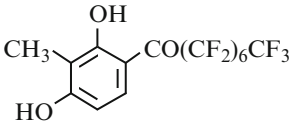
-Obtained by adding concentrated hydrochloric acid to a solution of 1-(4-hydroxyphenyl)-3-hydroxy-1-octanone [1634], in dioxane. The mixture obtained was stirred at 20° for 22.5 h (70 %) [1747, 1748].

m.p. 56–57° (d) [1747, 1748];
^{1}H NMR [1747, 1748], IR [1747, 1748], UV [1747, 1748].

2.2 Substituted Hydroxyketones

1-(2,4-Dihydroxy-3-methylphenyl)-2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-1-octanone

[65240-06-4] $C_{15}H_7F_{15}O_3$ mol. wt. 520.19



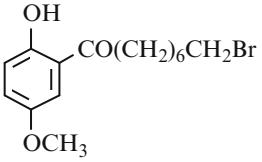
Synthesis

-Refer to: [450].

BIOLOGICAL ACTIVITY: Antimicrobial [450].

8-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-octanone

[173055-38-4] $C_{15}H_{21}BrO_3$ mol. wt. 329.23

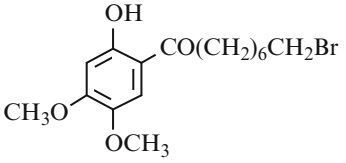


Synthesis

-Refer to: [2623].

8-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-octanone

[173055-44-2] $C_{16}H_{23}BrO_4$ mol. wt. 359.26

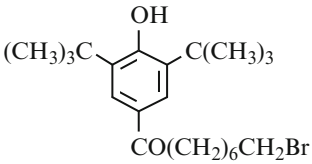


Synthesis

-Refer to: [2623].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-8-bromo-1-octanone

[158869-45-5] $C_{22}H_{35}BrO_2$ mol. wt. 411.42



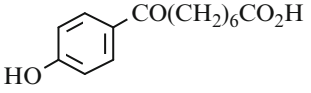
Synthesis
-Refer to: [1689].

3 Aromatic Hydroxyketones Derived from 8-Oxooctanoic Acids

3.1 Unsubstituted Hydroxyketones

8-(4-Hydroxyphenyl)-8-oxo-1-octanoic acid

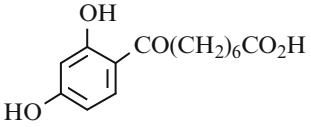
[22811-89-8] $C_{14}H_{18}O_4$ mol. wt. 250.29



Synthesis
-Refer to: [584].
m.p. 129° [584].

8-(2,4-Dihydroxyphenyl)-8-oxo-1-octanoic acid

[32246-77-8] $C_{14}H_{18}O_5$ mol. wt. 266.29



Syntheses
-Obtained by reaction of suberic acid with resorcinol in the presence of zinc chloride at 140° for 5 h (40 %) [445].
-Also refer to: [589, 3370].

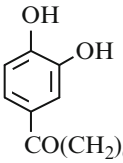
m.p. 145° [445], 143° [2606], 141° [589].

Methyl ester $C_{15}H_{20}O_5$ mol. wt. 280.32

$b.p._{\cdot 0.5}$ 260–264° [445]; m.p. 84° [445].

8-(3,4-Dihydroxyphenyl)-8-oxo-1-octanoic acid

$C_{14}H_{18}O_5$ mol. wt. 266.29



Synthesis
-Refer to: [1013].

Dimethyl ether [32246-94-9]
$C_{16}H_{22}O_5$ mol. wt. 294.35
-Obtained by heating of its ethyl ester below with 10 % aqueous NaOH on the steam bath for 1.5 h (88 %) [1013].

-Also refer to: [589].

white solid [1013]; m.p. 94–95° [1013], 85° [589];
IR [1013].

2,4-Dinitrophenylhydrazone of the dimethyl ether

[32340-79-7] $C_{22}H_{26}N_4O_8$ mol. wt. 474.47

m.p. 236° [589].

Ethyl ester of the dimethyl ether [57641-19-7] $C_{18}H_{26}O_5$ mol. wt. 322.40

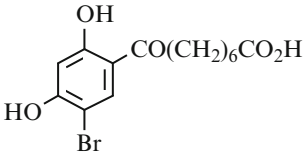
-Obtained by reaction of 8-chloro-8-oxooctanoic acid ethyl ester with 1,2-dimethoxybenzene in the presence of aluminium chloride in 1,1,2,2-tetrachloroethane first at 0–3° for 2.5 h, and overnight to 2° (59 %) [1013].

white solid [1013]; $b.p._{0.05}$ 192–193° [1013];
m.p. 40–43° [1013]; IR [1013]; GLC [1013].

3.2 Substituted Hydroxyketones

8-(2,4-Dihydroxy-5-bromophenyl)-8-oxo-1-octanoic acid

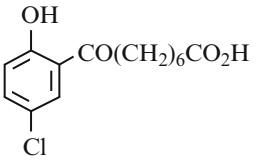
[32246-17-6] $C_{14}H_{17}BrO_5$ mol. wt. 345.19



Synthesis
-Refer to: [589].
m.p. 161° [589].

8-(2-Hydroxy-5-chlorophenyl)-8-oxo-1-octanoic acid

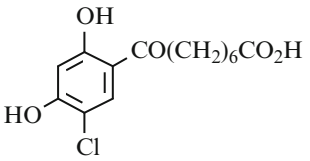
[22812-06-2] $C_{14}H_{17}ClO_4$ mol. wt. 284.74



Synthesis
-Refer to: [584].
m.p. 132° [584].

8-(2,4-Dihydroxy-5-chlorophenyl)-8-oxo-1-octanoic acid

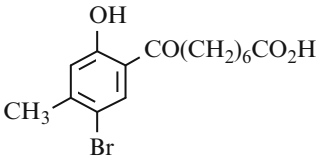
[32246-86-9] $C_{14}H_{17}ClO_5$ mol. wt. 300.74



Synthesis
-Refer to: [589].
m.p. 141° [589].

8-(2-Hydroxy-5-chloro-4-methylphenyl)-8-oxo-1-octanoic acid

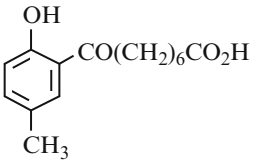
$C_{15}H_{19}ClO_4$ mol. wt. 298.77



Synthesis
-Refer to: [584].
m.p. 161° [584].

8-(2-Hydroxy-4-methylphenyl)-8-oxo-1-octanoic acid

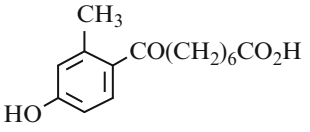
[22812-09-5] $C_{15}H_{20}O_4$ mol. wt. 264.32



Synthesis
-Refer to: [584].
m.p. 122° [584]; UV [1827].

8-(4-Hydroxy-2-methylphenyl)-8-oxo-1-octanoic acid

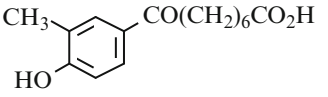
[22812-00-6] $C_{15}H_{20}O_4$ mol. wt. 264.32



Synthesis
-Refer to: [584].
m.p. 95° [584].

8-(4-Hydroxy-3-methylphenyl)-8-oxo-1-octanoic acid

[22811-96-7] $C_{15}H_{20}O_4$ mol. wt. 264.32



Synthesis
-Refer to: [584].
m.p. 102° [584].

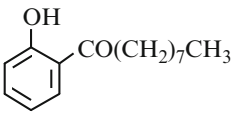
Chapter 7
Nonanones

1 Aromatic Hydroxyketones Derived from Nonanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-1-nonanone

[22362-60-3] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses

-Phenol was energetically mixed with finely divided aluminium chloride (1 mol) and heated to 100° (1 mol of hydrochloric acid is evolved); 1 mol. of n-pelargonoyl chloride was then added and heated to 125–130° for 1 h (55 %) [2700].

-Also obtained by stirring a solution of salicylaldehyde, 1-octene, $RhCl(PPh_3)_3$, acetonitrile and sodium acetate in methylene chloride at r.t. for 8 h under an argon atmosphere (82 %) [1434].

colourless oil [1434]; b.p.$_{10}$ 180° [2700]; m.p. 18.4° [2700];
^{1}H NMR [1434] (Sadtler standard N° 38630 M);
IR [1434] (Sadtler standard N° 65679 K), UV [1996], MS [1434];
$n_D^{25.5} = 1.5139$ [2700].

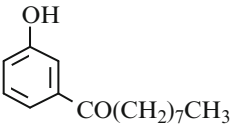
Oxime [439948-78-4] $C_{15}H_{23}NO_2$ mol. wt. 249.35

USE: Blocking agent, binders containing blocked PAPI and phenolic resins for wood composites [2077].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_7

1-(3-Hydroxyphenyl)-1-nonanone

[859995-51-0] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Obtained by treatment of its methyl ether with aluminium chloride in benzene by heating on a water bath for 2 h (80 %) [966].
-Also refer to: [967].

m.p. 54° [966, 967].

2,4-Dinitrophenylhydrazone $C_{21}H_{26}N_4O_5$ mol. wt. 414.46

m.p. 101° [967].

Methyl ether [172264-98-1] $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained by condensation of dodecylmagnesium bromide with m-methoxybenzamide in ethyl ether. The reaction was carried out at 60° for 48 h under hydrogen atmosphere (60–70 %) [966].
-Also refer to: [967, 1213, 1626].

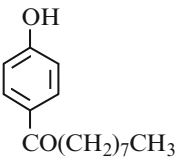
b.p.$_{14}$ 170° [966, 967];
^{1}H NMR [1626], ^{13}C NMR [1626]; $n_D^{37} = 1.5070$ [966].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{22}H_{28}N_4O_5$ mol. wt. 428.49

m.p. 90° [967].

1-(4-Hydroxyphenyl)-1-nonanone

[14392-69-9] $C_{15}H_{22}O_2$ mol. wt. 234.34



Syntheses
-Phenol was energetically mixed with finely divided aluminium chloride (1 mol) and heated to 100° (1 mol of hydrochloric acid is evolved); 1 mol. of n-pelargonoyl chloride was then added and heated to 125–130° for 1 h (35 %) [2700].

-Also obtained by reaction of nonanoyl chloride with phenol in the presence of aluminium chloride,
*in methylene chloride [64] for 14 h at r.t. (33 %) [1910];
*in nitrobenzene at r.t. overnight (70 %) [1769].
-Also obtained by Fries rearrangement of phenyl nonanoate with aluminium chloride in nitrobenzene at 38° for 2 days (60 %) [414].
-Also refer to: [62, 368, 442, 1730, 2658, 3100, 3457].

Isolation from natural sources

-From a cell suspension culture of *Humulus lupulus* cv Wye Northdown [602].

viscous oil [602]; b.p.$_4$ 195–199° [1769], b.p.$_{10}$ 232° [2700];
white solid [1910];
m.p. 57.2–57.6° [1910], 55.5–56.5° [1730], 55° (Sadtler standard N° 65675 K), 54.5° [2700], 50–52° [414], 42–46° [1769];
^{1}H NMR [602, 1910] (Sadtler standard N° 38626 M),
^{13}C NMR [602, 1910];
IR [602, 1910] (Sadtler standard N° 65675 K), UV [1995],
MS [602, 1910]; TLC [1910]; GC [1910].

BIOLOGICAL ACTIVITY: Inhibition of 17-β hydroxysteroid dehydrogenase 3 [1910]; Binary classification models for endocrine disrupter effects mediated through the estrogen receptor [2640].

Benzoate $C_{22}H_{26}O_3$ mol. wt. 338.45

m.p. 99.8–100° [2700].

Methyl ether [52754-68-4] $C_{16}H_{24}O_2$ mol. wt. 248.37

-Obtained from 1-nonene and (p-MeO-C_6H_4)$I^+PhBF_4^-$ (69 %) [1592].
-Also obtained by electrolyzing in an undivided cell a DMF solution containing n-octyl iodide and 4-iodoanisole, iron pentacarbonyl and a catalytic amount of a nickel 2,2′-bipyridine complex (35 %) [894].
-Also obtained by reaction of 1-(4-methoxyphenyl)-4-iodo-1-butanone with dipentylzinc in the presence of Ni(acac)$_2$ in THF/NMP and acetophenone at −35° (71 %) [1122].
-Obtained from 4-methoxybenzaldehyde and 1-octene (93 %) [3211].
-Also refer to: [1121, 1200, 1202, 2901, 3211, 3250].

m.p. 43° [2901];
^{1}H NMR [894, 3211], ^{13}C NMR [894, 3211], IR [894], MS [894, 3211].

USE: Photolysis of, energy transfer in, [3250].

Phenylhydrazone of the methyl ether $C_{22}H_{30}N_2O$ mol. wt. 338.49

m.p. 48° [2901].

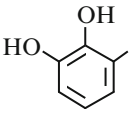
4-Bromophenyl ether [74261-29-3] $C_{21}H_{25}BrO_2$ mol. wt. 389.33

m.p. 79° [866].

USE: Prepn. nonmesogenic [865].

1-(2,3-Dihydroxyphenyl)-1-nonanone

[862666-37-3] $C_{15}H_{22}O_3$ mol. wt. 250.34



Synthesis
-Obtained by deprotection of its dimethyl ether with boron tribromide in methylene chloride at 0°. Then, the mixture was stirred overnight at r.t. (80 %) [82].

brown solid [82]; m.p. 41° [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

USE: Reactant for preparation of lithium gallium/titanium ketone complexes [82].

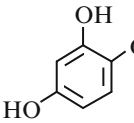
Dimethyl ether [862666-31-7] $C_{17}H_{26}O_3$ mol. wt. 278.39

-Obtained by treatment of 1-(2,3-dimethoxyphenyl)-1-nonanol in acetone with potassium dichromate in dilute sulfuric acid (Jones reagent) at r.t. for 3 h (61 %) [82].

colourless oil [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

1-(2,4-Dihydroxyphenyl)-1-nonanone

[27883-48-3] $C_{15}H_{22}O_3$ mol. wt. 250.34



Syntheses
-Obtained by reaction of nonanoyl chloride with resorcinol in the presence of aluminium chloride in 1,2-dichloro-ethane for 5 h at 65° [284].
-Also refer to: [893, 1655, 2112, 2114, 2673, 2704].

b.p.$_{12}$ 245–248° [893]; m.p. 73° [2704], 65° [2114], 50° [2673].
N.B.: There is a large disparity between the various melting points.
^{1}H NMR [3242].

USE: As colour developer [2704].

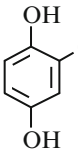
BIOLOGICAL ACTIVITY: Antifungal [2112, 2114].

2,4-Dinitrophenylhydrazone [95282-26-1] $C_{21}H_{26}N_4O_6$ mol. wt. 430.46

m.p. 145° [2673].

1-(2,5-Dihydroxyphenyl)-1-nonanone

$C_{15}H_{22}O_3$ mol. wt. 250.34



Synthesis

-Refer to: [2874].

Dimethyl ether [101741-11-1]

$C_{17}H_{26}O_3$ mol. wt. 278.39

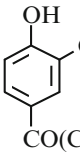
-Obtained by reaction of pelargonic acid chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in carbon disulfide first at 0°, kept overnight, heated to a boil [2874].

b.p.$_3$ 180–182° [2874].

1-(3,4-Dihydroxyphenyl)-1-nonanone

4-Nonanoylcatechol

$C_{15}H_{22}O_3$ mol. wt. 250.34



Synthesis

-Obtained by Fries rearrangement of pyrocatechol nonanoate (1 mol) with aluminium chloride (2 mol) in the presence of pyrocatechol (1 mol) in nitrobenzene at 80–100° for 2 h (40 %) [1283].

m.p. 92–93° [1283].

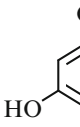
Dimethyl ether $C_{17}H_{26}O_3$ mol. wt. 278.39

-Refer to: [1347].

^{1}H NMR [1347], ^{13}C NMR [1347],
IR [1347], UV [1347], MS [1347].

1-(3,5-Dihydroxyphenyl)-1-nonanone

$C_{15}H_{22}O_3$ mol. wt. 250.34



Isolation from natural sources

-From the roots and stems of *Ardisia virens* Kurz (Myrsinaceae) [607].

-From the roots of *Ardisia cornudentata* Mez. [607].

colourless needles [607], m.p. 99–100° [607],
^{1}H NMR [607], ^{13}C NMR [607],
IR [607], UV [607], MS [607].

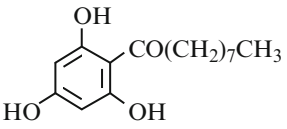
Dimethyl ether $C_{17}H_{26}O_3$ mol. wt. 278.39

-Obtained by reaction of n-octylmagnesium bromide with 3,5-dimethoxybenzamide (76 %) [30].
-Preparation in the usual way [25 (77 %), 2990].

b.p.$_{0.03}$ 150–156° [30], b.p.$_1$ 180° [25];
m.p. 35.5–36° [30].

1-(2,4,6-Trihydroxyphenyl)-1-nonanone
(Phlorononaphenone) [1026]

[74478-11-8] $C_{15}H_{22}O_4$ mol. wt. 266.34



Syntheses
-Obtained by reaction of nonanoyl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene and carbon disulfide mixture (57 %) [2113].
-Also refer to: [1026, 2111, 2781].

pale yellow needles [2113];
m.p. 82° [2781], 109° [2113];
N.B.: One of the reported melting point is obviously wrong.
IR [2113], UV [2113].

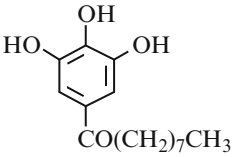
BIOLOGICAL ACTIVITY: Antifungal [2111, 2113].

Trimethyl ether $C_{18}H_{28}O_4$ mol. wt. 308.42

-Refer to: [16]; m.p. 34° [16].

1-(3,4,5-Trihydroxyphenyl)-1-nonanone

[100079-26-3] $C_{15}H_{22}O_4$ mol. wt. 266.34

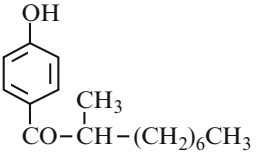


Syntheses
-Refer to: [1969, 3248].

BIOLOGICAL ACTIVITY: As platelet aggregation inhibitor and antiallergic agent [3248].

1-(4-Hydroxyphenyl)-2-methyl-1-nonanone

[120837-31-2] $C_{16}H_{24}O_2$ mol. wt. 248.37
[120837-03-8] (+)

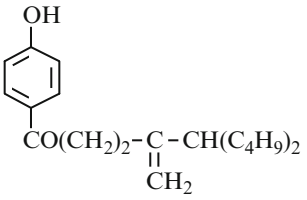


Syntheses
-Refer to: [1321, 1322, 2277].

Methyl ether [179037-21-9]
$C_{17}H_{26}O_2$ mol. wt. 262.39
-Refer to: [2277].

5-Butyl-1-(4-hydroxyphenyl)-4-methylene-1-nonanone

$C_{20}H_{30}O_2$ mol. wt. 302.36

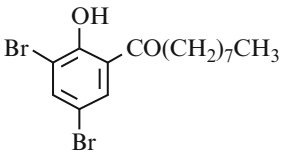


Synthesis
-Refer to: [532].
Methyl ether [465526-56-1]
$C_{21}H_{32}O_2$ mol. wt. 316.48
-Obtained by reaction of 2-butylpentylidene-cyclopropane and p-methoxyacetophenone in the presence of $Pd(PPh_3)_4$ (5 mol%) and $P(Bu)_3$ (10 mol%) at 120° for 3–4 days (71 %) [532].

1.2 Substituted Hydroxyketones

1-(3,5-Dibromo-2-hydroxyphenyl)-1-nonanone

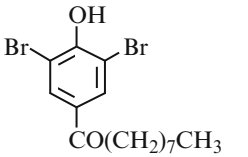
$C_{15}H_{20}Br_2O_2$ mol. wt. 392.13



Synthesis
-Refer to: [2002].
m.p. 55° (Sadtler standard N° 65681 K);
^{1}H NMR (Sadtler standard N° 38632 M);
IR (Sadtler standard N° 65681 K).

1-(3,5-Dibromo-4-hydroxyphenyl)-1-nonanone

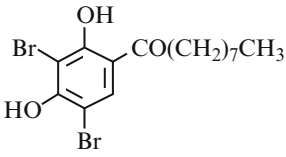
$C_{15}H_{20}Br_2O_2$ mol. wt. 392.13



Synthesis
-Refer to: [2002].
m.p. 38° (Sadtler standard N° 65677 K);
^{1}H NMR (Sadtler standard N° 38628 M);
IR (Sadtler standard N° 65677 K).

1-(3,5-Dibromo-2,4-dihydroxyphenyl)-1-nonanone

[76092-86-9] $C_{15}H_{20}Br_2O_3$ mol. wt. 408.13

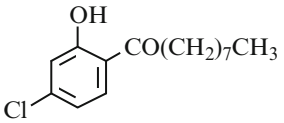


Synthesis
-Refer to: [2112].

BIOLOGICAL ACTIVITY: Antifungal compns. contg., [2112]

1-(4-Chloro-2-hydroxyphenyl)-1-nonanone

[67548-60-1] $C_{15}H_{21}ClO_2$ mol. wt. 268.78

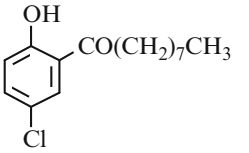


Syntheses
-Refer to: [1673, 1798].
$n_D^{20.5} = 1.4743$ [1673].

BIOLOGICAL ACTIVITY: Nematocide [1798].

1-(5-Chloro-2-hydroxyphenyl)-1-nonanone

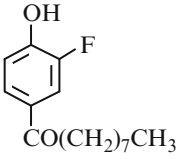
[1396756-57-2] $C_{15}H_{21}ClO_2$ mol. wt. 268.78



Synthesis
-Refer to: [3242].
colourless crystal [3242]; m.p. 46–48° [3242];
^{1}H NMR [3242], ^{13}C NMR [3242], MS [3242].

1-(3-Fluoro-4-hydroxyphenyl)-1-nonanone

$C_{15}H_{21}FO_2$ mol. wt. 252.33



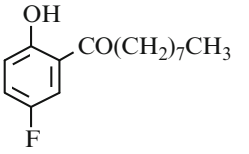
Synthesis
-Refer to: [2363].

Methyl ether [136936-71-5]
$C_{16}H_{23}FO_2$ mol. wt. 266.36

-Preparation by Friedel-Crafts acylation of 2-fluoroanisole with nonanoyl chloride (75 %) [2363].

1-(5-Fluoro-2-hydroxyphenyl)-1-nonanone

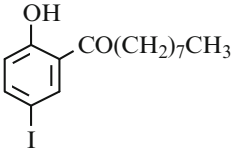
[1396756-56-1] $C_{15}H_{21}FO_2$ mol. wt. 252.33



Synthesis
-Refer to: [3242].
colourless crystal [3242]; m.p. 40–42° [3242];
^{1}H NMR [3242], ^{13}C NMR [3242], MS [3242].

1-(5-Iodo-2-hydroxyphenyl)-1-nonanone

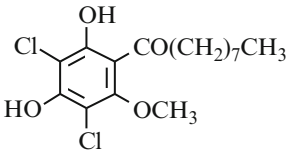
[1396756-58-3] $C_{15}H_{21}IO_2$ mol. wt. 360.24



Synthesis
-Refer to: [3242].
colourless crystal [3242]; m.p. 52–54° [3242];
^{1}H NMR [3242], ^{13}C NMR [3242], MS [3242].

1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-nonanone

[118191-35-8] $C_{16}H_{22}Cl_2O_4$ mol. wt. 349.25

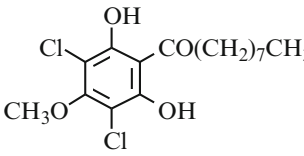


Synthesis
-Obtained by reaction of chlorine with 2,4-dihydroxy-6-methoxynonanophenone in water [2012].
^{1}H NMR [2012], MS [2012].

BIOLOGICAL ACTIVITY: Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-nonanone

[118191-36-9] $C_{16}H_{22}Cl_2O_4$ mol. wt. 349.25

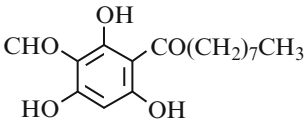


Synthesis
-Obtained by reaction of chlorine with 2,6-dihydroxy-4-methoxynonanophenone in water [2012].
^{1}H NMR [2012], MS [2012].

BIOLOGICAL ACTIVITY: Differentiation-inducing factor from the slime mould *Dictyostelium discoideum* [2012].

2,4,6-Trihydroxy-3-nonanoylbenzaldehyde

$C_{16}H_{22}O_5$ mol. wt. 294.35

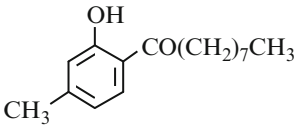


Synthesis
-Refer to: [3408].

BIOLOGICAL ACTIVITY: Effects on transpiration and stomatal closure [3408].

1-(2-Hydroxy-4-methylphenyl)-1-nonanone

$C_{16}H_{24}O_2$ mol. wt. 248.37

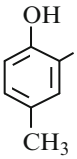


Synthesis
-Preparation by Fries rearrangement of m-cresyl pelargonate with aluminium chloride at 120–140° for 10–20 min (75 %) [243].

b.p.$_4$ 175–177° [243].

1-(2-Hydroxy-5-methylphenyl)-1-nonanone

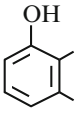
[75487-43-3] $C_{16}H_{24}O_2$ mol. wt. 248.37



Syntheses
-Refer to: [1355, 1356].

1-(2-Hydroxy-6-methylphenyl)-1-nonanone

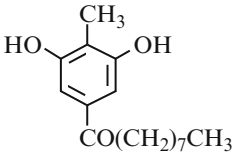
[1396756-55-0] $C_{16}H_{24}O_2$ mol. wt. 248.37



Synthesis
-Refer to: [3242].
Colourless crystal [3242]; ^{1}H NMR [3242], ^{13}C NMR [3242], MS [3242].

1-(3,5-Dihydroxy-4-methylphenyl)-1-nonanone

$C_{16}H_{24}O_3$ mol. wt. 264.36



Synthesis
-Refer to: [3132].
Dimethyl ether [196869-48-4]
$C_{18}H_{28}O_3$ mol. wt. 292.42

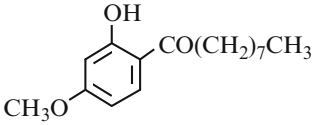
-Refer to: [3132 (80 %)].

colourless crystalline solid [3132];
^{1}H NMR [3132], ^{13}C NMR [3132].

USE: Preparation of striatol and related compounds [3132].

1-(2-Hydroxy-4-methoxyphenyl)-1-nonanone

[43221-42-7] $C_{16}H_{24}O_3$ mol. wt. 264.36

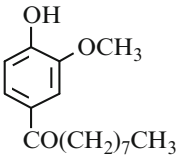


Synthesis
-Refer to: [3092, 3242].
m.p. 48.5–49° [3092];
^{1}H NMR [3242], ^{13}C NMR [3242], MS [3242].

USE: Light stabilizer, for polyolefins, [3092].

1-(4-Hydroxy-3-methoxyphenyl)-1-nonanone

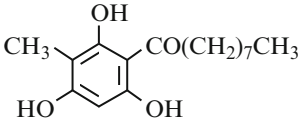
[143378-82-9] $C_{16}H_{24}O_3$ mol. wt. 264.36



Syntheses
-Refer to: [1427, 1429].

1-(2,4,6-Trihydroxy-3-methylphenyl)-1-nonanone

$C_{16}H_{24}O_4$ mol. wt. 280.36

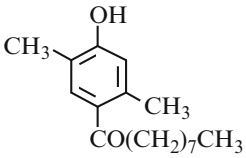


Syntheses
-Refer to: [1026, 1501, 1502].

BIOLOGICAL ACTIVITY: Antimicrobial [1026, 1501, 1502].

1-(4-Hydroxy-2,5-dimethylphenyl)-1-nonanone

[95102-38-8] $C_{17}H_{26}O_2$ mol. wt. 262.39

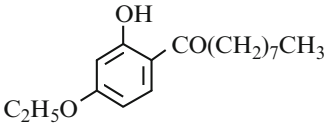


Syntheses
-Refer to: [1595, 2704] (Japanese patents).

USE: In preparation of thermographic recording material [1595].

1-(4-Ethoxy-2-hydroxyphenyl)-1-nonanone

$C_{17}H_{26}O_3$ mol. wt. 278.39



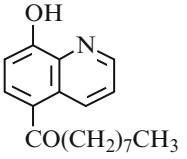
Synthesis
-Refer to: [1835].

Oxime [33488-76-5]
$C_{17}H_{27}NO_3$ mol. wt. 293.41

USE: Hydrogen bonding, spectra in relation to, [1835].

1-(8-Hydroxy-5-quinolinyl)-1-nonanone

[79111-56-1] $C_{18}H_{23}NO_2$ mol. wt. 285.39



Syntheses
-Obtained by reaction of nonanoyl chloride with 8-hydroxyquinoline in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].
-Also refer to: [938, 2638, 3108, 3173].

m.p. 66–67° [938], 64–65° [2261], 62–63° [3173];
^{1}H NMR [3173], ^{13}C NMR [2261, 2638], IR [3173],
MS [2261].

USE: For extraction of gallium [3172]; Amebicidal action [3108]

Hydrochloride [79111-55-0] $C_{18}H_{23}NO_2$, HCl mol. wt. 321.85

-Refer to: [3173].

m.p. 163–164° [3173].

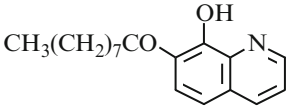
Hydrobromide $C_{18}H_{23}NO_2$, HBr mol. wt. 366.30

-Obtained by reaction of pelargonyl chloride with 8-quinolinol in the presence of aluminium chloride in nitrobenzene first at 75° for 16 h, then at r.t. for 20 h. Then, the acetone solution was saturated with hydrogen bromide (17 %) [938].

m.p. 229–231° (d) [938].

1-(8-Hydroxy-7-quinolinyl)-1-nonanone

[79111-54-9] $C_{18}H_{23}NO_2$ mol. wt. 285.39



Syntheses
-Obtained by reaction of nonanoyl chloride with 8-hydroxyquinoline in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].
-Also refer to: [2638, 3171, 3173].

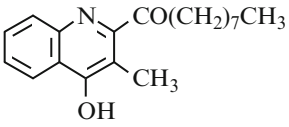
m.p. 64° [2261], 63–64° [3173];
^{1}H NMR [3173], ^{13}C NMR [2638], IR [3173], MS [2261].

Hydrazone [88559-43-7] $C_{18}H_{25}N_3O$ mol. wt. 299.42

m.p. 98–101° [3171].

1-(4-Hydroxy-3-methyl-2-quinolinyl)-1-nonanone

[331749-02-1] $C_{19}H_{25}NO_2$ mol. wt. 299.41



Synthesis
-Refer to: [2086].

BIOLOGICAL ACTIVITY: *In vitro* antibacterial activity against Helicobacter pylori [2086].

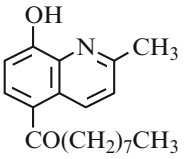
Acetate [331749-03-2] $C_{21}H_{27}NO_3$ mol. wt. 341.45

-Refer to: [279].

USE: Preparation of antibacterial quinoline derivatives for inhibition of Helicobacter pylori [2086].

1-(8-Hydroxy-2-methyl-5-quinolinyl)-1-nonanone

[217815-22-0] $C_{19}H_{25}NO_2$ mol. wt. 299.41



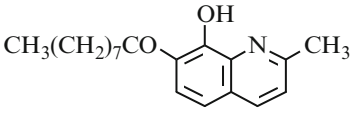
Synthesis

-Obtained by reaction of nonanoyl chloride with 8-hydroxyquinaldine in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

m.p. 72° [2261]; ^{1}H NMR [2261], ^{13}C NMR [2261], MS [2261].

1-(8-Hydroxy-2-methyl-7-quinolinyl)-1-nonanone

[217815-25-3] $C_{19}H_{25}NO_2$ mol. wt. 299.41



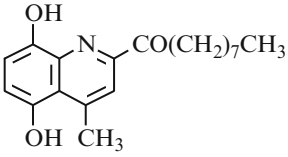
Synthesis

-Obtained by reaction of nonanoyl chloride with 8-hydroxyquinaldine in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

m.p. 58–60° [2261]; ^{1}H NMR [2261], ^{13}C NMR [2261], MS [2261].

1-(5,8-Dihydroxy-4-methyl-2-quinolinyl)-1-nonanone

$C_{19}H_{25}NO_3$ mol. wt. 315.41



Synthesis

-Refer to: [2266].

Dimethyl ether [67188-50-5]

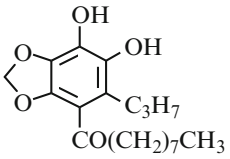
$C_{21}H_{29}NO_3$ mol. wt. 343.47

-Obtained by reaction of n-octylmagnesium bromide with 2-cyano-5,7-dimethoxy-4-methyl-quinoline in tetrahydrofuran (65 %) [2266].

m.p. 76–79° [2266].

1-(6,7-Dihydroxy-5-propyl-1,3-benzodioxol-4-yl)-1-nonanone

$C_{19}H_{28}O_5$ mol. wt. 336.43



Synthesis
-Refer to: [2179].

Dimethyl ether *(Pelargonyl dihydrodillapiole)*
[82652-29-7] $C_{21}H_{32}O_5$ mol. wt. 364.48

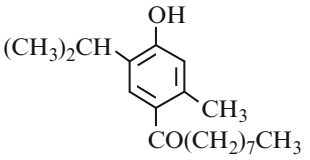
-Obtained by reaction of pelargonyl chloride with dihydrodillapiole in the presence of fused zinc chloride in methylene chloride for 3–4 h in an ice bath (70 %) [2179].

colourless solid [2179]; ^{1}H NMR [2179], IR [2179].

USE: Synergistic insecticidal activity of, with pyrethrum [2179].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-nonanone

$C_{19}H_{30}O_2$ mol. wt. 290.45



Synthesis
-Obtained (**XXIX**) by treatment of 1-[4-methoxy-2-methyl-5-(1-methylethyl)phenyl]-1-nonanone (**X**) with boiling pyridinium chloride (205–215°) for 5.5 h (7 %) [2660].

b.p.$_{17}$ 248–252° [2660]; m.p. 62° [2660].

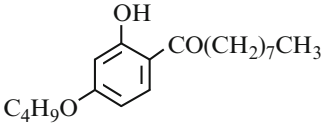
Methyl ether (**X**) $C_{20}H_{32}O_2$ mol. wt. 304.47

-Obtained by reaction of pelargonyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (47 %) [2660].

b.p.$_{14}$ 222° [2660]; $n_D^{23} = 1.5155$ [2660].

1-(4-Butoxy-2-hydroxyphenyl)-1-nonanone

[143286-92-4] $C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Obtained by reaction of butyl bromide with 1-(2,4-dihydroxyphenyl)-1-nonanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 33–34° [284].

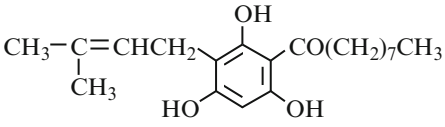
Oxime [143286-61-7] $C_{19}H_{31}NO_3$ mol. wt. 321.46

-Obtained by reaction of hydroxylamine hydrochloride with 1-(4-butoxy-2-hydroxyphenyl)-1-nonanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 43–45° [284].

1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-nonanone
2-Nonanoyl-4-(3-methylbuten-2-yl)phloroglucinol (**10**) [1026]

[85602-20-6] $C_{20}H_{30}O_4$ mol. wt. 334.46



Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and prenyl bromide to a solution of phlorononanophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

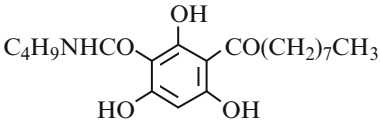
-Also prepared by adding prenyl bromide to a suspension of the sodium salt of phlorononanophenone in benzene, then the mixture obtained was refluxed for 3 h [1026].
-Also refer to: [3193].

^{13}C NMR [1026], IR [1026].

BIOLOGICAL ACTIVITY: Bactericidal and fungicidal activity of [3193].

1-[3-(Butylaminocarbonyl)-2,4,6-trihydroxyphenyl]-1-nonanone

$C_{20}H_{31}NO_5$ mol. wt. 365.47

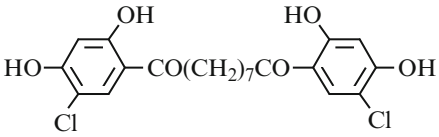


Syntheses
-Refer to: [3034, 3407].
m.p. 121–122° [3407].

BIOLOGICAL ACTIVITY: Cytotoxicity [3034]; Inhibition of Epstein-Barr virus early antigen activation [3034].

1,9-Bis(5-chloro-2,4-dihydroxyphenyl)-1,9-nonanedione

[26086-82-8] $C_{21}H_{22}Cl_2O_6$ mol. wt. 441.31



Syntheses
-Obtained by reaction of azelaic acid dichloride with 4-chlororesorcinol in the presence of aluminium chloride [591].
-Also refer to: [590].

m.p. 157° [590, 591]; IR [590].

Dioxime [37166-91-9] $C_{21}H_{24}Cl_2N_2O_6$ mol. wt. 471.34

m.p. 165–166° [590].

Tetramethyl ether [26086-85-1] $C_{25}H_{30}Cl_2O_6$ mol. wt. 497.42

-Obtained by reaction of azelaic acid dichloride with 4-chlororesorcinol dimethyl ether in the presence of aluminium chloride [591].
-Also refer to: [590].

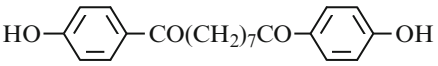
m.p. 147° [590, 591]; IR [590].

Dioxime of the tetramethyl ether [37166-94-2] $C_{25}H_{32}Cl_2N_2O_6$ mol. wt. 527.45

m.p. 140° [590].

1,9-Bis(4-hydroxyphenyl)-1,9-nonanedione

[2533-62-2] $C_{21}H_{24}O_4$ mol. wt. 340.42



Syntheses
-Obtained by reaction of azelaic acid dichloride (azeloyl chloride) with phenol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

-Also refer to: [1337].

rectangular plates [585]; m.p. 146.5–147° [1337], 142° [585].

Di-2,4-dinitrophenylhydrazone [2533-60-0] $C_{33}H_{32}N_8O_{10}$ mol. wt. 700.67

m.p. 240° [585].

Diacetate [2533-61-1] $C_{25}H_{28}O_6$ mol. wt. 424.49

m.p. 100.5–102° [1337].

Dimethyl ether [2525-89-5] $C_{23}H_{28}O_4$ mol. wt. 368.47

-Obtained by reaction of azelaic acid dichloride with anisole in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

m.p. 99° [585].

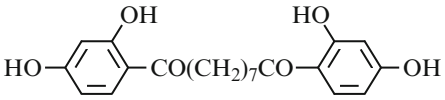
Di-2,4-dinitrophenylhydrazone of the dimethyl ether

[24336-93-4] $C_{35}H_{36}N_8O_{10}$ mol. wt. 728.72

m.p. 130° [585].

1,9-Bis(2,4-dihydroxyphenyl)-1,9-nonanedione

[7640-25-7] $C_{21}H_{24}O_6$ mol. wt. 372.42



Syntheses

-Obtained by adding resorcinol into the dinitrile of azelaic acid and hydrogen chloride in ethyl ether in the presence of zinc chloride.

Then, the diketimine dichloride obtained was hydrolyzed by boiling water (79 %) [2674].

-Also obtained by reaction of azelaic acid with resorcinol in the presence of zinc chloride at 140° for 5 h (60 %) [445].

-Also obtained by reaction of azelaic acid dichloride with resorcinol in the presence of aluminium chloride [591].

-Also refer to: [445, 590, 1735, 2504].

yellow crystals [445];
m.p. 141–143° [445], 116° [590], 115° [591], 114° [2504, 2674];
N.B.: One of the reported melting points is obviously wrong.
IR [590], UV [2504].

N.B.: Apparently the m.p. 141° was erroneously overstated [2674]. This diketone obtained according to the method in [445] had a m.p. of 114°; a mixed m.p. with the diketone synthetized according to Hoesh, showed no depression [2674].

Dioxime [37166-86-2] $C_{21}H_{26}N_2O_6$ mol. wt. 402.44

m.p. 217° [590].

Di-2,4-dinitrophenylhydrazone [124141-66-8] $C_{33}H_{32}N_8O_{12}$ mol. wt. 732.66

m.p. 275° [2674].

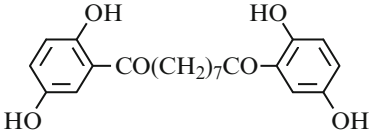
Tetramethyl ether [37166-89-5] $C_{25}H_{32}O_6$ mol. wt. 428.53

-Refer to: [590].

m.p. 96° [590]; IR [590].

1,9-Bis(2,5-dihydroxyphenyl)-1,9-nonanedione

$C_{21}H_{24}O_6$ mol. wt. 372.42



Synthesis

-Refer to: [1575].

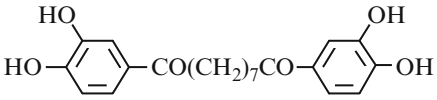
Tetramethyl ether [10365-25-0]
$C_{25}H_{32}O_6$ mol. wt. 428.53

-Obtained by reaction of azelaic acid dichloride (1 mol) with hydroquinone dimethyl ether (2.5 mol) in the presence of aluminium chloride (1 mol) (73 %) [1575].

m.p. 42° [1575].

1,9-Bis(3,4-dihydroxyphenyl)-1,9-nonanedione

$C_{21}H_{24}O_6$ mol. wt. 372.42



Synthesis
-Refer to: [1014].
Tetramethyl ether [50766-17-1]
$C_{25}H_{32}O_6$ mol. wt. 428.53

-Obtained by reaction of azelaic acid dichloride with pyrocatechol dimethyl ether in the presence of aluminium chloride [591].
-Also obtained by hydrogenating of its oxime in acetic acid in the presence of 10 % Pd/C in a Parr apparatus at r.t. and 45–50 psig for 12–36 h (66 %) [1014].
-Also refer to: [1012, 2342, 3364].

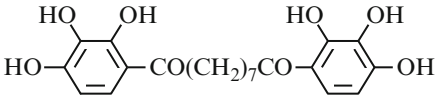
m.p. 102–103° [3059], 102° [591], 100–101° [3363], 98–100° [1014];
^{1}H NMR [2342], ^{13}C NMR [2342], IR [3364].

Dioxime of the tetramethyl ether [50766-31-9] $C_{25}H_{34}N_2O_6$ mol. wt. 458.56

m.p. 111–113° [1012], 108–110° [1014].

1,9-Bis(2,3,4-trihydroxyphenyl)-1,9-nonanedione

$C_{21}H_{24}O_8$ mol. wt. 404.41



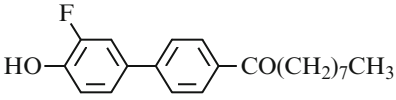
Synthesis
-Refer to: [1575].
Hexamethyl ether [10475-18-0]
$C_{27}H_{36}O_8$ mol. wt. 488.58

-Obtained by reaction of azelaic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride [591].
-Also obtained by reaction of dimethyl sulfate with 1,9-bis(2-hydroxy-3,4-dimethoxyphenyl)-1,9-nonanedione the presence of 30 % sodium hydroxide (65–90 %) [1574].
-Also refer to: [1575].

m.p. 117° [591], 74° [1574, 1575].
N.B.: One the reported melting point is obviously wrong.

1-(3′-Fluoro-4′-hydroxy[1,1′-biphenyl]-4-yl)-nonanone

$C_{21}H_{25}FO_2$ mol. wt. 328.43



Synthesis
-Refer to: [2107].

3-Methylpentyl ether (S) [112780-51-5] $C_{27}H_{37}FO_2$ mol. wt. 413.26

USE: Liq.-crystal compns. contg., for display devices [2107].

4-Methylhexyl ether (S) [112815-87-9] $C_{28}H_{39}FO_2$ mol. wt. 426.62

USE: Liq.-crystal compns. contg., for display devices [2107].

5-Methylheptyl ether (S) [112780-52-6] $C_{29}H_{41}FO_2$ mol. wt. 440.64

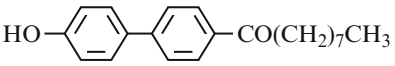
USE: Liq.-crystal compns. contg., for display devices [2107].

6-Methyloctyl ether (S) [112780-53-7] $C_{30}H_{43}FO_2$ mol. wt. 454.67

USE: Liq.-crystal compns. contg., for display devices [2107].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-nonanone

[121586-48-9] $C_{21}H_{26}O_2$ mol. wt. 310.44



Syntheses
-Refer to: [69, 1233, 1647, 1923].

Acetate [121586-49-0] $C_{23}H_{28}O_3$ mol. wt. 352.47

-Refer to: [1647].

Various ethers (11)

-Preparations and liquid crystalline properties of, [847].

Methyl ether [56116-81-5] $C_{22}H_{28}O_2$ mol. wt. 324.46

-Also refer to: [1923].

Ethyl ether [56116-90-6] $C_{23}H_{30}O_2$ mol. wt. 338.49

Propyl ether [56116-98-4] $C_{24}H_{32}O_2$ mol. wt. 352.52

Butyl ether [56117-06-7] $C_{25}H_{34}O_2$ mol. wt. 366.54

Pentyl ether [56117-15-8] $C_{26}H_{36}O_2$ mol. wt. 380.57

Hexyl ether [56117-24-9] $C_{27}H_{38}O_2$ mol. wt. 394.60

-Also refer to: [1233] (Japanese patent).

Heptyl ether [56189-90-3] $C_{28}H_{40}O_2$ mol. wt. 408.62

Octyl ether [56117-41-0] $C_{29}H_{42}O_2$ mol. wt. 422.65

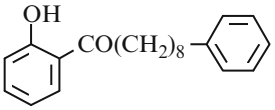
Nonyl ether [56117-50-1] $C_{30}H_{44}O_2$ mol. wt. 436.68

Decyl ether [56117-59-0] $C_{31}H_{46}O_2$ mol. wt. 450.71

Dodecyl ether [56117-68-1] $C_{33}H_{50}O_2$ mol. wt. 478.76

1-(2-Hydroxyphenyl)-9-phenyl-1-nonanone

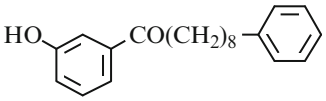
$C_{21}H_{26}O_2$ mol. wt. 310.44



Synthesis
-Refer to: [1368].
m.p. 47–48° [1368]; ^{1}H NMR [1368], IR [1368], MS [1368].

1-(3-Hydroxyphenyl)-9-phenyl-1-nonanone

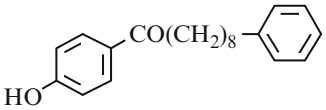
$C_{21}H_{26}O_2$ mol. wt. 310.44



Synthesis
-Refer to: [1368].
m.p. 79–81° [1368]; ^{1}H NMR [1368], MS [1368].

1-(4-Hydroxyphenyl)-9-phenyl-1-nonanone

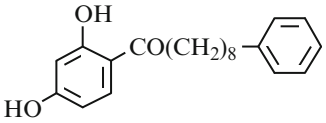
$C_{21}H_{26}O_2$ mol. wt. 310.44



Synthesis
-Refer to: [1368].
m.p. 45–47° [1368]; ^{1}H NMR [1368], IR [1368], MS [1368].

1-(2,4-Dihydroxyphenyl)-9-phenyl-1-nonanone

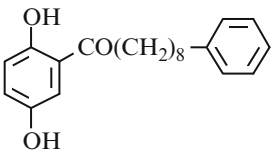
$C_{21}H_{26}O_3$ mol. wt. 326.44



Synthesis
-Refer to: [1368].
m.p. 49–50° [1368]; ^{1}H NMR [1368], IR [1368], MS [1368].

1-(2,5-Dihydroxyphenyl)-9-phenyl-1-nonanone

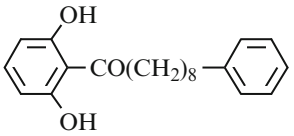
$C_{21}H_{26}O_3$ mol. wt. 326.44



Synthesis
-Refer to: [1368].
m.p. 76–77° [1368]; ^{1}H NMR [1368], IR [1368], MS [1368].

1-(2,6-Dihydroxyphenyl)-9-phenyl-1-nonanone
(Malabaricone A)

[63335-23-9] $C_{21}H_{26}O_3$ mol. wt. 326.44



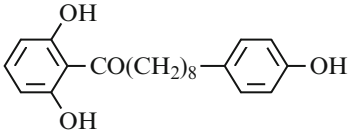
Isolation from natural sources
-From stem bark of *Myristica dactyloides* (Myristicaceae) [1786].
-From seed kernel of *Myristica dactyloides* (Myristicaceae) [719].

-From the fruit rind of *Myristica malabarica* (Myristicaceae) [2528].

bright yellow crystals [1786]; crystals [719];
m.p. 81–82° [2528], 80–82° [719], 80–81° [1786];
^{1}H NMR [2528], ^{13}C NMR [1786, 2528], IR [2528],
UV [2528], MS [2528].

1-(2,6-Dihydroxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone
(Malabaricone B)

[63335-24-0] $C_{21}H_{26}O_4$ mol. wt. 342.44



Isolation from natural sources
-From stem bark of Myristica dactyloides (Myristicaceae) [1786].
-From seed kernel of *Myristica dactyloides* (Myristicaceae) [719].

-From the fruit rind of *Myristica malabarica* (Myristicaceae) [2528].

pale yellow crystals [719];
m.p. 105–106° [1786], 102° [2528], 100–102° [719];
^{1}H NMR [2528], ^{13}C NMR [1786], IR [2528], UV [2528],
MS [2528].

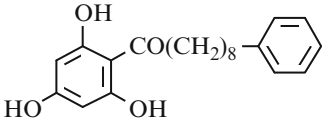
Trimethyl ether [114226-21-0] $C_{24}H_{32}O_4$ mol. wt. 384.52

-Obtained by treatment of 1-(2-hydroxy-6-methoxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone or 1-(2,6-dihydroxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone with diazomethane in ethyl ether [1786].

^{1}H NMR [1786], IR [1786], MS [1786].

1-(2,4,6-Trihydroxyphenyl)-9-phenyl-1-nonanone

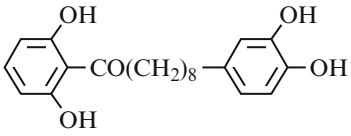
$C_{21}H_{26}O_4$ mol. wt. 342.44



Synthesis
-Refer to: [2489].
m.p. 71–72° [2489]; ^{1}H NMR [2489], IR [2489],
UV [2489], MS [2489].

1-(2,6-Dihydroxyphenyl)-9-(3,4-dihydroxyphenyl)-1-nonanone
(Malabaricone C)

[63335-25-1] $C_{21}H_{26}O_5$ mol. wt. 358.43



Isolation from natural sources
-From mace, aril of *Myristica fragrans* HOUTT (Myristicaceae) [2231].
-From seed kernel of *Myristica dactyloides* (Myristicaceae) [719].

-From the fruit rind of *Myristica malabarica* (Myristicaceae) [2528].

pale yellow prisms [2231]; yellow crystals [719];
pale yellow crystals [2528];
m.p. 123–124° [2231, 2528], 122–124° [719];
^{1}H NMR [2231, 2528], ^{13}C NMR [2231, 2528], IR [2231, 2528], UV [2231, 2528], MS [2231, 2528]; TLC [2231].

BIOLOGICAL ACTIVITY: Nematocidal [2231].

Tetramethyl ether $C_{25}H_{34}O_5$ mol. wt. 414.54

^{1}H NMR [1308], IR [1308], MS [1308].

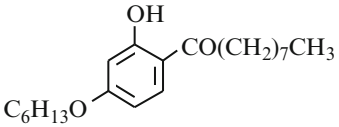
Tetraacetate $C_{29}H_{34}O_9$ mol. wt. 526.58

-Obtained by acetylation of malabaricone C with acetic anhydride in the presence of pyridine [2231].

oil [2231]; ^{1}H NMR [2231], MS [2231].

1-(4-Hexyloxy-2-hydroxyphenyl)-1-nonanone

[143286-93-5] $C_{21}H_{34}O_3$ mol. wt. 334.50



Synthesis
-Obtained by reaction of hexyl bromide with 1-(2,4-dihydroxyphenyl)-1-nonanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 38–40° [284].

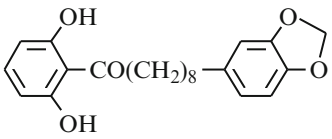
Oxime [143286-62-8] $C_{21}H_{35}NO_3$ mol. wt. 349.51

-Obtained by reaction of hydroxylamine hydrochloride with 1-(2,4-hydroxyphenyl)-1-nonanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 44–48° [284]; ^{1}H NMR [284].

9-(1,3-Benzodioxol-5-yl)-1-(2,6-dihydroxyphenyl)-1-nonanone
(Malabaricone D)

[63335-26-2] $C_{22}H_{26}O_5$ mol. wt. 370.45



Isolation from natural sources
-From stem bark of Myristica dactyloides (Myristicaceae) [1786].
-From seed kernel of *Myristica dactyloides* (Myristicaceae) [719].

-From the fruit rind of *Myristica malabarica* (Myristicaceae) [2528].

pale yellow crystals [719, 1786];
m.p. 90–91° [2528], 89–91° [719], 86–87° [1786];
^{1}H NMR [2528], ^{13}C NMR [1786], IR [2528], UV [2528], MS [2528].

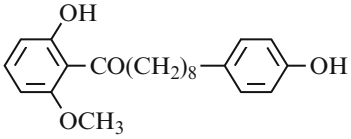
Dimethyl ether [114226-19-6] $C_{24}H_{30}O_5$ mol. wt. 398.50

-Obtained by treatment of the title ketone with diazomethane in ethyl ether [1786].

^{1}H NMR [1786], IR [1786], MS [1786].

1-(2-Hydroxy-6-methoxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone

[114226-26-5] $C_{22}H_{28}O_4$ mol. wt. 356.46

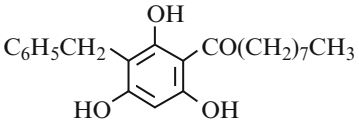


Isolation from natural sources
-From stem bark of Myristica dactyloides (Myristicaceae) [1786].
pale yellow crystals [1786];
m.p. 65–66° [1786];

^{1}H NMR [1786], ^{13}C NMR [1786], IR [1786], MS [1786].

1-[2,4,6-Trihydroxy-3-(phenylmethyl)phenyl]-1-nonanone
2-Nonanoyl-4-benzylphloroglucinol (**24**) [1026]

[85602-33-1] $C_{22}H_{28}O_4$ mol. wt. 356.46



Syntheses
-Obtained by adding cuprous chloride, a saturated aqueous solution of sodium carbonate and benzyl chloride to a solution of phlorononanophenone in ethyl ether at r.t., then to keep the mixture for 12 h at this temperature [1026].

-Also obtained by adding benzyl chloride to a two-phase mixture consisting of phlorononanophenone in diethyl ether and saturated aqueous sodium carbonate. A catalytic amount of CuCl was added and the mixture was stirred or shaken vigorously for 3 h at r.t. (48 %) [838].

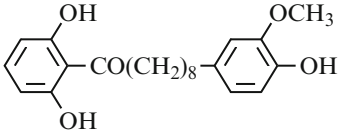
-Also obtained by reaction of benzyl chloride with phlorononanophenone in an alkaline two-phase (aqueous-ether) system and catalyzed by CuCl [838, 3193].
-Also refer to: [839].

m.p. 131–132° [838];
^{1}H NMR [1026], ^{13}C NMR [838, 1026],
IR [838, 1026], MS [838].

BIOLOGICAL ACTIVITY: Bactericidal, and fungicidal [1026, 3193].

1-(2,6-Dihydroxyphenyl)-9-(4-hydroxy-3-methoxyphenyl)-1-nonanone

[113201-69-7] $C_{22}H_{28}O_5$ mol. wt. 372.46

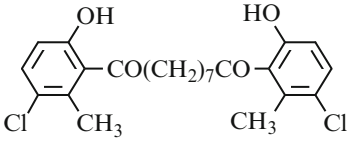


Isolation from natural sources
-From seed kernel of *Myristica dactyloides* (Myristicaceae) [719].
White needles [719];
m.p. 109–111° [719];

^{1}H NMR [719], ^{13}C NMR [719], IR [719], UV [719], MS [719].

1,9-Bis(3-chloro-6-hydroxy-2-methylphenyl)-1,9-nonanedione

$C_{23}H_{26}Cl_2O_4$ mol. wt. 437.36



Synthesis
-Obtained by reaction of azelaic acid dichloride (azeloyl chloride) with 4-chloro-3-methylphenol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

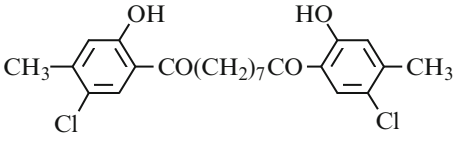
m.p. 105° [585].

Di-2,4-dinitrophenylhydrazone $C_{35}H_{34}Cl_2N_8O_{10}$ mol. wt. 797.61

m.p. 200° [585].

1,9-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,9-nonanedione

[25715-26-8] $C_{23}H_{26}Cl_2O_4$ mol. wt. 437.36



Synthesis
-Obtained by reaction of azelaic acid dichloride (azeloyl chloride) with 4-chloro-3-methylphenol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

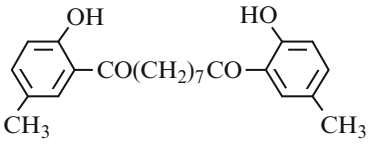
m.p. 105° [585].

Di-2,4-dinitrophenylhydrazone [25715-27-9] $C_{35}H_{34}Cl_2N_8O_{10}$ mol. wt. 797.61

m.p. 200° [585].

1,9-Bis(2-hydroxy-5-methylphenyl)-1,9-nonanedione

[113796-20-6] $C_{23}H_{28}O_4$ mol. wt. 368.47



Syntheses

-Obtained by Fries rearrangement of di (4-methyl-phenyl) azelate with aluminium chloride in refluxing chlorobenzene for 6 h (58 %) [3107].

-Also obtained by reaction of azelaic acid dichloride (azeloyl chloride) with p-cresol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

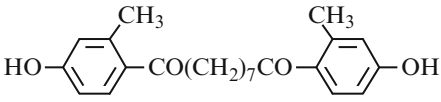
m.p. 79–80° [3107], 71° [585]; IR [3107].

Di-2,4-dinitrophenylhydrazone $C_{35}H_{36}N_8O_{10}$ mol. wt. 728.72

m.p. 84° [585].

1,9-Bis(4-hydroxy-2-methylphenyl)-1,9-nonanedione

[24336-97-8] $C_{23}H_{28}O_4$ mol. wt. 368.47



Synthesis

-Obtained by reaction of azelaic acid dichloride (azeloyl chloride) with m-cresol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

m.p. 100° [585].

Di-2,4-dinitrophenylhydrazone [24339-82-0] $C_{35}H_{36}N_8O_{10}$ mol. wt. 728.72

m.p. 250° [585].

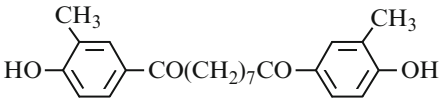
Dimethyl ether $C_{25}H_{32}O_4$ mol. wt. 396.53

-Obtained by methylation of 1,9-Bis(4-hydroxy-2-methylphenyl)-1,9-nonanedione [585].

m.p. 120° [585].

1,9-Bis(4-hydroxy-3-methylphenyl)-1,9-nonanedione

[24336-94-5] $C_{23}H_{28}O_4$ mol. wt. 368.47



Synthesis

-Obtained by reaction of azelaic acid dichloride (azeloyl chloride) with o-cresol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

needles [585]; m.p. 139° [585].

Di-2,4-dinitrophenylhydrazone $C_{35}H_{36}N_8O_{10}$ mol. wt. 728.72

m.p. 210° [585].

Dimethyl ether [24336-96-7] $C_{25}H_{32}O_4$ mol. wt. 396.53

-Obtained by reaction of azelaic acid dichloride with o-cresol methyl ether in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

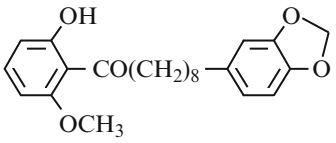
prismatic rods [585]; m.p. 140° [585].

Di-2,4-dinitrophenylhydrazone of the dimethyl ether $C_{37}H_{40}N_8O_{10}$ mol. wt. 756.77

m.p. 200° [585].

9-(1,3-Benzodioxol-5-yl)-1-(2-hydroxy-6-methoxyphenyl)-1-nonanone

[114226-25-4] $C_{23}H_{28}O_5$ mol. wt. 384.47



Isolation from natural sources

-From stem bark of Myristica dactyloides (Myristicaceae) [1786].

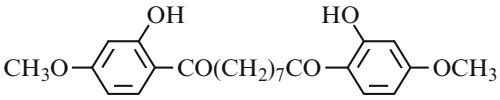
Synthesis

-Obtained by treatment of 1-(2,6-dihydroxyphenyl)-9-(3,4-dihydroxyphenyl)-1-nonanone with diazomethane in ethyl ether [1786].

m.p. 51–52° [1786]; ^{1}H NMR [1786], ^{13}C NMR [1786], IR [1786], MS [1786].

1,9-Bis(2-hydroxy-4-methoxyphenyl)-1,9-nonanedione

[26086-78-2] $C_{23}H_{28}O_6$ mol. wt. 400.47



Syntheses

-Obtained by reaction of azelaic acid dichloride with 3-methoxyphenol in the presence of aluminium chloride [591].

-Also refer to: [590].

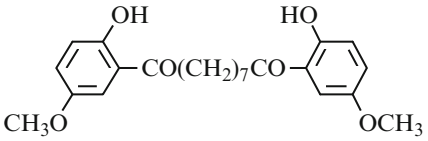
m.p. 89° [590, 591].

Di-2,4-dinitrophenylhydrazone [37402-33-8] $C_{35}H_{36}N_8O_{12}$ mol. wt. 760.72

m.p. 151° [590].

1,9-Bis(2-hydroxy-5-methoxyphenyl)-1,9-nonanedione

[10365-30-7] $C_{23}H_{28}O_6$ mol. wt. 400.47



Synthesis

-Obtained by reaction of azelaic acid dichloride with p-dimethoxybenzene in the presence of aluminium chloride [1575].

m.p. 73° [1575].

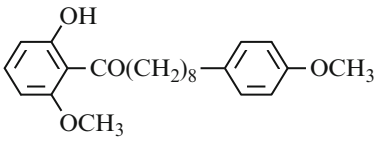
Diacetate [10365-36-3] $C_{27}H_{32}O_8$ mol. wt. 484.55

-Obtained by reaction of acetic anhydride (4 vol) with the title ketone in the presence of 1–2 drops concentrated sulfuric acid, the mixture warmed 5 min [1575].

m.p. 82° [1575].

1-(2-Hydroxy-6-methoxyphenyl)-9-(4-methoxyphenyl)-1-nonanone

[114226-20-9] $C_{23}H_{30}O_4$ mol. wt. 370.49



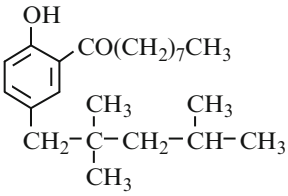
Synthesis

-Obtained by treatment of 1-(2-hydroxy-6-methoxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone or 1-(2,6-dihydroxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone with diazomethane in ethyl ether [1786].

^{1}H NMR [1786], IR [1786], MS [1786].

1-[2-Hydroxy-5-(2,2,4-trimethylpentyl)phenyl]-1-nonanone

$C_{23}H_{38}O_2$ mol. wt. 346.50

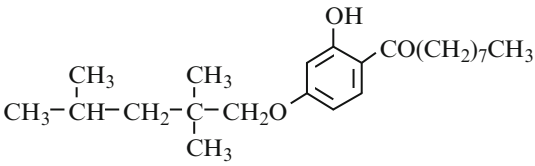


Synthesis
-Refer to: [1835].
Oxime [57073-45-7]
$C_{23}H_{39}NO_2$ mol. wt. 361.56

USE: Hydrogen bonding, spectra in relation to, [1835].

1-[2-Hydroxy-4-[(2,2,4-trimethylpentyl)oxy]phenyl]-1-nonanone

$C_{23}H_{38}O_3$ mol. wt. 362.50

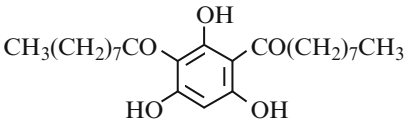


Synthesis
-Refer to: [1835].
Oxime [57073-43-5]
$C_{23}H_{39}NO_3$ mol. wt. 377.57

USE: Hydrogen bonding, spectra in relation to, [1835].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-nonanone

[3118-42-1] $C_{24}H_{38}O_5$ mol. wt. 406.56



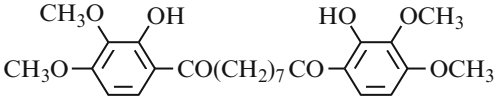
Syntheses
-Obtained by reaction of nonanoic anhydride with phloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].
-Also refer to: [457, 644, 2911].

m.p. 84–87° [457, 2911].

BIOLOGICAL ACTIVITY: Antiviral activity towards the replication of vesicular stomatitis virus in HEL cell cultures [644]; Anthelmintic [457].

1,9-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,9-nonanedione

[10483-68-8] $C_{25}H_{32}O_8$ mol. wt. 460.52



Syntheses
-Obtained by reaction of azelaic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride in tetrachloroethane [1574].

-Also refer to: [590, 1575].

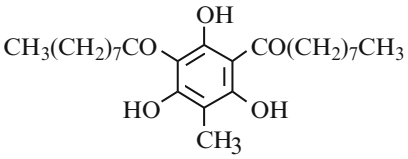
m.p. 117° [590]; 115° [1574, 1575].

Di-2,4-dinitrophenylhydrazone [37166-96-4] $C_{37}H_{40}N_8O_{14}$ mol. wt. 820.77

m.p. 175° [590].

1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-nonanone

[2999-12-4] $C_{25}H_{40}O_5$ mol. wt. 420.59



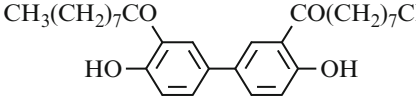
Syntheses
-Obtained by reaction of nonanoic anhydride with 2-methylphloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].
-Also refer to: [457, 600, 2911] .

m.p. 100–102° [457, 2911].

BIOLOGICAL ACTIVITY: For treatment of immune dysfunction associated with human immuno deficiency virus infection [600]; Anthelmintic [457].

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-nonanone

[104295-23-0] $C_{30}H_{42}O_4$ mol. wt. 466.66



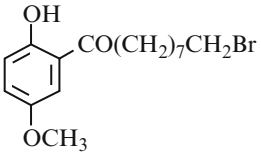
Synthesis
-Preparation by Fries rearrangement of 4,4′-biphenyl dipelargonate with aluminium chloride in refluxing chlorobenzene for 24 h (72 %) [2377].

m.p. 72–73° [2377]; IR [2377].

2 Aromatic Hydroxyketone Derived from 9-Bromononanoic Acid

9-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-nonanone

[173055-40-8] $C_{16}H_{23}BrO_3$ mol. wt. 343.26



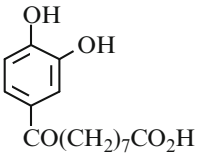
Synthesis
-Refer to: [2623].

3 Aromatic Hydroxyketones Derived from 9-Oxononanoic Acids

3.1 Unsubstituted Hydroxyketones

9-(3,4-Dihydroxyphenyl)-9-oxo-1-nonanoic acid

$C_{15}H_{20}O_5$ mol. wt. 280.32



Synthesis
-Refer to: [1013].

Dimethyl ether [57640-96-7]
$C_{17}H_{24}O_5$ mol. wt. 308.37

-Obtained by heating of its ethyl ester below with 10 % aqueous NaOH on the steam bath for 1.5 h (79 %) [1013].
-Also refer to: [3363, 3364].

m.p. 93–94° [1013], 92–93.5° [3363]; IR [1013, 3364].

2,4-Dinitrophenylhydrazone of the dimethyl ether $C_{23}H_{28}N_4O_8$ mol. wt. 488.50

m.p. 100–102° [3363].

Ethyl ester of the dimethyl ether [57641-20-0] $C_{19}H_{28}O_5$ mol. wt. 336.43

-Obtained by reaction of 9-chloro-9-oxononanoic acid ethyl ester with 1,2-dimethoxybenzene in the presence of aluminium chloride in 1,1,2,2-tetrachloroethane first at 0–3° for 2.5 h, then overnight to 2° (68 %) [1013].

$b.p._{\cdot 0.1}$ 195–197° [1013]; IR [1013]. GLC [1013].

Methyl ester of the methylenedioxy [72674-91-0] $C_{17}H_{22}O_5$ mol. wt. 306.36

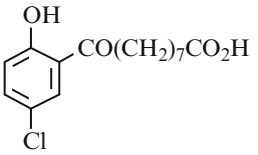
-Obtained by reaction of azelayl chloride monomethyl ester with methylene-1,2-dioxybenzene in the presence of stannic chloride in 1,1,2,2-tetrachloroethane for 15 h at r.t. (47 %) [2333].

m.p. 52–53° [2333];
^{1}H NMR [2333], IR [2333], UV [2333], MS [2333].

3.2 Substituted Hydroxyketones

9-(5-Chloro-2-hydroxyphenyl)-9-oxo-1-nonanoic acid

[24381-67-7] $C_{15}H_{19}ClO_4$ mol. wt. 298.77



Synthesis
-Obtained by reaction of azelaic acid dichloride (azeloyl chloride) with p-chlorophenol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

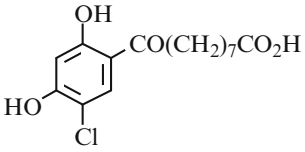
m.p. 85° [585].

2,4-Dinitrophenylhydrazone [24339-87-5] $C_{21}H_{23}ClN_4O_7$ mol. wt. 478.89

m.p. 150° [585].

9-(5-Chloro-2,4-dihydroxyphenyl)-9-oxo-1-nonanoic acid

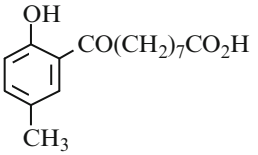
[37166-92-0] $C_{15}H_{19}ClO_5$ mol. wt. 314.77



Synthesis
-Refer to: [590].
m.p. 126° [590].

9-(2-Hydroxy-5-methylphenyl)-9-oxo-1-nonanoic acid

$C_{16}H_{22}O_4$ mol. wt. 278.35



Synthesis
-Obtained by reaction of azelaic acid dichloride (azeloyl chloride) with p-cresol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

m.p. 80° [585].

2,4-Dinitrophenylhydrazone $C_{22}H_{26}N_4O_7$ mol. wt. 458.47

m.p. 110° [585].

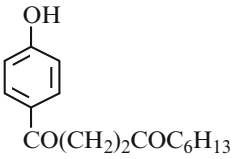
Chapter 8
Decanones

1 Aromatic Hydroxyketones Derived from Decanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(4-Hydroxyphenyl)-1,4-decanedione

$C_{16}H_{22}O_3$ mol. wt. 262.35



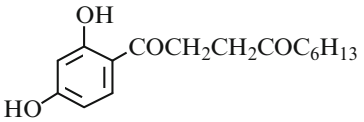
Synthesis
-Refer to: [2953].
Methyl ether [67756-15-4]
$C_{17}H_{24}O_3$ mol. wt. 276.38

-Obtained from heptanal and 1-(4-methoxyphenyl)-2-propen-1-one (60 %) [2953].

b.p.$_{0.1}$ 170° [2953];
m.p. 48° [2953];
^{1}H NMR [2953], IR [2953].

1-(2,4-Dihydroxyphenyl)-1,4-decanedione

$C_{16}H_{22}O_4$ mol. wt. 278.35



Synthesis
-Refer to: [2953].
Dimethyl ether [67756-21-2]
$C_{18}H_{26}O_4$ mol. wt. 306.40

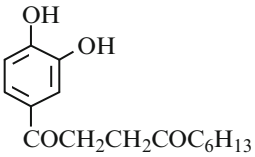
-Obtained from heptanal and 1-(2,4-dimethoxyphenyl)-2-propen-1-one (60 %) [2953].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_8

b.p.$_{0.4}$ 187° [2953];
m.p. 44–47° [2953],
^{1}H NMR [2953], IR [2953].

1-(3,4-Dihydroxyphenyl)-1,4-decanedione

$C_{16}H_{22}O_4$ mol. wt. 278.35



Synthesis
-Refer to: [2953].

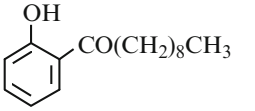
Dimethyl ether [67756-24-5]
$C_{18}H_{26}O_4$ mol. wt. 306.40

-Obtained from heptanal and 1-(3,4-dimethoxyphenyl)-2-propen-1-one (57 %) [2953].

b.p.$_{0.06}$ 175° [2953]; m.p. 55° [2953],
^{1}H NMR [2953], IR [2953].

1-(2-Hydroxyphenyl)-1-decanone

[14353-76-5] $C_{16}H_{24}O_2$ mol. wt. 248.37



Syntheses
-Obtained by reaction of decanoyl chloride with phenol in the presence of aluminium chloride,
*in nitrobenzene at 70° for 3 h (21 %) [2549];
*in carbon disulfide at 47° for 5.5 h (44 %) [2549];
*in tetrachloroethane at 55–60° for 6 h [2669].
-Also obtained by Fries rearrangement of phenyl decanoate with aluminium chloride,
*in tetrachloroethane [3169];
*first in refluxing carbon disulfide for 2 h, then at 136–140° for 4 h, after solvent elimination (46.3 %) [13].
-Also refer to: [1985, 2035, 2658].

b.p.$_{0.3}$ 130–133° [2035], b.p.$_6$ 174° [13];
prisms [13]; m.p. 35–35.5° [2549], 35° [2669, 3169], 33.5–34.5° [13];
IR [13], UV [1996]; TLC [1994].

2,4-Dinitrophenylhydrazone $C_{22}H_{28}N_4O_5$ mol. wt. 428.49

m.p. 111–112° [2549], 111° [3169], 84–85° [524].

Oxime [439948-79-5] $C_{16}H_{25}NO_2$ mol. wt. 263.38

-Refer to: [2077].

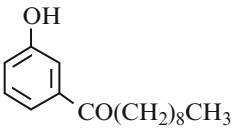
2,3-Epoxypropyl ether [18110-28-6] $C_{19}H_{28}O_3$ mol. wt. 304.43

-Obtained by reaction of epichlorohydrin with o-decanoylphenol (0.1 mol) in the presence of 30 % sodium hydroxide between 40 and 50° (61 %) [2669].

b.p.$_{0.5}$ 220–230° [2669].

1-(3-Hydroxyphenyl)-1-decanone

[63480-88-6] $C_{16}H_{24}O_2$ mol. wt. 248.37



Syntheses
-Refer to: [1984, 1985].
m.p. 30° [1984]; IR [1984].

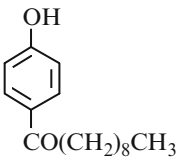
Methyl ether [63442-82-0] $C_{17}H_{26}O_2$ mol. wt. 262.39

-Refer to: [1984, 1985].

b.p.$_{15}$ 128–130° [1984]; IR [1984].

1-(4-Hydroxyphenyl)-1-decanone

[14353-77-6] $C_{16}H_{24}O_2$ mol. wt. 248.37



Syntheses
-Obtained by reaction of decanoyl chloride with phenol in the presence of aluminium chloride,
*in nitrobenzene at 70° for 3 h (74 %) [2549];
*in carbon disulfide at 47° for 5.5 h (52 %) [2549];
*in methylene chloride for 1 h at 0°, then at r.t. overnight (39–41 %) [114, 1977] or for 14 h at r.t. (14 %) [1910];
*in tetrachloroethane at 55–60° for 6 h [2669].
-Also obtained by Fries rearrangement of phenyl decanoate with aluminium chloride,
*at 110–120° for 1 h [3336];
*in tetrachloroethane [3169];
*in nitrobenzene (49 %) [2947];
*first in refluxing carbon disulfide for 2 h, then at 136–140° for 4 h, after solvent elimination (32.2 %) [13];
*in the presence of aluminium chloride in refluxing carbon disulfide for 5 h. Then, the mixture was kept at 80–90° for 2 h and at 140–150° for 1 h after solvent elimination [1222].
-Also obtained by Fries rearrangement of phenyl decanoate with boron trifluoride at 30–35° for 20 h (53.3 %) [1938].

-Also obtained by reaction of decanoic acid with phenol in the presence of boron trifluoride at 20–25° for 19.5 h (60 %) [142].
-Also refer to: [62, 1116, 1743, 2658, 3423].

b.p.$_{0.5}$ 160–200° [3336], b.p.$_{.6}$ 224° [13], b.p.$_{1}$ 225–228° [2947];
white solid [1910]; rhombic plates [3336]; short needles [13];
m.p. 67.2–67.8° [1910], 64–65° [3336], 63.5–64° [2549], 63–64° [1938], 63° [2669], 62.5–63.5° [142], 62–63° [13], 61–62° [3169], 60–61° [1977], 59° [1743];
^{1}H NMR [114, 1910], ^{13}C NMR [114, 1910],
IR [13, 1910, 1977], UV [1995], MS [1910];
TLC [1910, 1994]; GC [1910].

USE: Preparation of 2-hydroxy-3,5-dialkylbenzenesulfonate anionic surfactant for defoaming agent [3423]; Reactant in smectic C liquid crystal [1299].

BIOLOGICAL ACTIVITY: Inhibition of 17-β-hydroxysteroid dehydrogenase 3 [1910]; Antimicrobial [1743]; Antifungal [1743].

2,4-Dinitrophenylhydrazone [17744-45-5] $C_{22}H_{28}N_4O_5$ mol. wt. 428.49

m.p. 148–148.5° [2549], 148° [3169], 111–112° [2549].

iso-Nicotinylhydrazone [102701-26-8] $C_{22}H_{29}N_3O_2$ mol. wt. 367.49

m.p. 203° [520, 521].

USE: In chemotherapy of leprosy [520, 521].

Semicarbazone [14353-85-6] $C_{17}H_{27}N_3O_2$ mol. wt. 305.42

Refer to: [1743].

Semicarbazone dihydrate $C_{17}H_{27}N_3O_2$, 2 H_2O mol. wt. 341.46

m.p. 130° [1743].

Phosphate (93 %) [114]; ^{1}H NMR [114].

Methyl ether [101741-01-9] $C_{17}H_{26}O_2$ mol. wt. 262.39

-Obtained by acylation of anisole with decanoic acid,
*over a range of solid-acid catalysts under conventional heating and microwave stimulation [422];
*in the presence of a catalytic amount of p-toluenesulfonic acid and graphite for 3 h at 90° (92 %) [2709];

*on the surface of graphite in the presence of methanesulfonic acid at 80° for 20 min (90 %) [1369];
*in the presence of silica-supported phosphotungstic acid and Ce-exchanged zeolite catalysts for anisole acylation [1092].
-Also obtained by reaction of decanoic acid with anisole over three large pore zeolites-beta (BEA), faujasite (FAU) and mordenite (MOR) [3246].
-Also obtained by treatment of anisole with decanoic anhydride or decanoyl chloride in the presence of sulfated zirconia [867].
-Also refer to: [2016].

m.p. 49–50.5° [2016], 110° [2709];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [1369, 2709], IR [422, 1369, 2709].

iso-Nicotinylhydrazone of the methyl ether

[102753-19-5] $C_{23}H_{31}N_3O_2$ mol. wt. 381.52

m.p. 126° [520, 521].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{23}H_{30}N_4O_5$ mol. wt. 442.52

m.p. 114–115° [2016].

2-Acetoxyethyl ether [82944-57-8] $C_{20}H_{30}O_4$ mol. wt. 334.46

-Refer to: [1929].

2-Hydroxyethyl ether [82684-67-1] $C_{18}H_{28}O_3$ mol. wt. 292.42

-Refer to: [1929].

2-Chloroethyl ether [666836-96-0] $C_{18}H_{27}ClO_2$ mol. wt. 310.86

-Obtained by reaction of decanoyl chloride with 2-chloroethoxybenzene in the presence of aluminium chloride in carbon disulfide for 4 h at 50° (51 %) [476].

m.p. 74.5° [476].

N-Dimethylaminoethyl ether [666836-97-1] $C_{20}H_{33}NO_2$ mol. wt. 319.49

-Obtained by reaction of 4-(2-chloroethoxy)decanophenone with dimethylamine in a sealed tube for 2 h at 150° [476].

free base: b.p.$_{0.05}$ 199° [476]; m.p. 40–41° [476].
hydrochloride: m.p. 180° (88.5 %) [476].

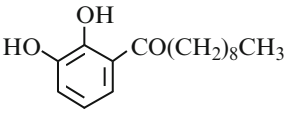
2,3-Epoxypropyl ether [18211-87-5] $C_{19}H_{28}O_3$ mol. wt. 304.43

-Obtained by reaction of epichlorohydrin (0.1 mol) with p-decanoylphenol (0.1 mol) in the presence of 30 % sodium hydroxide between 40 and 50° (53 %) [2669].

m.p. 112° [2669].

1-(2,3-Dihydroxyphenyl)-1-decanone

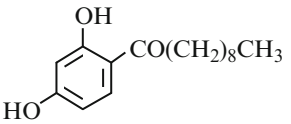
[7573-11-7] $C_{16}H_{24}O_3$ mol. wt. 264.36



Syntheses
-Refer to: [1228, 1229].
$b.p._{0.002}$ 130–140° [1228, 1229];
m.p. 53–54° [1228, 1229]; IR [1229], UV [1229].

1-(2,4-Dihydroxyphenyl)-1-decanone

[24313-95-9] $C_{16}H_{24}O_3$ mol. wt. 264.36



Syntheses
-Obtained by reaction of capric acid chloride with resorcinol in the presence of KU-2x8 cation-exchange resin [3145].
-Also obtained by reaction of decanoyl chloride with resorcinol (59 %) [3146] in the presence of aluminium chloride in 1,2-dichloroethane for 5 h at 65° [284].

-Also refer to: [76, 489, 490, 893, 1194, 1743, 2112, 2114, 2228, 2673, 2864, 3125].

$b.p._{.1}$ 180° [1743], $b.p._{2.5}$ 205–206° [3125], $b.p._{10}$ 240–245° [893];
m.p. 78° [2114], 74.2–75° [3125], 74–75° [3145], 69° [2673], 65° [1743];
IR [1194, 1195, 3145].

BIOLOGICAL ACTIVITY: Antimicrobial [1743]; Antifungal [1743, 2112, 2114]; Aldose reductase of eye lens inhibition by [2228]; Bactericidal action of, [76].

Hemihydrate $C_{16}H_{24}O_3$, 0.5 H_2O mol. wt. 273.37

m.p. 67–68° [3125].

2,4-Dinitrophenylhydrazone [95809-40-8] $C_{22}H_{28}N_4O_6$ mol. wt. 444.49

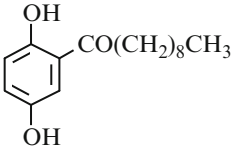
m.p. 153° [2673].

Dimethyl ether [430425-42-6] $C_{18}H_{28}O_3$ mol. wt. 292.42

-Obtained by reaction of decanoyl chloride with resorcinol dimethyl ether in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].

1-(2,5-Dihydroxyphenyl)-1-decanone

[7337-50-0] $C_{16}H_{24}O_3$ mol. wt. 264.36



Syntheses
-Refer to: [1743] (Japanese paper).
-Also refer to: [1691, 1950].
$b.p._{.2}$ 170–172° [1743]; m.p. 63° [1743].

BIOLOGICAL ACTIVITY: Antimicrobial [1743]; Antifungal [1743].

Dimethyl ether [49710-91-0] $C_{18}H_{28}O_3$ mol. wt. 292.42

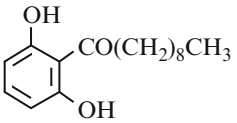
-Obtained by acylation of hydroquinone dimethyl ether in the presence of stannic chloride in benzene (30 %) [1040].
-Also obtained by reaction of decanoic acid chloride with hydroquinone dimethyl ether,
*in the presence of aluminium chloride in carbon disulfide first at 0°, kept overnight, heated to a boil [2874];
*in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].
-Also refer to: [1691].

$b.p._{.12}$ 230° [1040]; m.p. 38° [2874]; $n_D^{25} = 1.5075$ [1040].

USE: Radioprotective activity of, [1040].

1-(2,6-Dihydroxyphenyl)-1-decanone

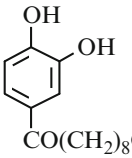
[185301-37-5] $C_{16}H_{24}O_3$ mol. wt. 264.36



Isolation from natural sources
-Of the andromeda lace bug *Stephanitis rhododendrii* [2334].
-In the wood of *Knema austrosiamensis* W. J. J. O. DeWilde (Myristaceae) [1133].

1-(3,4-Dihydroxyphenyl)-1-decanone

[2754-54-3] $C_{16}H_{24}O_3$ mol. wt. 264.36



Syntheses

-Obtained by Fries rearrangement of pyrocatechol decanoate with aluminium chloride in the presence of pyrocatechol at 135–140° for 5 h (15 %) [283].

-Also obtained by reaction of decanoic acid with catechol in the presence of boron trifluoride at 80° for 2 h (19 %) [2954].

-Also refer to: [1809].

b.p.$_{.2}$ 236–240° [283];
m.p. 102–104° [2954], 96–98° [283];
^{1}H NMR [283, 2954], ^{13}C NMR [2954], MS [2954].

BIOLOGICAL ACTIVITY: Protective agent against the lethal effects of X rays [1809].

Dimethyl ether [109558-46-5] $C_{18}H_{28}O_3$ mol. wt. 292.42

-Preparation by Friedel-Crafts acylation of veratrole [3056].
-Also obtained by reaction of decanoyl chloride with veratrole in the presence of zinc chloride in refluxing carbon disulfide,
*for 6 h and then left overnight (43 %) [2420];
*for 4 h and then left overnight (68 %) [2836].
-Also obtained by reaction of decanoyl chloride with veratrole in the presence of HY-zeolite. Before reaction, the zeolites were activated at 500° for 5 h in nitrogen flow [352].
-Also refer to: [2366, 2836, 3056].

white needles [2420, 2836];
b.p.$_{.2}$ 198–200° [2420], b.p.$_{.6}$ 205–208° [2836];
m.p. 62° [2420, 2836], 60–61° [3056].

2,4-Dinitrophenylhydrazone of the dimethyl ether

[113927-78-9] $C_{24}H_{32}N_4O_6$ mol. wt. 472.54

m.p. 90–91° [2420].

Semicarbazone of the dimethyl ether [102709-19-3] $C_{19}H_{31}N_3O_3$ mol. wt. 349.47

white prisms [2836]; m.p. 80° [2836].

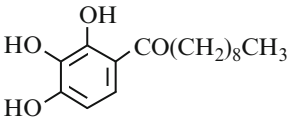
Dibenzyl ether $C_{30}H_{36}O_3$ mol. wt. 444.61

-Refer to: [2657].

m.p. 65° [2657].

1-(2,3,4-Trihydroxyphenyl)-1-decanone

[1154-72-9] $C_{16}H_{24}O_4$ mol. wt. 280.36



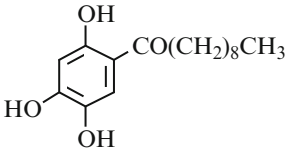
Syntheses
-Obtained by reaction of decanoic acid with pyrogallol in the presence of zinc chloride at 140–145° for 4 h (75–80 %) [506].
-Also refer to: [1101, 1810, 1883].

b.p.$_{13}$ 254–256° [506]; m.p. 78–79° [506].

BIOLOGICAL ACTIVITY: Protection against whole-body irradiation [1810]; Antitumor [1883]; Protection from O-poisoning [1101].

1-(2,4,5-Trihydroxyphenyl)-1-decanone

[108978-55-8] $C_{16}H_{24}O_4$ mol. wt. 280.36



Syntheses
-Obtained by reaction of decanoyl chloride with 1,2,4-trihydroxybenzene in the presence of aluminium chloride in nitrobenzene at r.t. several hrs, and heated 0.5 h at 65° [290].
-Also refer to: [1101, 1708].

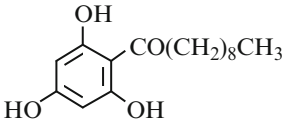
m.p. 108–111° [290].

USE: Antioxidant [1708]; Antioxidant in fats and oils [290]; Protection from O-poisoning [1101].

BIOLOGICAL ACTIVITY: Toxicity [1708].

1-(2,4,6-Trihydroxyphenyl)-1-decanone

[6048-89-1] $C_{16}H_{24}O_4$ mol. wt. 280.36



Syntheses
-Obtained by reaction of decanoyl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene and carbon disulfide mixture (46 %) [2113].
-Also obtained by reaction of caprinonitrile with phloroglucinol (Hoesch reaction) [1441].
-Preparation (23 %) [3202] using to the process [3201].
-Also refer to: [1441, 2111, 2433].

Isolation from natural sources

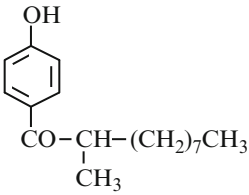
-In the wood of *Knema austrosiamensis* W. J. J. O. DeWilde (Myristaceae) [1133].
-From the Myristaceae family [3111].

white crystals [3202];
m.p. 133° [2113], 127° [3202], 109–110° [1441];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [3202], ^{13}C NMR [3202], IR [3202], UV [3202],
MS [3202]; TLC [3202].

BIOLOGICAL ACTIVITY: Antifungal [2111, 2113]; Antibiotic [3202]; Antibacterial [3202].

1-(4-Hydroxyphenyl)-2-methyl-1-decanone (*S*)

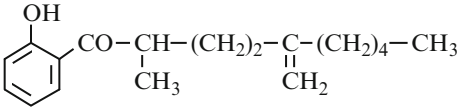
[120837-01-6] (+) $C_{17}H_{26}O_2$ mol. wt. 262.39



Syntheses
-Refer to: [1063, 1064, 1321].
Acetate (*S*) [152430-07-4]
$C_{19}H_{28}O_3$ mol. wt. 304.43
-Refer to: [1063, 1064].

1-(2-Hydroxyphenyl)-2-methyl-5-methylene-1-decanone

[526208-17-3] $C_{18}H_{26}O_2$ mol. wt. 274.40



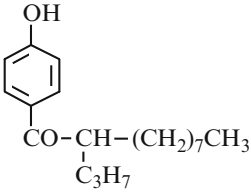
Syntheses
-Obtained by intermolecular hydroacylation between salicylaldehyde and 2-pentyl-1,5-hexadiene (6 equiv.) in the presence of $RhCl(PPh_3)_3$ (0.2 equiv.) in methylene chloride for 72 h at r.t. (53 %) [1435].

-Also refer to: [3066].

^{1}H NMR [1435].

1-(4-Hydroxyphenyl)-2-propyl-1-decanone (*S*)

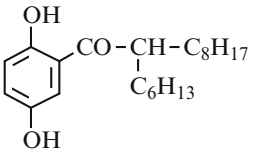
[120837-05-0] (+) $C_{19}H_{30}O_2$ mol. wt. 290.45



Syntheses
-Refer to: [1318, 1321].

1-(2,5-Dihydroxyphenyl)-2-hexyl-1-decanone

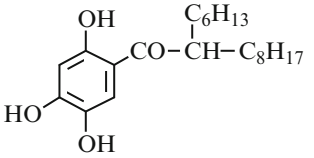
[295327-95-6] $C_{22}H_{36}O_3$ mol. wt. 348.53



Syntheses
-Refer to: [2352, 2717].

2-Hexyl-1-(2,4,5-trihydroxyphenyl)-1-decanone

[103449-10-1] $C_{22}H_{36}O_4$ mol. wt. 364.53

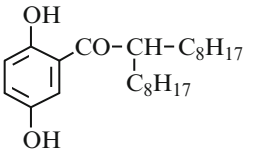


Synthesis
-Refer to: [2326].

USE: Colour photog. paper contg. antistaining agent from, [2326].

1-(2,5-Dihydroxyphenyl)-2-octyl-1-decanone

[375172-14-6] $C_{24}H_{40}O_3$ mol. wt. 376.58

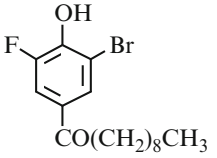


Synthesis
-Refer to: [2352].

1.2 Substituted Hydroxyketones

1-(3-Bromo-5-fluoro-4-hydroxyphenyl)-1-decanone

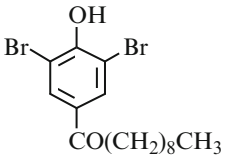
[402-81-3] $C_{16}H_{22}BrFO_2$ mol. wt. 345.25



Synthesis
-Obtained by reaction of bromine with 3-fluoro-4-hydroxy-decanophenone in acetic acid [516].
m.p. 68° [516].

1-(3,5-Dibromo-4-hydroxyphenyl)-1-decanone

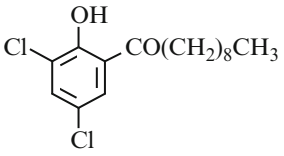
[20683-53-8] $C_{16}H_{22}Br_2O_2$ mol. wt. 406.16



Synthesis
-Obtained by reaction of bromine with 4-hydroxydecanophenone in aqueous acetic acid [516].
m.p. 54° [516].

1-(3,5-Dichloro-2-hydroxyphenyl)-1-decanone

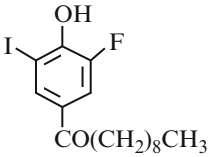
$C_{16}H_{22}Cl_2O_2$ mol. wt. 317.25



Synthesis
-Obtained by Fries rearrangement of 2,4-dichlorophenyl caprate with aluminium chloride [3170].
m.p. 53.5° [3170]; UV [3170].

1-(3-Fluoro-4-hydroxy-5-iodophenyl)-1-decanone

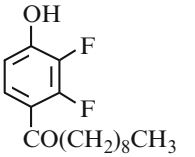
[402-82-4] $C_{16}H_{22}FIO_2$ mol. wt. 392.25



Synthesis
-Obtained by reaction of iodine with 3-fluoro-4-hydroxydecanophenone in ethanol in the presence of yellow mercuric oxide [519].
fine colourless needles [519];
m.p. 73° [519].

1-(2,3-Difluoro-4-hydroxyphenyl)-1-decanone

[144292-58-0] $C_{16}H_{22}F_2O_2$ mol. wt. 284.35

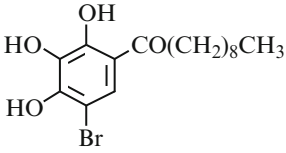


Syntheses
-Refer to: [2720, 2975].

Benzyl ether [144292-57-9]
$C_{23}H_{28}F_2O_2$ mol. wt. 374.47
-Refer to: [2975].

1-(5-Bromo-2,3,4-trihydroxyphenyl)-1-decanone

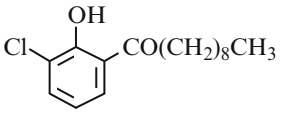
$C_{16}H_{23}BrO_4$ mol. wt. 359.26



Synthesis
-Obtained by reaction of bromine with 4-decanoylpyrogallol in acetic acid [506].
m.p. 86–87° [506].

1-(3-Chloro-2-hydroxyphenyl)-1-decanone

$C_{16}H_{23}ClO_2$ mol. wt. 282.81



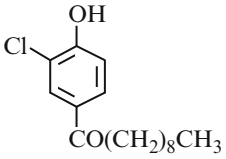
Synthesis

-Obtained by Fries rearrangement of 2-chlorophenyl caprate with aluminium chloride [3170].

$b.p._{.4}$ 146–147° [3170]; m.p. 42–43° [3170]; UV [3170].

1-(3-Chloro-4-hydroxyphenyl)-1-decanone

$C_{16}H_{23}ClO_2$ mol. wt. 282.81



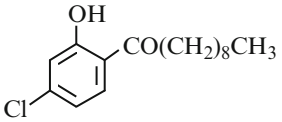
Synthesis

-Obtained by Fries rearrangement of 2-chlorophenyl caprate with aluminium chloride [3170].

m.p. 53–54° [3170]; UV [3170].

1-(4-Chloro-2-hydroxyphenyl)-1-decanone

[666836-99-3] $C_{16}H_{23}ClO_2$ mol. wt. 282.81



Syntheses

-Preparation by Fries rearrangement of 3-chlorophenyl caprate with aluminium chloride,

*without solvent at 130° for 2 h (52 %) [2802];

*in nitrobenzene at 25° for 6 h (79 %) [2802].

$b.p._{.40}$ 230° [2802].

Methyl ether $C_{17}H_{25}ClO_2$ mol. wt. 296.84

-Obtained by methylation of the above ketone in the usual way (85 %) [2802].

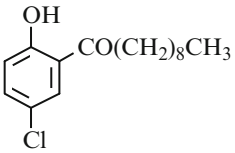
$b.p._{.29}$ 150° [2802].

2,4-Dinitrophenylhydrazone $C_{22}H_{27}ClN_4O_5$ mol. wt. 462.93

m.p. 126° [2802].

1-(5-Chloro-2-hydroxyphenyl)-1-decanone

[98813-29-7] $C_{16}H_{23}ClO_2$ mol. wt. 282.81



Syntheses

-Obtained by Fries rearrangement of 4-chlorophenyl caprate with aluminium chloride [3170].

-Also obtained by reaction of decanoyl chloride with 4-chlorophenol in the presence of aluminium chloride (49.6 %) [2680].

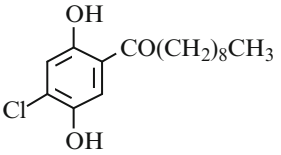
-Also refer to: [148].

b.p.$_1$ 158–160° [2680]; m.p. 69–70° [3170], 68–69° [2680]; UV [3170].

USE: Retard photodegradation of high-d polyethylene in air [148].

1-(4-Chloro-2,5-dihydroxyphenyl)-1-decanone

$C_{16}H_{23}ClO_3$ mol. wt. 298.81

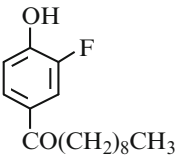


Synthesis
-Refer to: [418].

Dimethyl ether [434340-29-1]
$C_{18}H_{27}ClO_3$ mol. wt. 326.86
-Refer to: [418].

1-(3-Fluoro-4-hydroxyphenyl)-1-decanone

[403-08-7] $C_{16}H_{23}FO_2$ mol. wt. 266.36



Synthesis
-Obtained by refluxing 3-fluoro-4-methoxydecanophenone with pyridinium chloride for 15 min [516].
b.p.$_{20}$ 233–234° [516]; m.p. 67° [516].

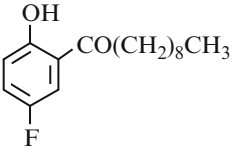
Methyl ether [455-77-6] $C_{17}H_{25}FO_2$ mol. wt. 280.38

-Obtained by Friedel-Crafts acylation of 2-fluoroanisole with decanoyl chloride in the presence of aluminium chloride in carbon disulfide (75–85 %) [516].

b.p.$_{20}$ 232–233° [516]; m.p. 72° [516].

1-(5-Fluoro-2-hydroxyphenyl)-1-decanone

[392-02-9] $C_{16}H_{23}FO_2$ mol. wt. 266.36



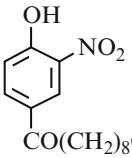
Synthesis
-Obtained by Fries rearrangement of 4-fluorophenyl caprate with aluminium chloride at 130° for 2 h (55 %) [1549].
b.p.$_5$ 270° [1549].

2,4-Dinitrophenylhydrazone [2546-82-9] $C_{22}H_{27}FN_4O_5$ mol. wt. 446.48

m.p. 98° [1549].

1-(4-Hydroxy-3-nitrophenyl)-1-decanone

[70079-27-5] $C_{16}H_{23}NO_4$ mol. wt. 293.36



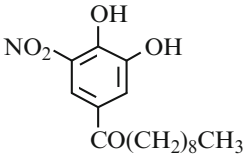
Synthesis

-Obtained by treatment of 4-decanoylphenol with concentrated nitric acid in concentrated sulfuric acid at 0° for 1 h 15 min [1222].

m.p. 63.5–64.5° [1222].

1-(3,4-Dihydroxy-5-nitrophenyl)-1-decanone

[125628-94-6] $C_{16}H_{23}NO_5$ mol. wt. 309.36



Syntheses

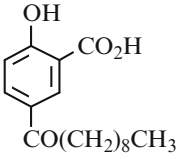
-Refer to: [322, 323, 429].

pKa [429].

2-Hydroxy-5-decanoylbenzoic acid

5-n-decanoylsalicylic acid

[78418-02-7] $C_{17}H_{24}O_4$ mol. wt. 292.37



Syntheses

-Obtained by saponification of the methyl ester [2522], (91 %) [689] with 15 % aqueous sodium hydroxide at reflux for 20 h (53 %) [782].

-Also obtained from methyl 2-(n-decyloxy)benzoate by a Fries rearrangement in carbon disulfide (38 % yield) followed by basic hydrolysis of the resulting methyl ester in 89 % yield [783].

-Also refer to: [849, 1743, 1844, 1855, 1857, 2439, 2477, 2643, 2884–2886, 3129, 3130].

m.p. 120.5–121.5° [2522], 120–122° [782], 118–119° [689], 117° [1743]; ^{1}H NMR [782], IR [782].

USE pattern: Refer to: [2885].

BIOLOGICAL ACTIVITY: Antimicrobial [1743]; Antifungal [1743].

Methyl ester [78417-97-7] $C_{18}H_{26}O_4$ mol. wt. 306.40

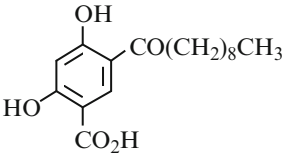
-Obtained by reaction of decanoyl chloride with methyl salicylate in the presence of aluminium chloride in carbon disulfide first at 5–10°, then at r.t. for 12 h (86 %) [689].

-Also obtained by Fries rearrangement of methyl 2-(n-decanoyloxy)benzoate [2522] with aluminium chloride in refluxing carbon disulfide for 2 h, then at 90–100° for 30 min after solvent elimination (67 %) [782].

b.p.$_{1.5}$ 180–190° [2522];
m.p. 66.5–67.5° [2522], 65–66° [782], 63–64° [689];
^{1}H NMR [782], IR [782].

2,4-Dihydroxy-5-decanoylbenzoic acid

$C_{17}H_{24}O_5$ mol. wt. 308.37

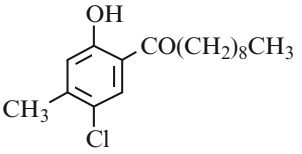


Synthesis
-Refer to: [1743] (Japanese paper).
m.p. 110° [1743].

BIOLOGICAL ACTIVITY: Antimicrobial [1743]; Antifungal [1743].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-decanone

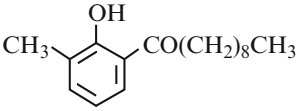
$C_{17}H_{25}ClO_2$ mol. wt. 296.84



Synthesis
-Refer to: [3138].
Fluorescence spectral data [3138].

1-(2-Hydroxy-3-methylphenyl)-1-decanone

[109251-96-9] $C_{17}H_{26}O_2$ mol. wt. 262.39



Synthesis
-Obtained by Fries rearrangement of o-cresyl caprate with aluminium chloride at 160–180° for 30 min (28 %) [1644].

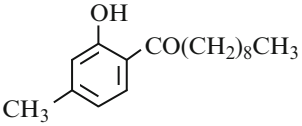
b.p.$_{.8}$ 190–193° [1644].

2,4-Dinitrophenylhydrazone $C_{23}H_{30}N_4O_5$ mol. wt. 442.52

m.p. 96–98° [1644].

1-(2-Hydroxy-4-methylphenyl)-1-decanone

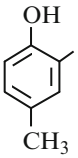
[109250-84-2] $C_{17}H_{26}O_2$ mol. wt. 262.39



Synthesis
-Preparation by Fries rearrangement of 3-methylphenyl caprate with aluminium chloride without solvent at 140–150° [906].
b.p.$_{1.5}$ 148–149° [906]; m.p. 32° [906].

1-(2-Hydroxy-5-methylphenyl)-1-decanone

[76115-96-3] $C_{17}H_{26}O_2$ mol. wt. 262.39



Syntheses
-Obtained by Fries rearrangement of p-cresyl caprate with aluminium chloride,
*at 120° for 10 min (53 %) [1644];
*at 125–130° for 45 min (69 %) [489].
-Also obtained by reaction of decanoyl chloride with p-cresol in the presence of aluminium chloride in ethylene chloride at 110–120° for 8 h (59 %) [1769].
-Also refer to: [142, 148, 490, 1921].

b.p.$_{0.7}$ 144–148° [489], b.p.$_1$ 145° [142], b.p.$_{60}$ 180–181° [1769], b.p.$_{6.5}$ 182–186° [1644];
^{1}H NMR [489], IR [489]; $n_D^{25} = 1.5110$ [142].

USE: Retard photodegradation of high-d polyethylene in air [148].

Oxime [71491-29-7] $C_{17}H_{27}NO_2$ mol. wt. 277.41

-Refer to: [123, 1768, 1769, 2706, 3321].

m.p. 92–93.5° [1769];
^{1}H NMR [1769], ^{13}C NMR [1769], IR [1769], UV [1769], MS [1921].

USE: Solvent extraction of copper (II) [1769, 2520]; Hydroxyoxime adsorption at octane-toluene/water interfaces [3321].

Oxime (*E*) [103582-40-7] $C_{17}H_{27}NO_2$ mol. wt. 277.41

-Refer to: [124, 1769, 1921, 2600].

m.p. 92–93.5° [1769];
^{1}H NMR [1769], ^{13}C NMR [1769], IR [1769], UV [1769], MS [1921].

USE: Copper (II) complexing and extracting ability from aqueous solutions [2600].

2,4-Dinitrophenylhydrazone [115098-09-4] $C_{23}H_{30}N_4O_5$ mol. wt. 442.52

m.p. 139–141° [1644], 99–100° [1769].

Methyl ether $C_{18}H_{28}O_2$ mol. wt. 276.42

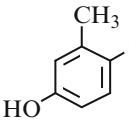
^{1}H NMR [879], ^{13}C NMR [879].

Oxime of the methyl ether [101396-10-5] $C_{18}H_{29}NO_2$ mol. wt. 291.43

USE: Palladium extn. and purifn. with [3191].

1-(4-Hydroxy-2-methylphenyl)-1-decanone

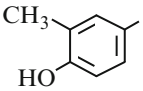
[1263095-96-0] $C_{17}H_{26}O_2$ mol. wt. 262.39



Synthesis
-Refer to: [2189].

1-(4-Hydroxy-3-methylphenyl)-1-decanone

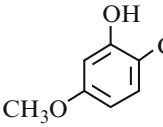
[109250-85-3] $C_{17}H_{26}O_2$ mol. wt. 262.39



Synthesis
-Refer to: [142].
m.p. 72.5–74° [142].

1-(2-Hydroxy-4-methoxyphenyl)-1-decanone

[393519-46-5] $C_{17}H_{26}O_3$ mol. wt. 278.39

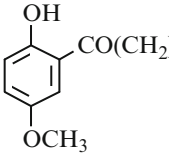


Synthesis
-Obtained by treatment of 2-(*t*-butyldimethylsilyloxy)-4-methoxy-2′-octylacetophenone (m.p. 129–131°) with $(n\text{-Bu})_4NF$ in THF at 0° for 45 min (79 %) [1467].

m.p. 151–153° [1467];
^{1}H NMR [1467], ^{13}C NMR [1467], IR [1467], MS [1467].

1-(2-Hydroxy-5-methoxyphenyl)-1-decanone

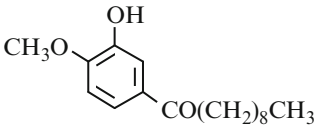
[80427-37-8] $C_{17}H_{26}O_3$ mol. wt. 278.39



Synthesis
-Obtained by Fries rearrangement of 4-methoxyphenyl decanoate with titanium tetrachloride for 1 h at 120° (60–74 %) [2000].
m.p. 39° [2000]; IR [2000], UV [2000].

1-(3-Hydroxy-4-methoxyphenyl)-1-decanone

[66476-00-4] $C_{17}H_{26}O_3$ mol. wt. 278.39



Syntheses
-Obtained in two steps: First, reaction of decanoyl chloride with 2-methoxyphenyl decanoate in the presence of stannic chloride in nitromethane at 20° for 1 h (61 %). Then, the m-ketoester obtained was hydrolyzed (82 %) [1999, 2000].

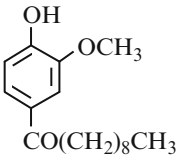
m.p. 58° [1999, 2000];
^{1}H NMR (Sadtler standard N° 28213M) [2000],
IR (Sadtler standard N° 55285) [1999, 2000], UV [1999, 2000].

Decanoate [66475-97-6] $C_{27}H_{44}O_4$ mol. wt. 432.65

m.p. 39° [1999, 2000];
IR (Sadtler standard N° 57342) [1999, 2000], UV [1999, 2000].

1-(4-Hydroxy-3-methoxyphenyl)-1-decanone

[66476-01-5] $C_{17}H_{26}O_3$ mol. wt. 278.39

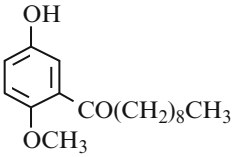


Syntheses
-Obtained by Fries rearrangement of 2-methoxyphenyl decanoate (1 mol) in the presence of various catalysts* (2 mol) in nitromethane at 20° for 24 h,
*stannic chloride (69 %) [1999];
*aluminium chloride (65 %) [1999];

*titanium tetrachloride (62 %) [1999];
*antimony pentachloride (28 %) [1999].

1-(5-Hydroxy-2-methoxyphenyl)-1-decanone

[80427-32-3] $C_{17}H_{26}O_3$ mol. wt. 278.39

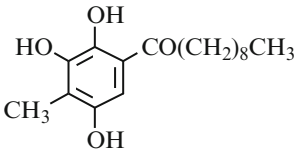


Syntheses
-Preparation by treatment of 3-decanoyl-4-methoxyphenyl decanoate with potassium hydroxide, itself obtained by acylation of 4-methoxyphenyl decanoate with decanoyl chloride in the presence of stannic chloride [2000].
-Also refer to: [2002].

m.p. 56° [2000], 55° (Sadtler standard N° 62646K);
^{1}H NMR (Sadtler standard N° 35278M), [2000];
IR (Sadtler standard N° 62646K), [2000], UV [2000].

1-(2,3,5-Trihydroxy-4-methylphenyl)-1-decanone

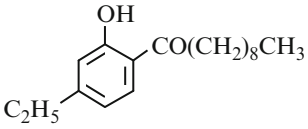
$C_{17}H_{26}O_4$ mol. wt. 294.39



Synthesis
-Refer to: [2681].
^{1}H NMR [2681], ^{13}C [2681], IR [2681], UV [2681], MS [2681].

1-(4-Ethyl-2-hydroxyphenyl)-1-decanone

$C_{18}H_{28}O_2$ mol. wt. 276.42



Syntheses
-Obtained by Fries rearrangement of 3-ethylphenyl n-caprate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (86 %) [2801];
*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (83 %) [2801].

b.p.$_{30}$ 200° [2801].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 108° [2801].

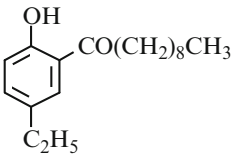
Methyl ether $C_{19}H_{30}O_2$ mol. wt. 290.45

-Obtained by reaction of dimethyl sulfate with 1-(4-ethyl-2-hydroxyphenyl)-1-decanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (83 %) [2801].

b.p.$_{36}$ 165° [2801].

1-(5-Ethyl-2-hydroxyphenyl)-1-decanone

$C_{18}H_{28}O_2$ mol. wt. 276.42



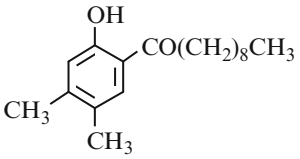
Synthesis
-Obtained by Fries rearrangement of 4-ethylphenyl caprate with aluminium chloride at 100° for 2 h (76 %) [2800].
b.p.$_{11}$ 182° [2800].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 115° [2800].

1-(2-Hydroxy-4,5-dimethylphenyl)-1-decanone

$C_{18}H_{28}O_2$ mol. wt. 276.42



Synthesis

Methyl ether [108623-73-0]

$C_{19}H_{30}O_2$ mol. wt. 290.45

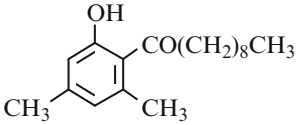
-Obtained by reaction of capryl chloride with 4-methyl-thymol methyl ether (4,5-dimethyl-2-isopropylanisole) (**II**) in the presence of aluminium chloride in carbon disulfide at r.t. for 48 h (4 %) [2663].

N.B.: There is an isopropyl group elimination [2663].

oil yellow [2663]; b.p.$_{0.2}$ 228–231° [2663]; $n_D^{24} = 1.4992$ [2663].

1-(2-Hydroxy-4,6-dimethylphenyl)-1-decanone

[101873-69-2] $C_{18}H_{28}O_2$ mol. wt. 276.42



Syntheses

-Obtained by Fries rearrangement of 3,5-dimethylphenyl n-caprate (1 equiv.),

*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (75 %) [2801];

*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (70 %) [2801].

-Also obtained by reaction of capric acid with 3,5-xylenol in the presence of boron trifluoride at 70° for 2 h (86 %) [1685].

b.p.$_1$ 182–183° [1685], b.p.$_2$ 190° [2801]; m.p. 33° [1685].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 195° [2801].

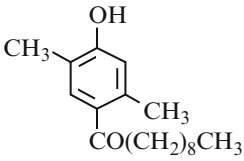
Methyl ether $C_{19}H_{30}O_2$ mol. wt. 290.45

-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxy-4,6-dimethylphenyl)-1-decanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (75 %) [2801].

b.p.$_{39}$ 220° [2801].

1-(4-Hydroxy-2,5-dimethylphenyl)-1-decanone

[95102-23-1] $C_{18}H_{28}O_2$ mol. wt. 276.42

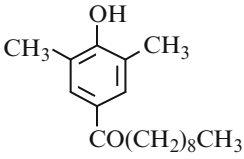


Synthesis
-Refer to: [2704].

USE: Colour developer, for thermal recording materials [2704].

1-(4-hydroxy-3,5-dimethylphenyl)-1-decanone

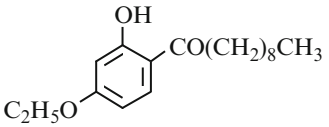
[29665-56-3] $C_{18}H_{28}O_2$ mol. wt. 276.42



Synthesis
-Obtained by Fries rearrangement of 2,6-dimethylphenyl decanoate in the presence of aluminium chloride in nitrobenzene [718], according to [380].
m.p. 48–49.5° [718].

1-(4-Ethoxy-2-hydroxyphenyl)-1-decanone

[20825-28-9] $C_{18}H_{28}O_3$ mol. wt. 292.42



Synthesis
-Obtained by reaction of decanoyl chloride with m-diethoxy-benzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°.

The temperature was then raised to 80° and stirring was continued at that temperature for 5 h (75 %) [1194, 1195].

m.p. 48.5° [1194, 1195]; UV [1194, 1195].

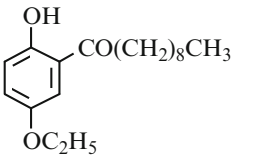
USE: UV absorber [1194]; Light-stabilizer of polymeric materials [1194].

Copper complex [66468-51-7].

-Refer to: [3181].

1-(5-Ethoxy-2-hydroxyphenyl)-1-decanone

[140943-34-6] $C_{18}H_{28}O_3$ mol. wt. 292.42



Synthesis
-Refer to: [285].

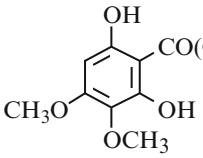
Oxime [141027-87-4]
$C_{18}H_{29}NO_3$ mol. wt. 307.43

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-decanone

[134081-96-2] $C_{18}H_{28}O_5$ mol. wt. 324.42

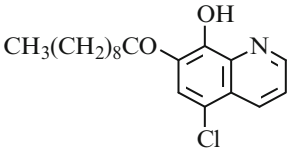


Synthesis
-Preparation by treatment of 1-[6-hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-decanone with potassium carbonate in refluxing methanol for 1–3 h (83 %) [1353].

m.p. 71–72.5° [1353]; ^{1}H NMR [1353].

1-(5-Chloro-8-hydroxy-7-quinolinyl)-1-decanone

[88559-39-1] $C_{19}H_{24}ClNO_2$ mol. wt. 333.86



Synthesis
-Obtained by Friedel-Crafts acylation of 5-chloro-8-hydroxyquinoline with decanoyl chloride in the presence of aluminium chloride in nitrobenzene for 15 to 24 h (10 %) [3171].

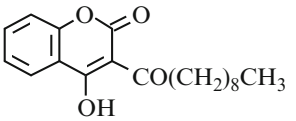
m.p. 68–69° [3171]; IR [3171].

Hydrazone [88559-45-9] $C_{19}H_{26}ClN_3O$ mol. wt. 347.89

m.p. 119–120° [3171].

4-Hydroxy-3-(1-oxodecyl)-2*H*-1-benzopyran-2-one

[20924-70-3] $C_{19}H_{24}O_4$ mol. wt. 316.40



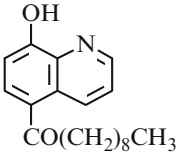
Syntheses
-Obtained by reaction of decanoyl chloride with 4-hydroxycoumarin in pyridine containing one drop of piperidine for 12 h on a water bath (62 %) [3174].

-Also refer to: [3143, 3144].

m.p. 108° [3174].

1-(8-Hydroxy-5-quinolinyl)-1-decanone

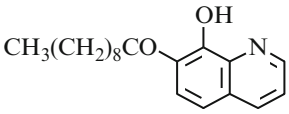
[88559-37-9] $C_{19}H_{25}NO_2$ mol. wt. 299.41



Synthesis
-Obtained by Friedel-Crafts acylation of 8-hydroxyquinoline in the presence of aluminium chloride in nitrobenzene for 15–24 h (20–25 %) [3171].
m.p. 60–61° [3171]; IR [3171].

1-(8-Hydroxy-7-quinolinyl)-1-decanone

[88559-38-0] $C_{19}H_{25}NO_2$ mol. wt. 299.41



Synthesis
-Obtained by Friedel-Crafts acylation of 8-hydroxyquinoline in the presence of aluminium chloride in nitrobenzene for 15–24 h (5–8 %) [3171].

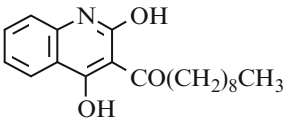
m.p. 61–62° [3171]; IR [3171].

Hydrazone [88559-44-8] $C_{19}H_{27}N_3O$ mol. wt. 313.44

m.p. 100–103° [3171].

1-(2,4-Dihydroxy-3-quinolinyl)-1-decanone

[94432-99-2] $C_{19}H_{25}NO_3$ mol. wt. 315.41



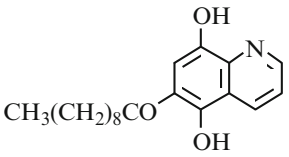
Synthesis
-Obtained by reaction of decanoyl chloride with 2,4-dihydroxyquinoline in the presence of aluminium chloride in nitrobenzene on the steam bath for 3 h (10 %) [3123].

m.p. 127–130° [3123]; UV [3123].

BIOLOGICAL ACTIVITY: Antibacterial properties (Staphylococcus aureus and Escherichia coli) [3123].

1-(5,8-Dihydroxy-6-quinolinyl)-1-decanone

$C_{19}H_{25}NO_3$ mol. wt. 315.41



Synthesis
-Refer to: [3016].

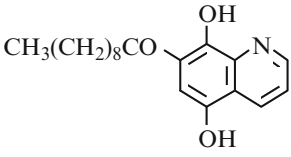
Diacetate

$C_{23}H_{29}NO_5$ mol. wt. 399.49

-Obtained by irradiation of an 6-halo-5,8-quinolinequinone and capraldehyde (decanal) mixture in acetic acid [3016].

1-(5,8-Dihydroxy-7-quinolinyl)-1-decanone

$C_{19}H_{25}NO_3$ mol. wt. 315.41



Synthesis
-Refer to: [3016].

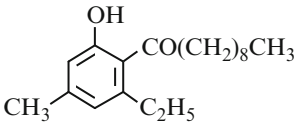
Diacetate

$C_{23}H_{29}NO_5$ mol. wt. 399.49

-Obtained by irradiation of an 7-halo-5,8-quinolinequinone and capraldehyde (decanal) mixture in acetic acid [3016].

1-(2-Ethyl-6-hydroxy-4-methylphenyl)-1-decanone

$C_{19}H_{30}O_2$ mol. wt. 290.45



Syntheses

-Preparation by Fries rearrangement of 3-ethyl-5-methylphenyl caprate with aluminium chloride,
*without solvent at 130° for 2 h (77 %) [2802];
*in nitrobenzene at 25° for 6 h (79 %) [2802].

m.p. 40° [2802].

Methyl ether $C_{20}H_{32}O_2$ mol. wt. 304.47

-Obtained by methylation of the above ketone in the usual way (77 %) [2802].

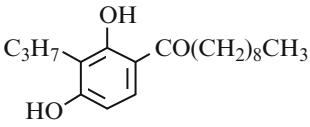
$b.p._{.27}$ 230° [2802].

2,4-Dinitrophenylhydrazone $C_{25}H_{34}N_4O_5$ mol. wt. 470.57

m.p. 115° [2802]

1-(2,4-Dihydroxy-3-propylphenyl)-1-decanone

[172932-00-2] $C_{19}H_{30}O_3$ mol. wt. 306.45

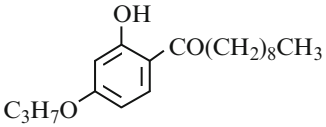


Synthesis

-Refer to: [2388].

1-(2-Hydroxy-4-propoxyphenyl)-1-decanone

[143286-94-6] $C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis

-Obtained by reaction of propyl bromide with 1-(2,4-dihydroxyphenyl)-1-decanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 38–40° [284].

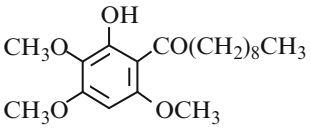
Oxime [143286-63-9] $C_{19}H_{31}NO_3$ mol. wt. 321.46

-Obtained by reaction of hydroxylamine hydrochloride with 1-(2-hydroxy-4-propoxyphenyl)-1-decanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 72–74.5° [284]; ^{1}H NMR [284].

1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-decanone

[134081-65-5] $C_{19}H_{30}O_5$ mol. wt. 338.44



Syntheses

-Obtained by partial selective demethylation of crude 2,3,4,6-tetramethoxydecanophenone with aluminium chloride in acetonitrile at 50° for 1–2 h (83 %) [1353].

-Also refer to: [1351].

m.p. 47.5–48.5° [1353]; ^{1}H NMR [1353].

p-Toluenesulfonic ether [134081-80-4] $C_{26}H_{36}O_7S$ mol. wt. 492.63

-Obtained by reaction of p-toluenesulfonyl chloride with 2-hydroxy-3,4,6-trimethoxy-decanophenone in the presence of potassium carbonate in refluxing acetone for 6–14 h (83 %) [1353].

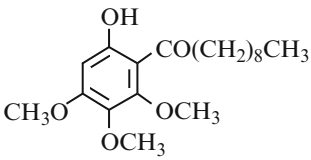
m.p. 84–85° [1353]; ^{1}H NMR [1353].

Methyl ether $C_{20}H_{32}O_5$ mol. wt. 352.47

-Obtained by reaction of decanoyl chloride with 1,2,3,5-tetramethoxybenzene in the presence of aluminium chloride in ethyl ether at 0° for 30 min [1353].

1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-decanone

[134081-72-4] $C_{19}H_{30}O_5$ mol. wt. 338.44



Syntheses

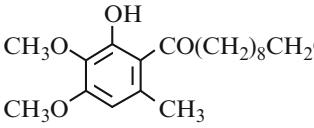
-Obtained by hydrogenation of (6-phenylmethoxy)-2,3,4-trimethoxydecanophenone over 10 % palladium on charcoal in ethyl acetate/methanol (1:1) until the uptake of hydrogen ceased (93 %) [1353].

-Also refer to: [1351].

m.p. 31–31.8° [1353]; ^{1}H NMR [1353].

10-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-decanone

[104966-97-4] $C_{19}H_{30}O_5$ mol. wt. 338.44



Synthesis

-Obtained by treatment of its 10-acetyl ester with sodium hydroxide in methanol for 2 h at r.t. (79 %) [1147].

colourless needles [1147]; m.p. 67° [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

10-Acetyl ester [104966-92-9] $C_{21}H_{32}O_6$ mol. wt. 380.48

-Obtained by Friedel-Crafts reaction of 10-acetoxydecanoyl chloride with 3,4,5-trimethoxy-toluene in 1,2-dichloroethane,
*in the presence of aluminium chloride (2.1 mol) at 20° for 72 h (79 %) [1147];
*in the presence of zinc chloride (2.1 mol) at 10° for 72 h (41 %) [1147].

colourless oil [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

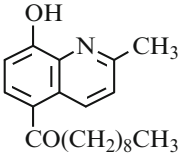
Methyl ether of the 10-acetyl ester [104967-07-9] $C_{22}H_{34}O_6$ mol. wt. 394.51

-Obtained by Friedel-Crafts reaction of 10-acetoxydecanoyl chloride with 3,4,5-trimethoxytoluene in 1,2-dichloroethane in the presence of aluminium chloride (1.1 mol) at 20° for 72 h (43 %) [1147].

colourless oil [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

1-(8-Hydroxy-2-methyl-5-quinolinyl)-1-decanone

[217815-23-1] $C_{20}H_{27}NO_2$ mol. wt. 313.44

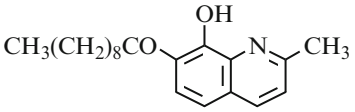


Synthesis
-Obtained by reaction of decanoyl chloride with 8-hydroxyquinaldine in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

m.p. 63° [2261];
^{1}H NMR [2261], ^{13}C NMR [2261], IR [2261].

1-(8-Hydroxy-2-methyl-7-quinolinyl)-1-decanone

[217815-26-4] $C_{20}H_{27}NO_2$ mol. wt. 313.44

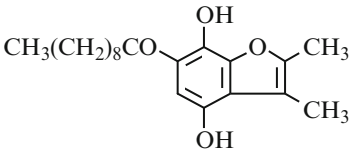


Synthesis
-Obtained by reaction of decanoyl chloride with 8-hydroxyquinaldine in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

m.p. 63° [2261]; ^{13}C NMR [2261].

1-(4,7-Dihydroxy-2,3-dimethyl-6-benzofuranyl)-1-decanone

[49710-89-6] $C_{20}H_{28}O_4$ mol. wt. 332.43



Synthesis
-Obtained by treatment of its dimethyl ether with pyridinium chloride (37 %) [1040].
m.p. 76° [1040]; LD_{50} [1040].

USE: Prepn. and radioprotective activity of, [1040].

Dimethyl ether [42782-77-4] $C_{22}H_{32}O_4$ mol. wt. 360.49

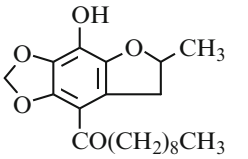
-Obtained by acylation of 4,7-dimethoxy-2,3-dimethylbenzofuran in the presence of stannic chloride in benzene (73 %) [1040].

m.p. 58.5° [1040]; LD_{50} [1040].

USE: Prepn. and radioprotective activity of, [1040].

1-(6,7-Dihydro-4-hydroxy-6-methylfuro[2,3-f]-1,3-benzodioxol-8-yl)-1-decanone

$C_{20}H_{28}O_5$ mol. wt. 348.44



Synthesis
-Refer to: [2179].
Methyl ether [82652-37-7]
$C_{21}H_{30}O_5$ mol. wt. 362.47
Decanoyl furapiole

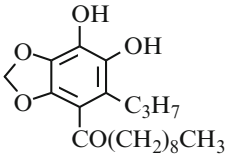
-Obtained by reaction of decanoyl chloride with furapiole in the presence of fused zinc chloride in methylene chloride for 3–4 h in an ice bath (70 %) [2179].

colourless plates; m.p. 53° [2179]; ^{1}H NMR [2179], IR [2179].

USE: Synergistic insecticidal activity of, with pyrethrum [2179].

1-(6,7-Dihydroxy-5-propyl-1,3-benzodioxol-4-yl)-1-decanone

$C_{20}H_{30}O_5$ mol. wt. 350.46



Synthesis
-Refer to: [2179].
Dimethyl ether [82652-30-0]
$C_{22}H_{34}O_5$ mol. wt. 378.51
Decanoyl dihydrodillapiole

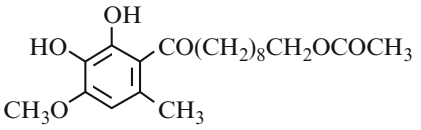
-Obtained by reaction of decanoyl chloride with dihydrodillapiole in the presence of fused zinc chloride in methylene chloride for 3–4 h in an ice bath (70 %) [2179].

colourless solid [2179]; ^{1}H NMR [2179], IR [2179].

USE: Synergistic insecticidal activity of, with pyrethrum [2179].

10-(Acetyloxy)-1-(2,3-dihydroxy-4-methoxy-6-methylphenyl)-1-decanone

[104967-09-1] $C_{20}H_{30}O_6$ mol. wt. 366.45



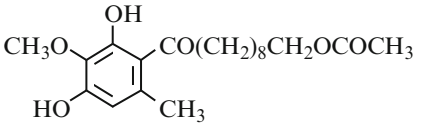
Synthesis
-Obtained by Friedel-Crafts reaction of 10-acetoxy-decanoyl chloride with 3,4,5-trimethoxytoluene in 1,2-dichloroethane in the presence of aluminium chloride (3.1 mol) at 20° for 72 h (35 %) (total of two isomers) [1147].

colourless oil [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

and

10-(Acetyloxy)-1-(2,4-dihydroxy-3-methoxy-6-methylphenyl)-1-decanone

[104967-08-0] $C_{20}H_{30}O_6$ mol. wt. 366.45



Synthesis
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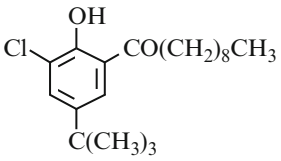
colourless oil [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-decanone

[102370-52-5] $C_{20}H_{31}ClO_2$ mol. wt. 338.92



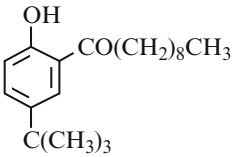
Synthesis
-Obtained by Fries rearrangement of 2-chloro-4-tert-butylphenyl caprate with aluminium chloride at 110° (68 %) [3119].
b.p.$_{13}$ 162° [3119].

2,4-Dinitrophenylhydrazone [102946-84-9] $C_{26}H_{35}ClN_4O_5$ mol. wt. 519.04

m.p. 185° [3119].

1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-decanone

[60170-85-6] $C_{20}H_{32}O_2$ mol. wt. 304.47

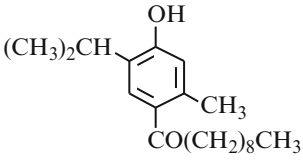


Synthesis
-Obtained by photo-Fries rearrangement of 4-tert-butylphenyl decanoate [148].

USE: Retard photodegradation of high-d polyethylene in air [148].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-decanone

$C_{20}H_{32}O_2$ mol. wt. 304.47



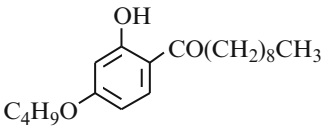
Synthesis
-Refer to: [2660].

Methyl ether (XI) $C_{21}H_{34}O_2$ mol. wt. 318.50
-Obtained by reaction of capryl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (50 %) [2660].

b.p.$_{14}$ 230–231° [2660]; $n_D^{24} = 1.5125$ [2660].

1-[4-(Butyloxy)-2-hydroxyphenyl]-1-decanone

[24313-96-0] $C_{20}H_{32}O_3$ mol. wt. 320.47

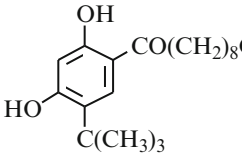


Synthesis
-Obtained by reaction of decanoyl chloride with m-dibutoxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°. The temperature was then raised to 80° and stirring was continued at that temperature for 5 h [1194].

IR [1194, 1195].

1-[5-(1,1-Dimethylethyl)-2,4-dihydroxyphenyl]-1-decanone

$C_{20}H_{32}O_3$ mol. wt. 320.47



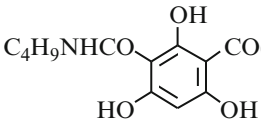
Syntheses
-Refer to: [1051, 3089].

Oxime, nickel complex [82322-05-2]

USE: Colour photog. stabilizer [1051]; Singlet oxygen quencher, laser recording materials contg. cyanine dye and, [3089].

1-[3-(Butylaminocarbonyl)-2,4,6-trihydroxyphenyl]-1-decanone

$C_{21}H_{33}NO_5$ mol. wt. 379.50

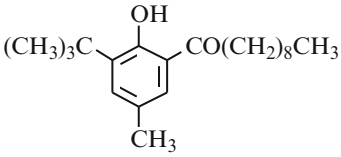


Syntheses
-Refer to: [3034, 3407].
m.p. 105–106° [3407].

BIOLOGICAL ACTIVITY: Cytotoxicity [3034]; Inhibition of Epstein-Barr virus early antigen activation [3034].

1-[3-(1,1-Dimethylethyl)-2-hydroxy-5-methylphenyl]-1-decanone

$C_{21}H_{34}O_2$ mol. wt. 318.50

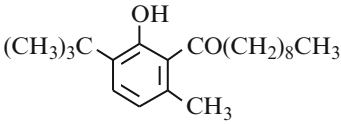


Synthesis
-Refer to: [148].

USE: Retard photodegradation of high-d polyethylene in air [148].

1-[3-(1,1-Dimethylethyl)-2-hydroxy-6-methylphenyl]-1-decanone

$C_{21}H_{34}O_2$ mol. wt. 318.50



Syntheses
-Obtained by Fries rearrangement of 2-tert-butyl-5-methylphenyl decanoate,
*in the presence of aluminium chloride (1.5 equiv.) in nitrobenzene at 25° for 6 h (74 %) [3118];
*in the presence of aluminium chloride (3 equiv.) at 110° for 2 h (74 %) [3118].

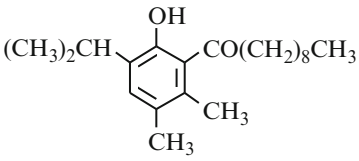
b.p.$_{.8}$ 180° [3117, 3118].

2,4-Dinitrophenylhydrazone $C_{27}H_{38}N_4O_5$ mol. wt. 498.62

m.p. 113° [3117, 3118].

1-[2-Hydroxy-5,6-dimethyl-3-(1-methylethyl)phenyl]-1-decanone

[102456-07-5] $C_{21}H_{34}O_2$ mol. wt. 318.50

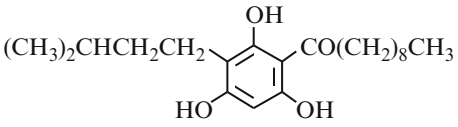


Synthesis
-Obtained (**XXXVII**) by reaction of capryl chloride with 4-methylthymol methyl ether (4,5-dimethyl-2-isopropyl-anisole) (**II**) in the presence of aluminium chloride in carbon disulfide at r.t. for 48 h (12 %) [2663].

yellow oil [2663]; b.p.$_{0.6}$ 170° [2663]; m.p. 0° [2663].

1-[2,4,6-Trihydroxy-3-(3-methylbutyl)phenyl]-1-decanone

[74478-13-0] $C_{21}H_{34}O_4$ mol. wt. 350.50

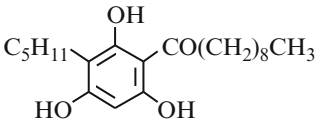


Synthesis
-Refer to: [2111].

BIOLOGICAL ACTIVITY: Fungicidal [2111].

1-(2,4,6-Trihydroxy-3-pentylphenyl)-1-decanone

[74478-12-9] $C_{21}H_{34}O_4$ mol. wt. 350.50

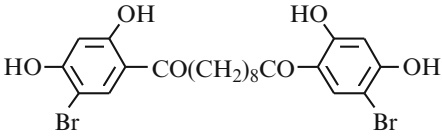


Synthesis
-Refer to: [2111].

BIOLOGICAL ACTIVITY: Fungicidal [2111].

1,10-Bis(5-bromo-2,4-dihydroxyphenyl)-1,10-decanedione

[37174-78-0] $C_{22}H_{24}Br_2O_6$ mol. wt. 544.24



Synthesis
-Refer to: [590].
m.p. 210° [590].

Dioxime [37402-01-0] $C_{22}H_{26}Br_2N_2O_6$ mol. wt. 574.27

m.p. 110° [590].

Tetramethyl ether [37174-79-1] $C_{26}H_{32}Br_2O_6$ mol. wt. 600.34

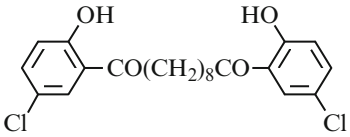
m.p. 173° [590].

Dioxime of the tetramethyl ether [37174-80-4] $C_{26}H_{34}Br_2N_2O_6$ mol. wt. 630.37

m.p. 143° [590].

1,10-Bis-(5-chloro-2-hydroxyphenyl)-1,10-decanedione

[113455-31-5] $C_{22}H_{24}Cl_2O_4$ mol. wt. 423.34



Synthesis
-Obtained by Fries rearrangement of bis-4-chlorophenyl sebacate with aluminium chloride at 150° for 1 h [3235].

m.p. 176° [3235].

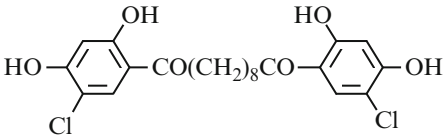
Dimethyl ether [10400-56-3] $C_{24}H_{28}Cl_2O_4$ mol. wt. 451.39

-Refer to: [1575].

m.p. 125° [1575].

1,10-Bis(5-chloro-2,4-dihydroxyphenyl)-1,10-decanedione

[26195-11-9] $C_{22}H_{24}Cl_2O_6$ mol. wt. 455.33



Syntheses
-Obtained by reaction of sebacic acid dichloride with 4-chlororesorcinol in the presence of aluminium chloride [591].
-Also refer to: [590].

m.p. 202° [590, 591].

Dioxime [37401-99-3] $C_{22}H_{26}Cl_2N_2O_6$ mol. wt. 485.36

m.p. 171–172° [590].

Tetramethyl ether [26086-86-2] $C_{26}H_{32}Cl_2O_6$ mol. wt. 511.44

-Obtained by reaction of sebacic acid dichloride with 4-chlororesorcinol dimethyl ether in the presence of aluminium chloride [591].
-Also refer to: [590].

m.p. 157° [590, 591].

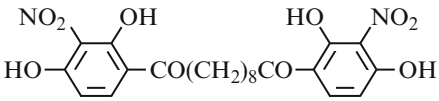
Di-2,4-dinitrophenylhydrazone of the tetramethyl ether

[37174-76-8] $C_{38}H_{40}Cl_2N_8O_{12}$ mol. wt. 871.69

m.p. 187° [590].

1,10-Bis(2,4-dihydroxy-3-nitrophenyl)-1,10-decanedione

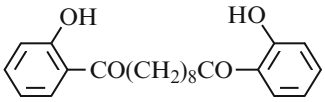
[113752-04-8] $C_{22}H_{24}N_2O_{10}$ mol. wt. 476.44



Synthesis
-Refer to: [1337].
m.p. 227° [1337].

1,10-Bis(2-hydroxyphenyl)-1,10-decanedione

[10401-05-5] $C_{22}H_{26}O_4$ mol. wt. 354.45



Syntheses
-Obtained by Fries rearrangement of phenyl sebacate with aluminium chloride (15–20 %) [1576] in tetrachloroethane for 4 h at 50–60° (21 %) [3207].

-Also refer to: [1575].

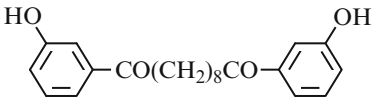
m.p. 103° [1575, 1576], 101–102° [3207]; UV [3207].

Oxime [102758-43-0] $C_{22}H_{28}N_2O_4$ mol. wt. 384.48

m.p. 145° [3207].

1,10-Bis(3-hydroxyphenyl)-1,10-decanedione

[10365-55-6] $C_{22}H_{26}O_4$ mol. wt. 354.45



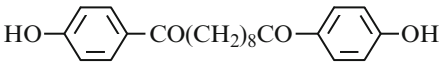
Syntheses
-Obtained by diazotization of 1,10-bis(3-aminophenyl)-1,10-decanedione (40–50 %) [1576].

-Also refer to: [1575].

m.p. 164° [1575, 1576].

1,10-Bis(4-hydroxyphenyl)-1,10-decanedione

[2533-59-7] $C_{22}H_{26}O_4$ mol. wt. 354.45



Syntheses
-Obtained by Fries rearrangement of phenyl sebacate with aluminium chloride in tetrachloroethane for 4 h at 50–60° (40 %) [3207].
-Obtained by reaction of sebacic acid dichloride (sebasoyl chloride) with phenol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].
-Also refer to: [445, 1337].

m.p. 212° [1337], 197° [585], 196° [445], 136° [3207].

Dioxime $C_{22}H_{28}N_2O_4$ mol. wt. 384.48

m.p. 127–129° [1337].

Di-2,4-dinitrophenylhydrazone [2630-99-1] $C_{34}H_{34}N_8O_{10}$ mol. wt. 714.69

m.p. 224° [585].

Diacetate [2619-46-7] $C_{26}H_{30}O_6$ mol. wt. 438.52

m.p. 117–118° [1337], 117° [445].

Dimethyl ether [2525-88-4] $C_{24}H_{30}O_4$ mol. wt. 382.50

-Obtained by reaction of sebacic acid with anisole in the presence of boron trifluoride at 75–80° for 45 min (>60 %) [2597].
-Also obtained by reaction of sebacic acid dichloride with anisole [585] in the presence of aluminium chloride (80–90 %) [1576], (82 %) [905].
-Also obtained by methylation of 1,10-bis(4-hydroxyphenyl)-1,10-decanedione [585].
-Also refer to: [1337, 1575, 2596 (90 %)].

m.p. 130° [585], 120–121° [1337, 2597], 120° [1575, 1576], 119–119.5° [2596], 118.5–119.5° [905].

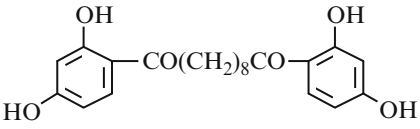
Di-2,4-dinitrophenylhydrazone of the dimethyl ether

[24339-81-9] $C_{36}H_{38}N_8O_{10}$ mol. wt. 742.75.

m.p. 142° [585].

1,10-Bis(2,4-dihydroxyphenyl)-1,10-decanedione
1,8-Di(2,4-dihydroxy-1-benzoyl)octane (**X**) [3207]

[3088-14-0] $C_{22}H_{26}O_6$ mol. wt. 386.45



Syntheses
-Obtained by reaction of sebacic acid with resorcinol,
*in the presence of zinc chloride for 3–5 h at 140° (85 %) or for 3–5 h at 110–115° (31 %) [445];
*in the presence of p-toluenesulfonic acid in xylene at 170–180° for 12 h (30 %) [3207];
*in the presence of boron trifluoride in anisole at 75–80° for 45 min (65 %) [2597].
-Also obtained by adding resorcinol into the dinitrile of sebacic acid and hydrogen chloride in ethyl ether in the presence of zinc chloride. Then, the diketimine dichlorhydrate obtained was hydrolyzed by boiling water (90 %) [2674].
-Also obtained by reaction of sebacic acid dichloride with resorcinol in the presence of aluminium chloride [591].
-Also refer to: [381, 590, 1735, 2504, 2607, 3468].

m.p. 174° [2597], 172° [2504, 2674], 171° [590, 591], 168° [381, 445, 2607, 3207]; UV [2504].

Monohydrate $C_{22}H_{26}O_6$, H_2O mol. wt. 404.46

-Refer to: [2597].

2,4-Dinitrophenylhydrazone $C_{28}H_{30}N_4O_9$ mol. wt. 566.57

m.p. 68° [2674].

Di-2,4-dinitrophenylhydrazone [37166-99-7] $C_{34}H_{34}N_8O_{12}$ mol. wt. 746.69

-Refer to: [2597].

m.p. 268° [2674], 266° [590].

Tetraacetate [13379-59-4] $C_{30}H_{34}O_{10}$ mol. wt. 554.59

-Obtained by treatment of this diketone with boiling an excess of acetic anhydride for some min [2597].
-Also refer to: [445, 2607].

m.p. 108–109° [445], 108° [2607], 105° [2597].

Tetramethyl ether [37167-02-5] $C_{26}H_{34}O_6$ mol. wt. 442.55

-Refer to: [590, 1337].

m.p. 128° [590], 127° [1337].

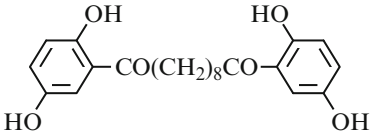
Di-2,4-dinitrophenylhydrazone of the tetramethyl ether

[37402-34-9] $C_{38}H_{42}N_8O_{12}$ mol. wt. 802.80

m.p. 137° [590].

1,10-Bis(2,5-dihydroxyphenyl)-1,10-decanedione

$C_{22}H_{26}O_6$ mol. wt. 386.45



Synthesis
-Refer to: [2331].

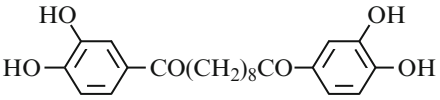
Tetramethyl ether [10365-10-3]
$C_{26}H_{34}O_6$ mol. wt. 442.55

-Preparation from hydroquinone dimethyl ether and sebacoyl chloride [2331].
-Obtained by reaction of sebacic acid dichloride (1 mol) with hydroquinone dimethyl ether (2.5 mol) in the presence of aluminium chloride (1 mol) (88 %) [1575].
-Also refer to: [1575].

needles [2331]; m.p. 103° [1575], 99–100° [2331].

1,10-Bis(3,4-dihydroxyphenyl)-1,10-decanedione

$C_{22}H_{26}O_6$ mol. wt. 386.45



Synthesis
-Obtained by reaction of sebacic acid with pyrocatechol in the presence of boron trifluoride in anisole at 75–80° for 45 min [2597].

Tetramethyl ether [859742-49-7] $C_{26}H_{34}O_6$ mol. wt. 442.55

-Obtained by reaction of sebacic acid dichloride with pyrocatechol dimethyl ether in the presence of aluminium chloride [591].
-Also refer to: [2342, 3060].

m.p. 106–107° [3060], 103° [591];
^{1}H NMR [2342], ^{13}C NMR [2342].

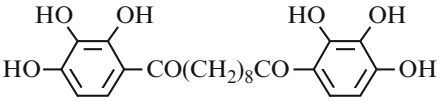
1,10-Bis(3,5-dihydroxyphenyl)-1,10-decanedione

$C_{22}H_{26}O_6$ mol. wt. 386.45

Synthesis
-Refer to: [1316].
m.p. 170–175° [1316].

1,10-Bis(2,3,4-trihydroxyphenyl)-1,10-decanedione

[13178-17-1] $C_{22}H_{26}O_8$ mol. wt. 418.44



Synthesis
-Obtained by reaction of sebacic acid with pyrogallol in the presence of boron trifluoride in anisole at 75–80° for 45 min (46 %) [2597].

m.p. 182–183° [2597].

Di-2,4-dinitrophenylhydrazone $C_{34}H_{34}N_8O_{14}$ mol. wt. 778.69

Refer to: [2597].

Hexaacetate $C_{34}H_{38}O_{14}$ mol. wt. 670.67

-Obtained by reaction of acetic anhydride with the title ketone [2597].

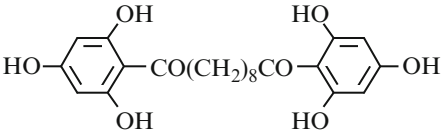
Hexamethyl ether [10373-33-8] $C_{28}H_{38}O_8$ mol. wt. 502.61

-Obtained by reaction of sebacic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride [591].
-Also obtained by reaction of dimethyl sulfate with 1,10-bis(2-hydroxy-3,4-dimethoxyphenyl)-1,10-decanedione the presence of 30 % sodium hydroxide (65–90 %) [1574].
-Also refer to: [1575].

m.p. 126° [591], 77° [1574, 1575].
N.B.: One the reported melting point is obviously wrong.

1,10-Bis(2,4,6-trihydroxyphenyl)-1,10-decanedione

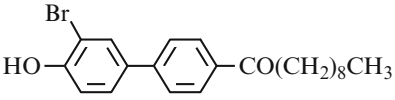
[98333-38-1] $C_{22}H_{26}O_8$ mol. wt. 418.44



Synthesis
-Refer to: [2673].
m.p. 198° [2673].

1-(3′-Bromo-4′-hydroxy[1,1′-biphenyl]-4-yl)-1-decanone

$C_{22}H_{27}BrO_2$ mol. wt. 403.36

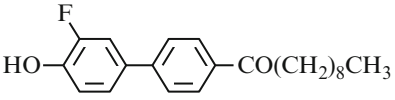


Synthesis
-Refer to: [1444].
6-Methyloctyl ether (S) [112780-54-8]
$C_{31}H_{45}BrO_2$ mol. wt. 529.60

-Refer to: [1444].

1-(3′-Fluoro-4′-hydroxy[1,1′-biphenyl]-4-yl)-1-decanone

$C_{22}H_{27}FO_2$ mol. wt. 342.63

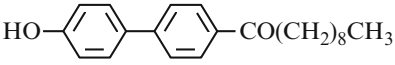


Synthesis
-Refer to: [1444].
Methyl ether [112780-70-8]
$C_{23}H_{29}FO_2$ mol. wt. 356.48

-Refer to: [1444].

1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-decanone

[93249-83-3] $C_{22}H_{28}O_2$ mol. wt. 324.46



Syntheses
-Refer to: [68, 1647, 2995, 3075].

USE: In preparation of liquid crystals [1647].

Acetate [93249-88-8] $C_{24}H_{30}O_3$ mol. wt. 366.49

-Refer to: [1647, 3075].

USE: In preparation of liquid crystals [1647].

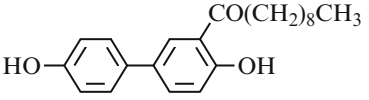
Various ethers (11)

-Preparations and liquid crystalline properties of, [847].

Methyl ether	[56116-82-6]	$C_{23}H_{30}O_2$	mol. wt. 338.49
Ethyl ether	[56116-91-7]	$C_{24}H_{32}O_2$	mol. wt. 352.52
Propyl ether	[56116-99-5]	$C_{25}H_{34}O_2$	mol. wt. 366.54
Butyl ether	[56117-07-8]	$C_{26}H_{36}O_2$	mol. wt. 380.57
Pentyl ether	[56117-16-9]	$C_{27}H_{38}O_2$	mol. wt. 394.60
Hexyl ether	[56117-25-0]	$C_{28}H_{40}O_2$	mol. wt. 408.62
Heptyl ether	[56117-33-0]	$C_{29}H_{42}O_2$	mol. wt. 422.65
Octyl ether	[56117-42-1]	$C_{30}H_{44}O_2$	mol. wt. 436.68
Nonyl ether	[56117-51-2]	$C_{31}H_{46}O_2$	mol. wt. 450.71
Decyl ether	[56117-60-3]	$C_{32}H_{48}O_2$	mol. wt. 464.73
Dodecyl ether	[56117-69-2]	$C_{34}H_{52}O_2$	mol. wt. 492.19

1-(4,4′-Dihydroxy[1,1′-biphenyl]-3-yl)-1-decanone

[36756-42-0] $C_{22}H_{28}O_3$ mol. wt. 340.46



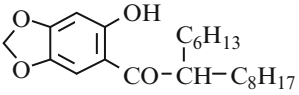
Synthesis

-Preparation by Fries rearrangement of 4,4′-biphenyl dicaprate with aluminium chloride in refluxing chlorobenzene for 24 h (19 %) [2091].

m.p. 90–91° [2091].

2-Hexyl-1-(6-hydroxy-1,3-benzodioxol-5-yl)-1-decanone

[103449-09-8] $C_{23}H_{34}O_4$ mol. wt. 374.52



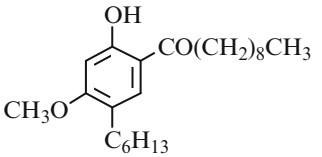
Synthesis

-Refer to: [2326].

USE: In prepn. of antistaining agent for colour photog. paper [2326].

1-(5-Hexyl-2-hydroxy-4-methoxyphenyl)-1-decanone

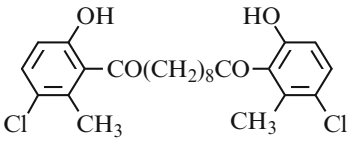
[143287-08-5] $C_{23}H_{38}O_3$ mol. wt. 362.55



Synthesis
-Obtained (**12c**) by reaction of bromomethane with 1-(2,4-dihydroxy-5-hexylphenyl)-1-decanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].
m.p. 49–50° [284].

1,10-Bis(3-chloro-6-hydroxy-2-methylphenyl)-1,10-decanedione

[25715-28-0] $C_{24}H_{28}Cl_2O_4$ mol. wt. 451.39



Synthesis
-Obtained by reaction of sebacic acid dichloride (sebasoyl chloride) with 4-chloro-3-methylphenol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

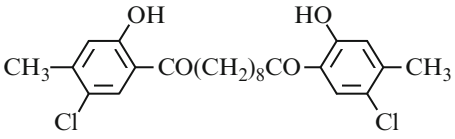
needles [585].

Di-2,4-dinitrophenylhydrazone [25779-68-4] $C_{36}H_{36}Cl_2N_8O_{10}$ mol. wt. 811.64

m.p. 193° [585].

1,10-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,10-decanedione

$C_{24}H_{28}Cl_2O_4$ mol. wt. 451.39



Synthesis
-Obtained by reaction of sebacic acid dichloride (sebasoyl chloride) with 4-chloro-3-methylphenol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

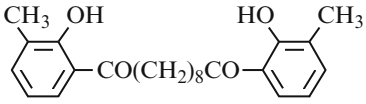
needles [585].

Di-2,4-dinitrophenylhydrazone $C_{36}H_{36}Cl_2N_8O_{10}$ mol. wt. 811.64

m.p. 193° [585].

1,10-Bis(2-hydroxy-3-methylphenyl)-1,10-decanedione

[10483-69-9] $C_{24}H_{30}O_4$ mol. wt. 382.50



Syntheses

-Obtained by Fries rearrangement of o-cresyl sebacate with aluminium chloride (15–20 %) [1576] in tetrachloroethane for 4 h at 50–60° (13 %) [3207].

-Also refer to: [1575].

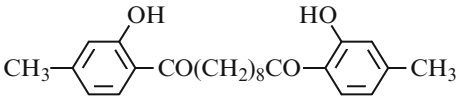
m.p. 107° [1575, 1576], 106° [3207]; UV [3207].

Dioxime [115097-69-3] $C_{24}H_{32}N_2O_4$ mol. wt. 412.53

m.p. 170° [184].

1,10-Bis(2-hydroxy-4-methylphenyl)-1,10-decanedione

[10400-43-8] $C_{24}H_{30}O_4$ mol. wt. 382.50



Syntheses

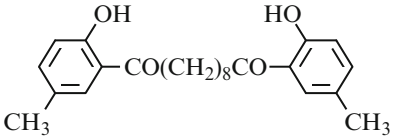
-Obtained by Fries rearrangement of m-cresyl sebacate with aluminium chloride (70–80 %) [1576] in tetrachloroethane for 4 h at 50–60° (53 %) [3207].

-Also refer to: [1575].

m.p. 121° [1575, 1576], 120.5° [3207]; UV [3207].

1,10-Bis(2-hydroxy-5-methylphenyl)-1,10-decanedione

[13282-28-5] $C_{24}H_{30}O_4$ mol. wt. 382.50



Syntheses

-Obtained by Fries rearrangement of di-p-cresyl sebacate with aluminium chloride,

*in refluxing chlorobenzene for 6 h (79 %) [3107];

*in tetrachloroethane for 4 h at 50–60° (62 %) [3207].

-Also obtained by reaction of sebacic acid dichloride (sebasoyl chloride) with p-cresol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

m.p. 126–127° [3107], 126° [585], 110.5° [3207];
IR [3107], UV [3207].

Dioxime [115096-86-1] $C_{24}H_{32}N_2O_4$ mol. wt. 412.53

m.p. 178° [3207].

Di-2,4-dinitrophenylhydrazone [24340-07-6] $C_{36}H_{38}N_8O_{10}$ mol. wt. 742.75

m.p. 200° [585].

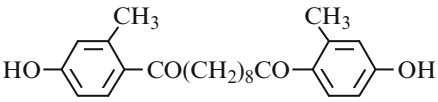
Dimethyl ether [10400-51-8] $C_{26}H_{34}O_4$ mol. wt. 410.55

-Obtained by reaction of sebacic acid dichloride with 4-methylanisole in the presence of aluminium chloride (50–70 %) [1576].
-Also refer to: [1575].

m.p. 88° [1575, 1576].

1,10-Bis(4-hydroxy-2-methylphenyl)-1,10-decanedione

[24340-00-9] $C_{24}H_{30}O_4$ mol. wt. 382.50



Synthesis
-Obtained by reaction of sebacic acid dichloride (sebasoyl chloride) with m-cresol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

needles [585].

Di-2,4-dinitrophenylhydrazone [24340-01-0] $C_{36}H_{38}N_8O_{10}$ mol. wt. 742.75

m.p. 190° [585].

Dimethyl ether [24340-02-1] $C_{26}H_{34}O_4$ mol. wt. 410.55

-Obtained by reaction of dimethyl sulfate with 1,10-bis(4-hydroxy-2-methylphenyl)-1,10-decanedione in the presence of alkali [585].
-Also obtained by reaction of sebacic acid dichloride with m-cresol methyl ether in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

m.p. 110° [585].

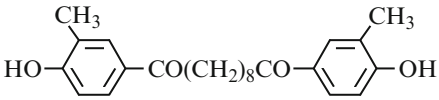
Di-2,4-dinitrophenylhydrazone of the dimethyl ether

[24340-03-2] $C_{38}H_{42}N_8O_{10}$ mol. wt. 770.80

m.p. 150° [585].

1,10-Bis(4-hydroxy-3-methylphenyl)-1,10-decanedione

[13178-43-3] $C_{24}H_{30}O_4$ mol. wt. 382.50



Syntheses

-Obtained by Fries rearrangement of di-o-cresyl sebacate with aluminium chloride in tetrachloroethane for 4 h at 50–60° (47 %) [3207].

-Also obtained by reaction of sebacic acid with o-cresol in the presence of boron trifluoride in chlorobenzene, first at 60°, then at 80° for 90 min (55 %) [2597].

-Also obtained by reaction of sebacic acid dichloride (sebasoyl chloride) with o-cresol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

m.p. 196° [585, 3207], 195–196° [2597].

Di-2,4-dinitrophenylhydrazone $C_{36}H_{38}N_8O_{10}$ mol. wt. 742.75

m.p. 152° [585].

Dimethyl ether [24339-99-9] $C_{26}H_{34}O_4$ mol. wt. 410.55

-Obtained by reaction of dimethyl sulfate with 1,10-bis(4-hydroxy-3-methylphenyl)-1,10-decanedione in the presence of alkali [585].

-Also obtained by reaction of sebacic acid dichloride with o-cresol methyl ether [585].

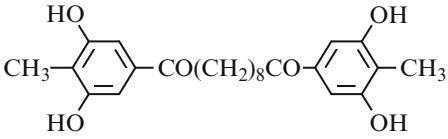
m.p. 131° [585].

Di-2,4-dinitrophenylhydrazone of the dimethyl ether $C_{38}H_{42}N_8O_{10}$ mol. wt. 770.80

m.p. 207° [585].

1,10-Bis(3,5-dihydroxy-4-methylphenyl)-1,10-decanedione

$C_{24}H_{30}O_6$ mol. wt. 414.50



Synthesis

-Refer to: [3132].

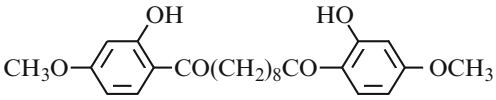
Tetramethyl ether [196869-44-0]
$C_{28}H_{38}O_6$ mol. wt. 470.61

-Synthesis from 3,5-dimethoxy-4-methylbenzaldehyde (75 %) [3132].

Colourless crystalline solid [3132];
^{1}H NMR [3132], ^{13}C NMR [3132].

1,10-Bis(2-hydroxy-4-methoxyphenyl)-1,10-decanedione

[13969-78-3] $C_{24}H_{30}O_6$ mol. wt. 414.50



Syntheses
-Obtained by reaction of sebacic acid dichloride with 3-methoxyphenol in the presence of aluminium chloride [590, 591].

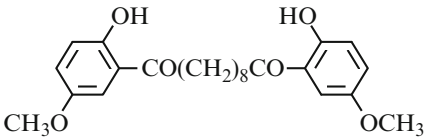
m.p. 122° [590, 591].

Di-2,4-dinitrophenylhydrazone [37167-01-4] $C_{36}H_{38}N_8O_{12}$ mol. wt. 774.74

m.p. 119° [590].

1,10-Bis(2-hydroxy-5-methoxyphenyl)-1,10-decanedione

[10365-31-8] $C_{24}H_{30}O_6$ mol. wt. 414.50



Syntheses
-Obtained by reaction of sebacic acid dichloride with p-dimethoxybenzene in the presence of aluminium chloride [1575].
-Also refer to: [1575] (Japanese paper).

m.p. 109° [1575].

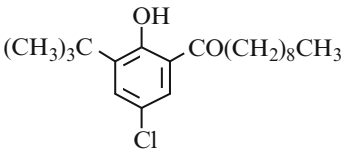
Diacetate [10365-37-4] $C_{28}H_{34}O_8$ mol. wt. 498.57

-Obtained by reaction of acetic anhydride (4 vol) with the title ketone in the presence of 1–2 drops concentrated sulfuric acid, the mixture warmed 5 min [1575].
-Also refer to: [1575].

m.p. 77° [1575].

1-[5-Chloro-3-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-decanone

$C_{24}H_{31}ClO_2$ mol. wt. 386.96

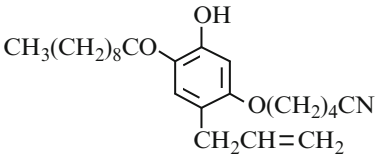


Synthesis
-Refer to: [148].

USE: Retard photodegradation of high-d polyethylene in air [148].

5-[5-Hydroxy-4-(1-oxodecyl)-2-(2-propenyl)phenoxy]pentanenitrile

[117706-06-6] $C_{24}H_{35}NO_3$ mol. wt. 385.55

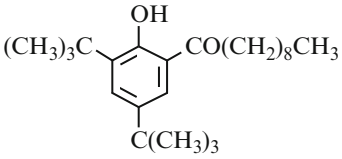


Synthesis
-Refer to: [1313] compound 74, method L, procedure 2 (5 %).
m.p. 49–51° [1313];
^{1}H NMR [1313], MS [1313].

BIOLOGICAL ACTIVITY: Inhibition of [^{3}H]LTB_4 Binding to Human PMN [1313].

1-[3,5-Bis(1,1-dimethylethyl)-2-hydroxyphenyl]-1-decanone

$C_{24}H_{40}O_2$ mol. wt. 360.58

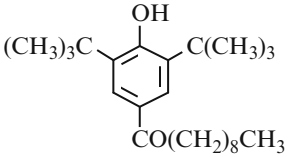


Synthesis
-Refer to: [148].

USE: Retard photodegradation of high-d polyethylene in air [148].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-decanone

$C_{24}H_{40}O_2$ mol. wt. 360.58

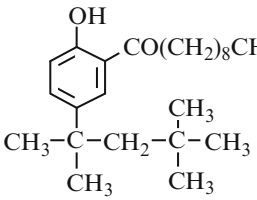


Synthesis
-Refer to: [1408].

O-Methyloxime [169888-15-7]
$C_{25}H_{43}NO_2$ mol. wt. 389.61
-Refer to: [1408].

1-[2-Hydroxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-decanone

[94899-68-0] $C_{24}H_{40}O_2$ mol. wt. 360.58



Synthesis
-Refer to: [3361].

Oxime [94613-09-9]
$C_{24}H_{41}NO_2$ mol. wt. 375.60
IR [3362].

USE: As copper extg. agent, [3361, 3362].

Methyl ether [94899-67-9] $C_{25}H_{42}O_2$ mol. wt. 374.61

-Refer to: [3361].

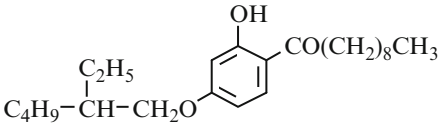
Oxime of the methyl ether [94613-10-2] $C_{25}H_{43}NO_2$ mol. wt. 389.61

IR [3362].

USE: As copper extg. agent, [3361, 3362].

1-[4-[(2-Ethylhexyl)oxy]-2-hydroxyphenyl]-1-decanone

$C_{24}H_{40}O_3$ mol. wt. 376.58

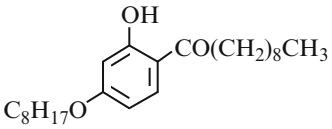


Synthesis
-Refer to: [1050].
Oxime, nickel complex [80848-71-1]

USE: Photog. stabilizer compns. contg. phenol derivs. and, for magenta images [1050].

1-[2-Hydroxy-4-(octyloxy)phenyl]-1-decanone

[143286-95-7] $C_{24}H_{40}O_3$ mol. wt. 376.58



Synthesis
-Obtained by reaction of octyl bromide with 1-(2,4-dihydroxyphenyl)-1-decanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 45-47° [284].

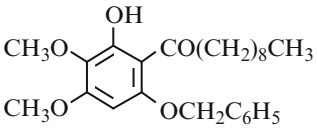
Oxime [143286-64-0] $C_{24}H_{41}NO_3$ mol. wt. 391.59

-Obtained by reaction of hydroxylamine hydrochloride with 1-(4-octyloxy-2-hydroxyphenyl)-1-decanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 53–57° [284].

1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-decanone

[134082-04-5] $C_{25}H_{34}O_5$ mol. wt. 414.54

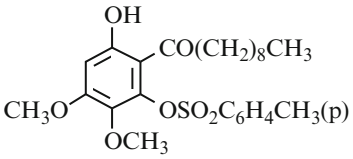


Synthesis
-Obtained by elimination of one phenylmethyl group in 2-position by treatment of 1-(2,6-dibenzyloxy-3,4-dimethoxyphenyl)-1-decanone with concentrated hydrochloric acid and acetic acid at r.t. for 2–3 h (80 %) [1353].

m.p. 83–83.5° [1353]; ^{1}H NMR [1353].

1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-decanone

[134081-88-2] $C_{25}H_{34}O_7S$ mol. wt. 478.61



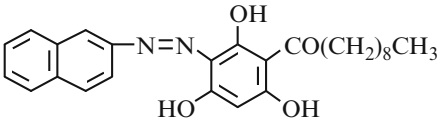
Synthesis

-Obtained by treatment of 1-(2-tosyloxy-3,4,6-trimethoxyphenyl)-1-decanone with 25 % aluminium bromide in acetonitrile at r.t. for 2–3 h (90 %) [1353].

m.p. 59–60° [1353]; ^{1}H NMR [1353].

3-[(2-Naphthylazo)-2,4,6-trihydroxyphenyl]-1-decanone

$C_{26}H_{30}N_2O_4$ mol. wt. 434.54

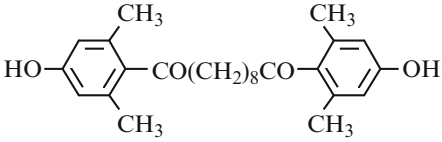


Synthesis

-Obtained by coupling diazotized 2-naphthyl-amine with 2,4,6-trihydroxyphenyl nonyl ketone [872].

1,10-Bis(4-hydroxy-2,6-dimethylphenyl)-1,10-decanedione

[107259-37-0] $C_{26}H_{34}O_4$ mol. wt. 410.55



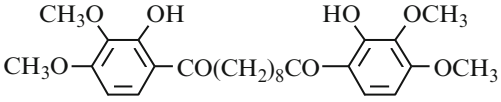
Synthesis

-Refer to: [875].

m.p. 128–130° [875].

1,10-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,10-decanedione

[10351-93-6] $C_{26}H_{34}O_8$ mol. wt. 474.55



Syntheses

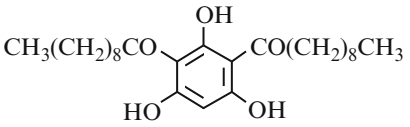
-Obtained by reaction of sebacic acid dichloride with pyrogallol trimethyl ether in the presence of aluminium chloride [3058] in tetrachloroethane [1574].

-Also refer to: [590, 1575].

m.p. 126° [590], 125–126.5° [3058], 125° [1574, 1575].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-decanone

[2999-11-3] $C_{26}H_{42}O_5$ mol. wt. 434.62



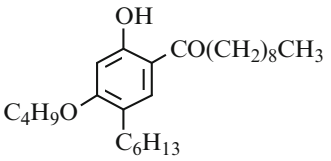
Syntheses
-Obtained by reaction of decanoic anhydride with phloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].
-Also refer to: [457, 644, 2911].

m.p. 80–82° [457, 2911].

BIOLOGICAL ACTIVITY: Antiviral activity towards the replication of vesicular stomatitis virus in HEL cell cultures [644]; Anthelmintic [457].

1-(4-Butoxy-5-hexyl-2-hydroxyphenyl)-1-decanone

[143287-09-6] $C_{26}H_{44}O_3$ mol. wt. 404.63



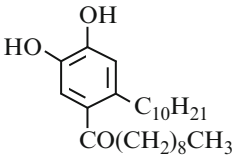
Synthesis
-Obtained (**12d**) by reaction of 1-bromobutane with 1-(2,4-dihydroxy-5-hexylphenyl)-1-decanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].
m.p. 38° [284].

Oxime [143287-10-9] $C_{26}H_{45}NO_3$ mol. wt. 419.65

m.p. 48–50° [284].

1-(2-Decyl-4,5-dihydroxyphenyl)-1-decanone

$C_{26}H_{44}O_3$ mol. wt. 404.63



Synthesis
-Refer to: [2366].

Dimethyl ether [919800-80-9]
$C_{28}H_{48}O_3$ mol. wt. 432.69

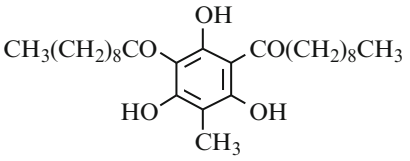
-Refer to: [2366].

^{1}H NMR [2366].

USE: Supramolecular fibers and microbelts from a phthalhydrazide derivative of crown ether with alkyl chains [2366].

1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-decanone

[4807-43-6] $C_{27}H_{44}O_5$ mol. wt. 448.64



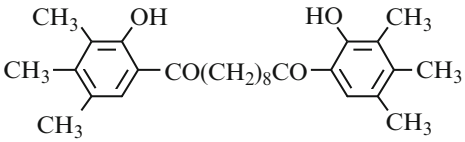
Syntheses
-Obtained by reaction of decanoic anhydride with 2-methylphloroglucinol in the presence of boron trifluoride etherate on heating for 4 h [457].
-Also refer to: [457, 2911].

m.p. 99–101° [457, 2911].

BIOLOGICAL ACTIVITY: Anthelmintic [457].

1,10-Bis(2-hydroxy-3,4,5-trimethylphenyl)-1,10-decanedione

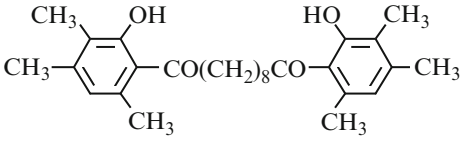
[84978-22-3] $C_{28}H_{38}O_4$ mol. wt. 438.61



Synthesis
-Refer to: [2325].
m.p. 135–142° [2325]; ^{1}H NMR [2325], IR [2325].

1,10-Bis(2-hydroxy-3,4,6-trimethylphenyl)-1,10-decanedione

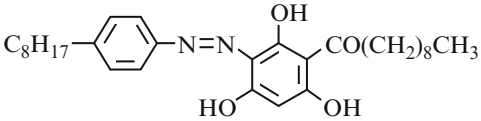
[84978-16-5] $C_{28}H_{38}O_4$ mol. wt. 438.61



Synthesis
-Refer to: [2325].
m.p. 125–129.5° [2325]; ^{1}H NMR [2325], IR [2325].

3-[(4-Octylphenylazo)-2,4,6-trihydroxyphenyl]-1-decanone

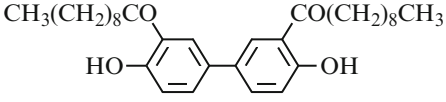
$C_{30}H_{44}N_2O_4$ mol. wt. 496.69



Synthesis
-Obtained by coupling p-octylazobenzene with 2,4,6-trihydroxyphenyl nonyl ketone [872].

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-decanone

[36677-71-1] $C_{32}H_{46}O_4$ mol. wt. 494.71

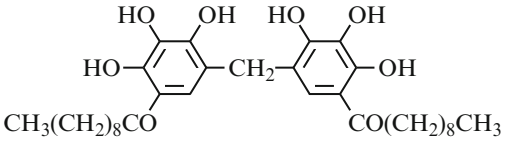


Synthesis
-Preparation by Fries rearrangement of 4,4′-biphenyl dicaprate with aluminium chloride in refluxing chlorobenzene for 24 h (75 %) [2091].

m.p. 74–75° [2091].

1,1′-[Methylenebis(2,3,4-trihydroxy-5,1-phenylene)]bis-1-decanone

$C_{33}H_{48}O_8$ mol. wt. 572.74

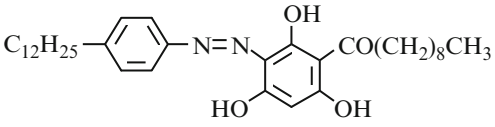


Synthesis
-Obtained by treatment of 4-decanoyl-pyrogallol with 35 % aqueous solution of formaldehyde in refluxing ethanol for 10 min [506].

m.p. 147–148° [506].

3-[(4-Dodecylphenylazo)-2,4,6-trihydroxyphenyl]-1-decanone
3′-(p-Dodecylphenylazo)-2′,4′,6′-trihydroxydecanophenone

$C_{34}H_{52}N_2O_4$ mol. wt. 552.80



Syntheses
-Obtained by coupling diazotized dodecylaniline with 2,4,6-trihydroxy-phenyl nonyl ketone [872].
-Also refer to: [2433].

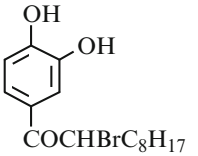
USE: As water-repellent dye for wood [2433].

2 Aromatic Hydroxyketones Derived from Various Halogenodecanoic Acids

2.1 Unsubstituted Hydroxyketones

2-Bromo-1-(3,4-dihydroxyphenyl)-1-decanone

$C_{16}H_{23}BrO_3$ mol. wt. 343.26



Synthesis
-Refer to: [2657].

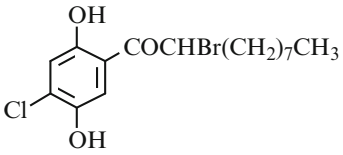
Dibenzyl ether $C_{30}H_{35}BrO_3$ mol. wt. 523.51
-Obtained by reaction of N-bromosuccinimide with 3,4-(dibenzyloxy)capriphenone in carbon tetrachloride in the presence of benzoyl peroxide at 50° (85–90 %) [2657].

m.p. 90° [2657].

2.2 Substituted Hydroxyketones

2-Bromo-1-(4-chloro-2,5-dihydroxyphenyl)-1-decanone

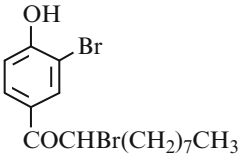
$C_{16}H_{22}BrClO_3$ mol. wt. 377.71



Synthesis
-Refer to: [418].
Dimethyl ether [434340-30-4]
$C_{18}H_{26}BrClO_3$ mol. wt. 405.76
-Refer to: [418].

2-Bromo-1-(3-bromo-4-hydroxyphenyl)-1-decanone

$C_{16}H_{22}Br_2O_2$ mol. wt. 406.16



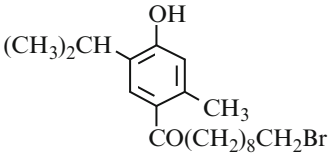
Synthesis
-Refer to: [441].
Methyl ether (2S) [306972-97-4]
$C_{17}H_{24}Br_2O_2$ mol. wt. 420.18

-Preparation of nonracemic α-bromoketones by stereoselective bromination of aryl alkyl tartrate acetals followed by hydrolysis (43 %, >98 % ee) [441].

m.p. 58–59° [441]; ^{1}H NMR [441], ^{13}C NMR [441], IR [441], MS [441].

10-Bromo-1-[4-hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-decanone

$C_{20}H_{31}BrO_2$ mol. wt. 383.37



Synthesis
-Refer to: [220].
Methyl ether [72236-95-4]
$C_{21}H_{33}BrO_2$ mol. wt. 397.39

-Obtained by reaction of 10-bromodecanoyl chloride with thymol methyl ether in the presence of aluminium chloride in methylene chloride at r.t. (90 %) [220].

$n_D^{20} = 1.5262$ [220].

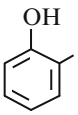
BIOLOGICAL ACTIVITY: Amebicidal and bactericidal and molluscicidal activity of, [220].

3 Aromatic Hydroxyketones Derived from 10-Oxodecanoic Acids

3.1 Unsubstituted Hydroxyketones

10-(2-Hydroxyphenyl)-10-oxo-1-decanoic acid

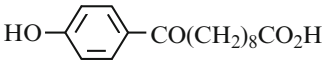
[101253-68-3] $C_{16}H_{22}O_4$ mol. wt. 278.35



Syntheses
-Refer to: [3122, 3135].
m.p. 91° [3122], 84° [3135].

10-(4-Hydroxyphenyl)-10-oxo-1-decanoic acid

[24339-95-5] $C_{16}H_{22}O_4$ mol. wt. 278.35



Syntheses

-Obtained by reaction of sebacic acid dichloride (sebasoyl chloride) with phenol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].
-Also refer to: [445, 1131, 2392, 3135].

m.p. 114° [585], 113° [3135], 110° [445]; ^{1}H NMR [1131].

BIOLOGICAL ACTIVITY: Refer to: [1131].

2,4-Dinitrophenylhydrazone [24339-96-6] $C_{22}H_{26}N_4O_7$ mol. wt. 458.47

m.p. 160° [585].

Methyl ether [24339-93-3] $C_{17}H_{24}O_4$ mol. wt. 292.37

-Obtained by reaction of ω-carbethoxypelargonoyl chloride with anisole in the presence of aluminium chloride in tetrachloroethane at 0° for 3–4 h (96 %) [2392].
-Also obtained by reaction of sebacic anhydride with anisole in the presence of aluminium chloride in a mixture of nitrobenzene and tetrachloroethane first at 0°, then at <5° for 3 days (51 %) [2367].
-Also obtained by reaction of sebacic acid dichloride with anisole [585].

colourless needles [2367];
m.p. 130° [585], 101.5–102° [2392], 98–98.5° [2367].
N.B.: One of the reported melting point is obviously wrong.

2,4-Dinitrophenylhydrazone of the methyl ether

[24339-80-8] $C_{23}H_{28}N_4O_7$ mol. wt. 472.50

m.p. 79° [585].

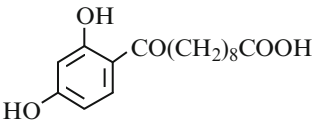
Ethyl ether $C_{18}H_{26}O_4$ mol. wt. 306.40

-Obtained by reaction of ω-carbethoxypelargonoyl chloride with phenetole in the presence of aluminium chloride in tetrachloroethane at 0° for 3–4 h (90 %) [2392].

m.p. 101–101.5° [2392].

10-(2,4-Dihydroxyphenyl)-10-oxo-1-decanoic acid

[858189-64-7] $C_{16}H_{22}O_5$ mol. wt. 294.35



Syntheses

-Preparation by reaction of sebacic acid dinitrile with resorcinol (Hoesch reaction) (90 %) [445].

-Also obtained by reaction of sebacic acid with resorcinol in the presence of zinc chloride at 140° for 5 h [445].

-Also refer to: [1056, 2606, 2607].

m.p. 122° [445, 2606], 121.5–122.5° [1056], 119° [2607].

BIOLOGICAL ACTIVITY: Antibacterial [1056].

Methyl ester [854909-05-0] $C_{17}H_{24}O_5$ mol. wt. 308.37

-Refer to: [445].

$b.p._{.0.3}$ 245° [445].

Ethyl ester [859994-77-7] $C_{18}H_{26}O_5$ mol. wt. 322.40

-Preparation by adding the acid chloride of ethyl hydrogen azelate to a mixture of resorcinol and aluminium chloride in tetrachlorethane over 1 h. Then, the mixture was stirred 24 h at r.t. (51 %) [489].

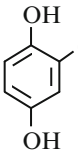
-Also refer to: [1056 (60 %)].

$b.p._{.0.3}$ 220–225° [1056], $b.p._{.0.5}$ 222–226° [489], $b.p._{.0.5}$ 233–234° [1056];
m.p. 47° [1056];
^{1}H NMR [489], IR [489].

BIOLOGICAL ACTIVITY: Antibacterial [1056].

10-(2,5-Dihydroxyphenyl)-10-oxo-1-decanoic acid

[502139-81-3] $C_{16}H_{22}O_5$ mol. wt. 294.35



Syntheses
-Refer to: [1056, 1131].
m.p. 95–97° [1056]; ^{1}H NMR [1131].

BIOLOGICAL ACTIVITY: Antibacterial [1056].

Ethyl ester [858189-97-6] $C_{18}H_{26}O_5$ mol. wt. 322.40

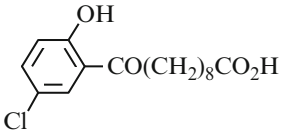
-Refer to: [1056] (40 %).

b.p.$_{0.5}$ 210° [1056]; m.p. 45° [1056].

3.2 Substituted Hydroxyketones

10-(5-Chloro-2-hydroxyphenyl)-10-oxo-1-decanoic acid

[24340-04-3] $C_{16}H_{21}ClO_4$ mol. wt. 312.79



Synthesis
-Obtained by reaction of sebacic acid dichloride (sebasoyl chloride) with p-chlorophenol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

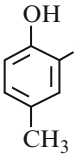
m.p. 134° [585].

2,4-Dinitrophenylhydrazone [24340-05-4] $C_{22}H_{25}ClN_4O_7$ mol. wt. 492.92

m.p. 198° [585].

10-(2-Hydroxy-5-methylphenyl)-10-oxo-1-decanoic acid

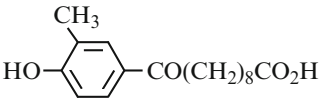
$C_{17}H_{24}O_4$ mol. wt. 292.37



Synthesis
-Refer to: [1827].
UV [1827].

10-(4-Hydroxy-3-methylphenyl)-10-oxo-1-decanoic acid

[24339-89-7] $C_{17}H_{24}O_4$ mol. wt. 292.37



Synthesis
-Obtained by reaction of sebacic acid dichloride (sebasoyl chloride) with o-cresol in the presence of aluminium chloride in nitrobenzene first at 0–5° for 1 h, then at r.t. for 4 h [585].

m.p. 83° [585].

BIOLOGICAL ACTIVITY: Refer to: [2770].

2,4-Dinitrophenylhydrazone [24339-88-6] $C_{23}H_{28}N_4O_7$ mol. wt. 472.50

m.p. 105° [585].

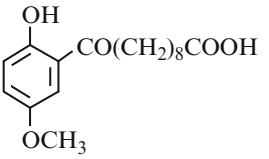
Methyl ether $C_{18}H_{26}O_4$ mol. wt. 306.40

-Obtained by reaction of dimethyl sulfate with 10-(4-hydroxy-3-methylphenyl)-10-oxo-1-decanoic acid in the presence of alkali [585].

m.p. 100° [585].

10-(2-Hydroxy-5-methoxyphenyl)-10-oxo-1-decanoic acid

$C_{17}H_{24}O_5$ mol. wt. 308.37



Synthesis
-Refer to: [1056] (Japanese paper).
m.p. 65–66° [1056].

Ethyl ester $C_{19}H_{28}O_5$ mol. wt. 336.43

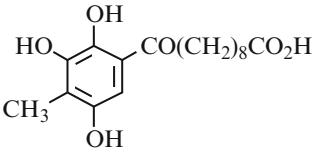
-Refer to: [1056 20 %)].

$b.p._{\cdot 0.5}$ 199–206° [1056].

BIOLOGICAL ACTIVITY: Antibacterial [1056].

10-(4-Methyl-2,3,5-trihydroxyphenyl)-10-oxo-1-decanone

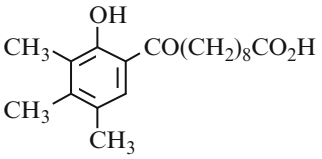
$C_{17}H_{24}O_6$ mol. wt. 324.37



Synthesis
-Refer to: [2681].
yellow crystal [2681]; ^{1}H NMR [2681], ^{13}C NMR [2681], IR [2681], UV [2681], MS [2681].

10-(2-Hydroxy-3,4,5-trimethylphenyl)-10-oxo-1-decanone

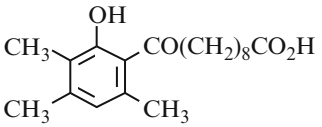
[84978-21-2] $C_{19}H_{28}O_4$ mol. wt. 320.43



Synthesis
-Refer to: [2325].
m.p. 97–98° [2325]; ^{1}H NMR [2325], IR [2325].

10-(2-Hydroxy-3,4,6-trimethylphenyl)-10-oxo-1-decanone

[58185-77-6] $C_{19}H_{28}O_4$ mol. wt. 320.43



Synthesis
-Refer to: [2149, 2325].
m.p. 97–100° [2149, 2325]; ^{1}H NMR [2149, 2325],
IR [2149, 2325].

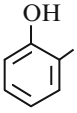
Chapter 9
Undecanones

1 Aromatic Hydroxyketones Derived from Undecanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-1-undecanone

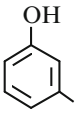
$C_{17}H_{26}O_2$ mol. wt. 262.39



Synthesis
-Refer to: [2077].
Oxime [439948-80-8]
$C_{17}H_{27}NO_2$ mol. wt. 277.41

1-(3-Hydroxyphenyl)-1-undecanone

$C_{17}H_{26}O_2$ mol. wt. 262.39



Synthesis
-Refer to: [928].
Methyl ether [72424-10-3]
$C_{18}H_{28}O_2$ mol. wt. 276.42

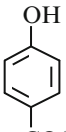
-The ethereal Grignard reagent solution from n-decyl bromide, magnesium and ether was treated with cadmium chloride and the cooled mixture refluxed (2 h) with 3-methoxybenzoyl chloride in ether (41 %) [928].
-Also refer to: [2893].

oil [928]; ^{1}H NMR [928], IR [928].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_9

1-(4-Hydroxyphenyl)-1-undecanone

[137034-61-8] $C_{17}H_{26}O_2$ mol. wt. 262.39



Syntheses

-Obtained by reaction of undecanoyl chloride with phenol in the presence of aluminium chloride in methylene chloride for 14 h at r.t. (43 %) [1910].

-Also obtained by Fries rearrangement of phenyl undecanoate with boron trifluoride at 45–50° for 6 h (70.6 %) [1938].

-Also refer to: [2698].

light brown solid [1910];
m.p. 61.5–62° [1938], 53.7–54.2° [1910];
^{1}H NMR [1910], ^{13}C NMR [1910], IR [1910], MS [1910];
TLC [1910]; GC [1910].

BIOLOGICAL ACTIVITY: Inhibition of 17β-hydroxysteroid dehydrogenase 3 [1910]; Polyoxyethylene ether, as emulsifier for pesticides, [2698].

Methyl ether [69657-36-9] $C_{18}H_{28}O_2$ mol. wt. 276.42

-Obtained by Friedel-Crafts acylation of anisole with tert-butyl undecanoate in the presence of indium tribromide using dimethylchlorosilane (**1r**) (52 %) [2287].

-Also obtained by reaction of undecanoic acid with anisole in the presence of $HSiMe_2Cl$ and $InCl_3$ in 1,2-dichloroethane, first 1 h at r.t., then heated at 80° for 4 h (73 %) [218].

-Also obtained by reaction of 4-methoxybenzaldehyde with 1-decene (90–95 %) [1918].

-Also refer to: [1963, 2255].

m.p. 51–52° [1918], 49° [1963], 44–46° [218];
^{1}H NMR [218, 1918, 2287], ^{13}C NMR [218, 1918, 2287];
IR [218, 1918], MS [218].

2-Chloroethyl ether $C_{19}H_{29}ClO_2$ mol. wt. 324.89

-Obtained by reaction of undecanoyl chloride with 2-chloroethoxybenzene in the presence of aluminium chloride in carbon disulfide for 4 h at 50° (45 %) [476].

m.p. 73–74° [476].

N-Dimethylaminoethyl ether $C_{21}H_{35}NO_2$ mol. wt. 333.51

-Obtained by reaction of 4-(2-chloroethoxy)undecanophenone with dimethylamine in a sealed tube for 2 h at 150° [476].

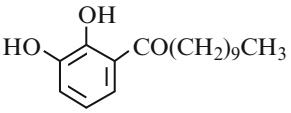
free base: $b.p._{.0.005}$ 185° [476]; m.p. 57–58° [476].
hydrochloride (92 %): m.p. 183° [476].

Benzyldimethylethylammonium chloride ether $C_{28}H_{42}NO_2{*}Cl$ mol. wt. 460.10

m.p. 105–106° [476].

1-(2,3-Dihydroxyphenyl)-1-undecanone

[862666-38-4] $C_{17}H_{26}O_3$ mol. wt. 278.39



Synthesis
-Obtained by deprotection of its dimethyl ether with boron tribromide in methylene chloride at 0°. Then, the mixture was stirred overnight at r.t. (86 %) [82].

brown solid [82]; m.p. 52° [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

USE: Reactant for preparation of lithium gallium/titanium ketone complexes [82].

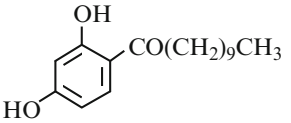
Dimethyl ether [862666-32-8] $C_{19}H_{30}O_3$ mol. wt. 306.45

-Obtained by treatment of 1-(2,3-dimethoxyphenyl)-1-undecanol in acetone with potassium dichromate in dilute sulfuric acid (Jones reagent) at r.t. for 3 h (40 %) [82].

colourless oil [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

1-(2,4-Dihydroxyphenyl)-1-undecanone

[19810-04-9] $C_{17}H_{26}O_3$ mol. wt. 278.39



Syntheses
-Obtained by reaction of undecanoic acid with resorcinol in the presence of zinc chloride for 2 h at 160° (35 %) [3442].
-Also obtained by the Hoesch method (62 %) [2673].
-Also obtained by reaction of undecanoic acid with resorcinol in the presence of concentrated sulfuric acid in refluxing xylene for 24 h (17.4 %) [2543].
-Also refer to: [893, 2114, 2673].

b.p.$_{11}$ 255–260° [893];
m.p. 80° [2114], 78.3–79.4° [2543], 72° [2673], 68–70° [3442];
^{1}H NMR [2543], IR [2543], UV [2543].

BIOLOGICAL ACTIVITY: Antifungal [2114].

2,4-Dinitrophenylhydrazone [95958-93-3] $C_{23}H_{30}N_4O_6$ mol. wt. 458.51

m.p. 158° [2673].

Di-3,5-dinitrobenzoate [19810-05-0] $C_{31}H_{30}N_4O_{13}$ mol. wt. 666.60

-Obtained by treatment of 1-(2,4-dihydroxyphenyl)-1-undecanone with 3,5-dinitrobenzoyl chloride under standard conditions [2543].

m.p. 94.8–96.5° [2543]; IR [2543].

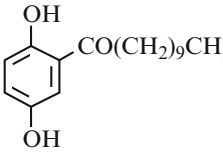
4-Undecanoate [19810-03-8] $C_{28}H_{46}O_4$ mol. wt. 446.67

-Obtained by reaction of undecanoic acid with resorcinol in the presence of concentrated sulfuric acid in refluxing xylene for 24 h (1.8 %) [2543].

m.p. 55.2–55.7° [2543]; IR [2543], UV [2543].

1-(2,5-Dihydroxyphenyl)-1-undecanone

$C_{17}H_{26}O_3$ mol. wt. 278.39



Syntheses

-Obtained by reaction of undecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156] in carbon disulfide [159].

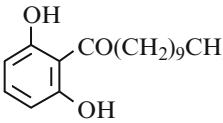
m.p. 73.5–74.5° [156, 159].

Dibenzoate $C_{31}H_{34}O_5$ mol. wt. 486.61

m.p. 93–94.5° [156, 159].

1-(2,6-Dihydroxyphenyl)-1-undecanone

[85298-88-0] $C_{17}H_{26}O_3$ mol. wt. 278.39



Syntheses

-Refer to: [1047, 1621].

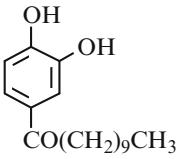
USE: Photog. black coupler [1621]; Photog. materials contg. aminobenzylideneaniline deriv. developing agent precursor and, [1047]; Multilayer colour photog. film assembly contg. organometallic stabilizer and primary amine developer and, for superior image formation and storage stability [1049].

Dimethyl ether [85298-95-9] $C_{19}H_{30}O_3$ mol. wt. 306.44

-Refer to: [1621].

1-(3,4-Dihydroxyphenyl)-1-undecanone
(4-Undecanoylcatechol)

$C_{17}H_{26}O_3$ mol. wt. 278.39



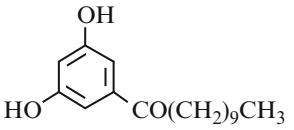
Synthesis
-Obtained by treatment of a pyrocatechol and undecanoic acid mixture with zinc chloride at 135–140° for 2 h (15 %) [1283].
m.p. 105° [1283].

Dibenzyl ether $C_{31}H_{38}O_3$ mol. wt. 458.64

USE: Bromination of, [2657].

1-(3,5-Dihydroxyphenyl)-1-undecanone

[85298-90-4] $C_{17}H_{26}O_3$ mol. wt. 278.39



Syntheses
-Refer to: [543, 1621].

USE: Photog. black coupler [1621].

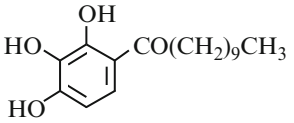
Dimethyl ether [41497-33-0] $C_{19}H_{30}O_3$ mol. wt. 306.45

-Refer to: [543].

m.p. 43–43.5° [543]; ^{1}H NMR [543], IR [543].

1-[2,3,4-Trihydroxyphenyl]-1-undecanone
(4-Undecanoylpyrogallol)

$C_{17}H_{26}O_4$ mol. wt. 294.39

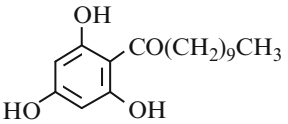


Synthesis
-Obtained by reaction of undecanoic acid with pyrogallol in the presence of zinc chloride (Nencki reaction) at 135–140° for 2 h (35 %) [1283].

m.p. 76–77° [1283].

1-(2,4,6-Trihydroxyphenyl)-1-undecanone

[74478-14-1] $C_{17}H_{26}O_4$ mol. wt. 294.39



Syntheses

-Obtained by reaction of undecanoyl chloride with phloroglucinol in the presence of aluminium chloride in nitrobenzene and carbon disulfide mixture (49 %) [2113].

-Also obtained by reaction of undecanonitrile with phloroglucinol (Hoesch reaction) [1441].

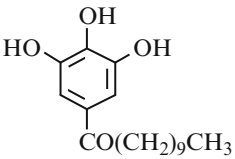
-Also refer to: [2111].

m.p. 117–118° [1441], 114° [2113].

BIOLOGICAL ACTIVITY: Antifungal [2111, 2113].

1-(3,4,5-Trihydroxyphenyl)-1-undecanone

[353499-39-5] $C_{17}H_{26}O_4$ mol. wt. 294.39

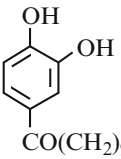


Synthesis

-Refer to: [1969].

1-(3,4-Dihydroxyphenyl)-11-hydroxy-1-undecanone

$C_{17}H_{26}O_4$ mol. wt. 294.39



Synthesis

-Refer to: [2749].

11-Acetate [22421-08-5]

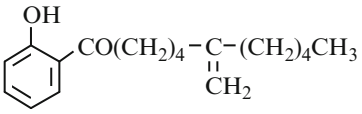
$C_{19}H_{28}O_5$ mol. wt. 336.43

-Obtained by reaction of sodium acetate with 4-(11-bromoundecanoyl)pyrocatechine in refluxing acetic acid for 14 h (81 %) [2749].

m.p. 108.5–110.5° [2749].

1-(2-Hydroxyphenyl)-6-methylene-1-undecanone

[526208-18-4] $C_{18}H_{26}O_2$ mol. wt. 274.40



Syntheses

-Obtained by intermolecular hydroacylation between salicylaldehyde and 2-pentyl-1,5-hexadiene (6 equiv.) in the presence of $RhCl(PPh_3)_3$ (0.2 equiv.) in methylene chloride for 72 h at r.t. (8 %) [1435].

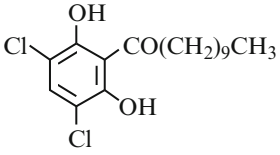
-Also refer to: [3066].

^{1}H NMR [1435].

1.2 Substituted Hydroxyketones

1-(3,5-Dichloro-2,6-dihydroxyphenyl)-1-undecanone

[85298-94-8] $C_{17}H_{24}Cl_2O_3$ mol. wt. 347.28



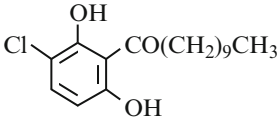
Synthesis

-Refer to: [1621].

USE: Photog. black coupler [1621].

1-(3-Chloro-2,6-dihydroxyphenyl)-1-undecanone

[85298-89-1] $C_{17}H_{25}ClO_3$ mol. wt. 312.83



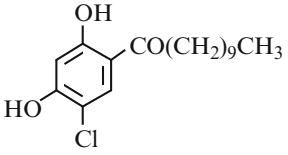
Synthesis

-Refer to: [1621].

USE: Photog. black coupler [1621].

1-(5-Chloro-2,4-dihydroxyphenyl)-1-undecanone

[19809-99-5] $C_{17}H_{25}ClO_3$ mol. wt. 312.83



Synthesis

-Obtained by reaction of undecanoic acid with 4-chloro-resorcinol in the presence of concentrated sulfuric acid in refluxing xylene for 24 h (4,6 %) [2543].

m.p. 98–98.5° [2543]; ^{1}H NMR [2543], IR [2543], UV [2543].

2,4-Dinitrophenylhydrazone [19810-00-5] $C_{23}H_{29}ClN_4O_6$ mol. wt. 492.96

-Refer to: [2543].

m.p. 167.5–168.1° [2543].

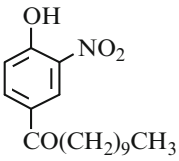
4-Undecanoate [19809-98-4] $C_{28}H_{45}ClO_4$ mol. wt. 481.12

-Obtained by reaction of undecanoic acid with 4-chlororesorcinol in the presence of concentrated sulfuric acid in refluxing xylene for 24 h (1,2 %) [2543].

m.p. 58.2–59.3° [2543]; IR [2543], UV [2543].

1-(4-Hydroxy-3-nitrophenyl)-1-undecanone

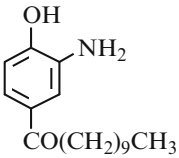
[141124-94-9] $C_{17}H_{25}NO_4$ mol. wt. 307.39



Synthesis
-Refer to: [3046].

1-(3-Amino-4-hydroxyphenyl)-1-undecanone

[141124-96-1] $C_{17}H_{27}NO_2$ mol. wt. 277.41

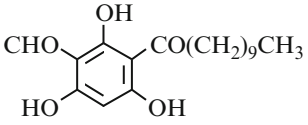


Syntheses
-Refer to: [1478, 3046].

USE: Liquid crystal compound and its containing liquid crystal composition used in liquid crystal display [1478].

2,4,6-Trihydroxy-3-undecanoylbenzaldehyde

$C_{18}H_{26}O_5$ mol. wt. 322.40

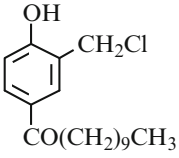


Synthesis
-Refer to: [3408].

BIOLOGICAL ACTIVITY: Effects on transpiration and stomatal closure [3408].

1-[3-(Chloromethyl)-4-hydroxyphenyl]-1-undecanone

$C_{18}H_{27}ClO_2$ mol. wt. 310.86

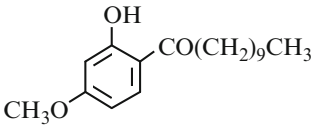


Synthesis
-Refer to: [2255].

Methyl ether [69657-35-8]
$C_{19}H_{29}ClO_2$ mol. wt. 324.89
-Refer to: [2255].

1-(2-Hydroxy-4-methoxyphenyl)-1-undecanone

[55896-05-4] $C_{18}H_{28}O_3$ mol. wt. 292.42

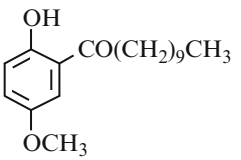


Synthesis
-Refer to: [3091].

USE: Light stabilizers, for polypropylene, [3091].

1-(2-Hydroxy-5-methoxyphenyl)-1-undecanone

$C_{18}H_{28}O_3$ mol. wt. 292.42



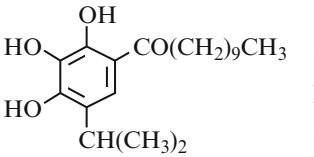
Syntheses
-Obtained by reaction of undecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156] in carbon disulfide [159].
m.p. 47.5–48.5° [156].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_6$ mol. wt. 472.54

m.p. 125–127° [156, 159].

1-[2,3,4-Trihydroxy-5-(1-methylethyl)phenyl]-1-undecanone

[877877-92-4] $C_{20}H_{32}O_4$ mol. wt. 336.47

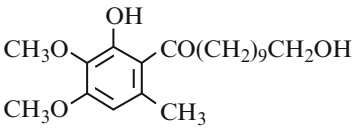


Synthesis
-Refer to: [3267].

BIOLOGICAL ACTIVITY: As inhibitors of antiapoptotic Bcl-2 [3267].

11-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-undecanone

[77712-08-4] $C_{20}H_{32}O_5$ mol. wt. 352.47



Synthesis
-Obtained by treatment of its 11-acetyl ester with sodium hydroxide in methanol for 2 h at r.t. (81 %) [1147].

colourless needles [1147]; m.p. 81° [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

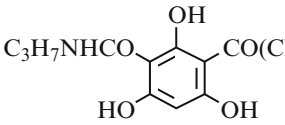
11-Acetyl ester [77712-07-3] $C_{22}H_{34}O_6$ mol. wt. 394.51

-Obtained by Friedel-Crafts reaction of 11-acetoxyundecanoyl chloride with 3,4,5-trimethoxy-toluene in 1,2-dichloroethane in the presence of aluminium chloride (2.1 mol) at 20° for 72 h [1147].

colourless oil [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

1-[3-(Propylaminocarbonyl)-2,4,6-trihydroxyphenyl]-1-undecanone

$C_{21}H_{33}NO_5$ mol. wt. 379.50

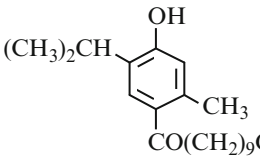


Synthesis
-Refer to: [3034].
m.p. 106–107° [3034]; ^{1}H NMR [3034], IR [3034].

BIOLOGICAL ACTIVITY: Cytotoxicity [3034]; Inhibition of Epstein-Barr virus early antigen activation [3034].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-undecanone

$C_{21}H_{34}O_2$ mol. wt. 318.50



Synthesis
-Refer to: [2660].

Methyl ether (XII)

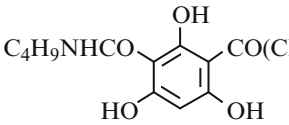
$C_{22}H_{36}O_2$ mol. wt. 332.53

-Obtained by reaction of undecanoyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (57 %) [2660].

b.p.$_{15}$ 234–236° [2660]; $n_D^{23} = 1.5125$ [2660].

1-[3-(Butylaminocarbonyl)-2,4,6-trihydroxyphenyl]-1-undecanone

$C_{22}H_{35}NO_5$ mol. wt. 393.52

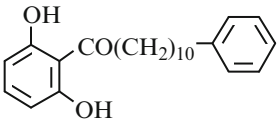


Syntheses
-Refer to: [3034, 3407].
m.p. 110–111° [3407].

BIOLOGICAL ACTIVITY: Cytotoxicity [3034]; Inhibition of Epstein-Barr virus early antigen activation [3034].

1-(2,6-Dihydroxyphenyl)-11-phenyl-1-undecanone

[82427-57-4] $C_{23}H_{30}O_3$ mol. wt. 354.49



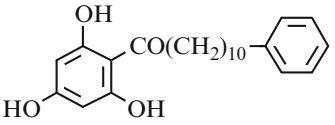
Syntheses
-Refer to: [1368, 1622, 2336].
Isolation from natural sources
-From H*orsfieldia glabra* warb [2489];
-From seeds of *Virola peruviana* [570];
-From ripening fruits of *Virola sebifera* Aubl. [1905].

m.p. 76–77° [1368], 69–71° [1905];
^{1}H NMR [1368, 1905, 2336], ^{13}C NMR [1368, 1622],
IR [1368, 1905, 2336], UV [1905],
MS [1368, 1905, 2336].

BIOLOGICAL ACTIVITY: Nematocidal activity against second-stage larvae of *Toxocara canis* [1368].

1-(2,4,6-Trihydroxyphenyl)-11-phenyl-1-undecanone

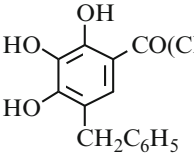
[129684-20-4] $C_{23}H_{30}O_4$ mol. wt. 370.49



Synthesis
-Refer to: [1623].
IR [1623], MS [1623].

1-[2,3,4-Trihydroxy-5-(phenylmethyl)phenyl]-1-undecanone

[877877-98-0] $C_{24}H_{32}O_4$ mol. wt. 384.52

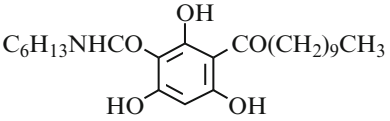


Synthesis
-Refer to: [3267].
^{1}H NMR [3267], ^{13}C NMR [3267].

BIOLOGICAL ACTIVITY: As inhibitors of antiapoptotic Bcl-2 [3267].

1-[3-(Hexylaminocarbonyl)-2,4,6-trihydroxyphenyl]-1-undecanone

$C_{24}H_{39}NO_5$ mol. wt. 421.58

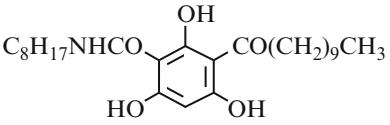


Synthesis
-Refer to: [3034].
m.p. 102–103° [3034]; ^{1}H NMR [3034],
IR [3034].

BIOLOGICAL ACTIVITY: Cytotoxicity [3034]; Inhibition of Epstein-Barr virus early antigen activation [3034].

1-[3-(Octylaminocarbonyl)-2,4,6-trihydroxyphenyl]-1-undecanone

$C_{26}H_{43}NO_5$ mol. wt. 449.63

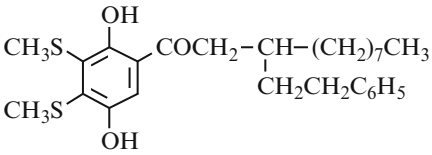


Synthesis
-Refer to: [3034].
m.p. 102–104° [3034]; IR [3034].

BIOLOGICAL ACTIVITY: Cytotoxicity [3034]; Inhibition of Epstein-Barr virus early antigen activation [3034].

1-[2,5-Dihydroxy-3,4-bis(methylthio)phenyl]-3-(2-phenylethyl)-1-undecanone

[357172-24-8] $C_{27}H_{38}O_3S_2$ mol. wt. 474.73

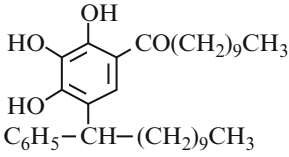


Synthesis
-Refer to: [2352].

USE: Prepn. of alkylbenzenediol derivs. by redn. of Ph ketones to benzyl alc. derivs. and catalytic hydrogenation, [2352].

1-[2,3,4-Trihydroxy-5-(1-phenylundecyl)phenyl]-1-undecanone

[877878-00-7] $C_{34}H_{52}O_4$ mol. wt. 524.78



Synthesis
-Refer to: [3267].

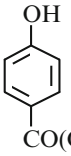
BIOLOGICAL ACTIVITY: As inhibitors of antiapoptotic Bcl-2 [3267].

2 Aromatic Hydroxyketones Derived from 11-Bromoundecanoic Acids

2.1 Unsubstituted Hydroxyketones

11-Bromo-1-(4-hydroxyphenyl)-1-undecanone

$C_{17}H_{25}BrO_2$ mol. wt. 341.29



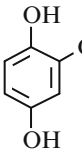
Synthesis
-Refer to: [2709].

Methyl ether [867213-74-9]
$C_{18}H_{27}BrO_2$ mol. wt. 355.31
-Obtained by acylation of anisole with 11-bromo-undecanoic acid in the presence of a catalytic amount of p-toluenesulfonic acid and graphite for 4 h at 90° (84 %) [2709].

m.p. 190° [2709];
^{1}H NMR [2709], ^{13}C NMR [2709], IR [2709], MS [2709].

11-Bromo-1-(2,5-dihydroxyphenyl)-1-undecanone

$C_{17}H_{25}BrO_3$ mol. wt. 357.28



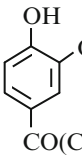
Synthesis
-Refer to: [3385].

Dimethyl ether [374808-62-5]
$C_{19}H_{29}BrO_3$ mol. wt. 385.34

USE: Linking agents for fluorescent labelling of nanocrystals or quantum dots [2653].

11-Bromo-1-(3,4-dihydroxyphenyl)-1-undecanone

[22421-07-4] $C_{17}H_{25}BrO_3$ mol. wt. 357.29



Synthesis
-Obtained by reaction of 11-bromoundecanoic acid with pyrocatechine in the presence of boron trifluoride at 70–80° for 2 h 30 min (70 %) [2749].
m.p. 88–94° [2748, 2749].

Diacetate [34767-67-4] $C_{21}H_{29}BrO_5$ mol. wt. 441.36

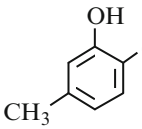
-Refer to: [2749].

m.p. 73–75° [2748].

2.2 Substituted Hydroxyketones

11-Bromo-1-(2-hydroxy-4-methylphenyl)-1-undecanone

[218784-30-6] $C_{18}H_{27}BrO_2$ mol. wt. 355.32

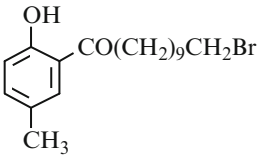


Syntheses
-Obtained by direct acylation of m-cresol with 11-bromo-undecanoic acid in the presence of AMA, a mixture of alumina and methanesulfonic acid, at 140° for 5 min (80 %) [2833].
-Also obtained by Fries rearrangement of m-cresyl 11-bromoundecanoate in the presence of AMA, a mixture of alumina and methanesulfonic acid, at 160° for 30 min (80 %) [2833].

white crystals [2833]; m.p. 62° [2833];
^{1}H NMR [2833], IR [2833], UV [2833], MS [2833].

11-Bromo-1-(2-hydroxy-5-methylphenyl)-1-undecanone
2-(11-Bromo-1-undecanoyl)-5-methylphenol

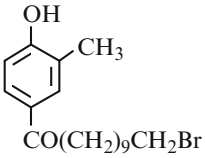
$C_{18}H_{27}BrO_2$ mol. wt. 355.32



Synthesis
-Refer to: [2834].
^{1}H NMR [2834], ^{13}C NMR [2834].

11-Bromo-1-(4-hydroxy-3-methylphenyl)-1-undecanone

$C_{18}H_{27}BrO_2$ mol. wt. 355.27



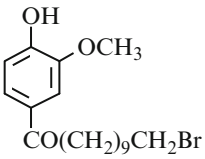
Synthesis
-Refer to: [218].
Methyl ether [927911-89-5]
$C_{19}H_{29}BrO_2$ mol. wt. 369.34

-Obtained by reaction of 11-bromoundecanoic acid with 2-methylanisole in the presence of $HSiMe_2Cl$ and $InCl_3$ (or $InBr_3$) in 1,2-dichloroethane, first 1 h at r.t., then heated at 80° for 4 h (71 %) (or 74 %) [218].

m.p. 35–37° [218];
^{1}H NMR [218], ^{13}C NMR [218], IR [218], MS [218].

11-Bromo-1-(4-hydroxy-3-methoxyphenyl)-1-undecanone

[13149-43-4] $C_{18}H_{27}BrO_3$ mol. wt. 371.32



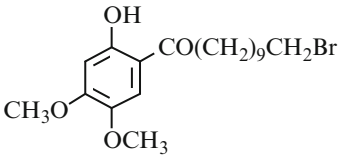
Synthesis
-Obtained by reaction of 11-bromoundecanoic acid with guaiacol in the presence of boron trifluoride first at 40°, then at 70° for 2.5 h (44.9 %) [2750].
m.p. 68–69° with softening at 63° [2750].

Allyl ether [13149-44-5] $C_{21}H_{31}BrO_3$ mol. wt. 411.38

-Obtained by reaction of allyl bromide with the title ketone in the presence of potassium carbonate in refluxing acetone for 9 h [2750].
m.p. 68–70° with sintering at 65° [2750].

11-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-undecanone

[173055-46-4] $C_{19}H_{29}BrO_4$ mol. wt. 401.34

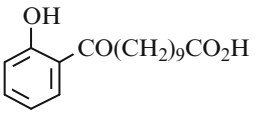


Synthesis
-Refer to: [2623].

3 Aromatic Hydroxyketone Derived from 11-Oxoundecanoic Acid

11-(2-Hydroxyphenyl)-11-oxo-1-undecanoic acid

$C_{17}H_{24}O_4$ mol. wt. 292.38



Synthesis
-Refer to: [1131].
m.p. 85–87° [1131]; ^{1}H NMR [1131].

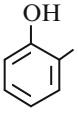
Chapter 10
Dodecanones

1 Aromatic Hydroxyketones Derived from Dodecanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-1-dodecanone

[2589-83-5] $C_{18}H_{28}O_2$ mol. wt. 276.42



Syntheses

-Preparation by reaction of lauric acid with phenol,

*in the presence of melted zinc chloride for 6 h (65–70 %) [2398];

*in the presence of the Japanese acid clay at 190° for 2 h [1785].

-Also obtained by Fries rearrangement of phenyl laurate [12],

*with aluminium chloride at 70° for 10 h (28 %) [2550], at 150° for 1 h [293] or in tetrachloroethane [3169].

*in the presence of aluminium chloride in refluxing carbon disulfide for 5 h. Then, the mixture was kept at 80–90° for 2 h and at 140–150° for 1 h after solvent elimination (33 %) [1222];

*in the presence of aluminium chloride in nitrobenzene [718] according to [380];

*in the presence of aluminium chloride in nitrobenzene for 15 h at 50° (10 %) [378];

*in the presence of titanium tetrachloride at high temperature [718] according to [1762].

-Also obtained by reaction of lauroyl chloride with phenol in the presence of aluminium chloride,

*in tetrachloroethane for 6 h at 55–60° (33 %) [2548];

*in nitrobenzene for 3 h at 70° (21 %) [2549];

*in carbon disulfide for 5.5 h at 47° (41 %) [2549].

-Also refer to: [12, 77, 110, 718, 873, 1230, 1271, 1456, 1985, 2316, 3122].

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b.p.$_{1.6}$ 180–204° [293];
m.p. 45–46.5° [718], 44–45.5° [2548], 44–45° [12, 3169], 44° [2398], 43.8–44.6° [293];
IR [12]; TLC [1456].

USE: Textile rot proofing by, [873].

BIOLOGICAL ACTIVITY: Effect on bacteria (*staphylococcus aureus and tricophyton asteroides*) [3122].

Oxime [20803-93-4] $C_{18}H_{29}NO_2$ mol. wt. 291.43

-Refer to: [12, 110].

m.p. 75–76° [12]; IR [12].

USE: In extn. of copper and nickel from sulfate solns. [110].

Oxime, nickel complex [55917-79-8]

USE: Quenchers for singlet oxygen, [3483].

Semicarbazone [20803-53-6] $C_{19}H_{31}N_3O_2$ mol. wt. 333.47

m.p. 139–145° (d) [12]; IR [12].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 92–93° [2548], 91° [3169], 89–89.2° [293].

Methyl ether $C_{19}H_{30}O_2$ mol. wt. 290.45

-Obtained by reaction of dimethyl sulfate with the above ketone in the presence of potassium carbonate in boiling acetone for 6 h [2398].

colourless liquid [2398]; b.p.$_{50}$ 110° [2398].
^{1}H NMR [1596], ^{13}C NMR [1596], MS [1596].

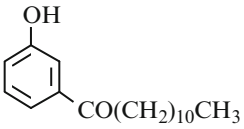
2,3-Epoxypropyl ether [18110-29-7] $C_{21}H_{32}O_3$ mol. wt. 332.48

-Obtained by reaction of epichlorohydrin with o-dodecanoylphenol (0.1 mol) in the presence of 30 % sodium hydroxide between 40 and 50° (62 %) [2669].

b.p.$_{0.7}$ 235–240° [2669].

1-(3-Hydroxyphenyl)-1-dodecanone

[63442-86-4] $C_{18}H_{28}O_2$ mol. wt. 276.42



Syntheses
-Refer to: [1984, 1985].
m.p. 40° [1984]; IR [1984].

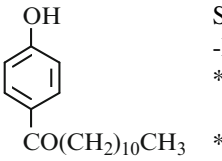
Methyl ether [63442-83-1] $C_{19}H_{30}O_2$ mol. wt. 290.45

-Refer to: [1984, 1985, 2725].

b.p.$_{10}$ 132–135° [1984]; IR [1984].

1-(4-Hydroxyphenyl)-1-dodecanone

[2589-74-4] $C_{18}H_{28}O_2$ mol. wt. 276.42



Syntheses
-Preparation by reaction of lauric acid with phenol,
*in the presence of boron trifluoride for 2 h at 70° (84 %) [1685] or for 3 h at 80–90° (68.6 %) [1938];
*in the presence of the Japanese acid clay at 190° for 2 h [1785].

-Also obtained by Fries rearrangement of phenyl laurate with aluminium chloride, (65 %) [414],
*for 10 h at 70° (46 %) [2550] or for 1 h at 150° [293, 2163];
*in tetrachloroethane [3169];
*in nitrobenzene (67 %) [2947], at 38° for 48 h (65 %) [414, 415] or at r.t. overnight (56 %) [1769];
*in the presence of aluminium chloride in nitrobenzene [718] according to [380];
*in the presence of aluminium chloride in nitrobenzene for 15 h at 50° (60 %) [378];
*in the presence of aluminium chloride in refluxing carbon disulfide for 5 h. Then, the mixture was kept at 80–90° for 2 h and at 140–150° for 1 h after solvent elimination (42 %) [1222].
-Also obtained by demethylation of its methyl ether [2398].
-Also obtained by reaction of lauroyl chloride with phenol in the presence of aluminium chloride,
*in tetrachlorethane for 6 h at 55–60° (25 %) [2548];
*in nitrobenzene at 70° for 3 h (73 %) [2549];
*in carbon disulfide at 47° for 5.5 h (55 %) [2549].
-Also obtained by reaction of dodecanoyl chloride with phenol in the presence of aluminium chloride in methylene chloride for 14 h at r.t. (28 %) [1910].
-Also obtained by heating 2-hydroxy-5-(1-oxododecyl)benzoic acid in quinoline in the presence of copper for 1 h at 210° (96 %) [448].
-Also obtained by reaction of lauric acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3277].

-Also refer to: [12, 293, 378, 379, 513, 1271, 1299, 1456, 1863, 1908, 1985, 2035, 2316, 2697, 2945, 3109, 3122, 3371, 3424].

b.p.$_{.0.2}$ 195° [448], b.p.$_{.0.3}$ 198° [2035], b.p.$_{.10}$ 250–257° [2947], b.p.$_{.15}$ 275° [2163]; b.p.$_{.15}$ 277° [293];
off-white solid [1910];
m.p. 72° [2398], 71.2–71.6° [1863], 71–72° [2548], 71–71.5° [3277], 71° [12, 1685, 3169],
70.5–71° [293], 70–72° [1938], 70–71° [378, 2163, 2549], 70° [414, 415],
69.6–70.4° [1910], 68–70° [1769], 62° [3424], 61–62° [379];
^{1}H NMR [1910, 3424], ^{13}C NMR [1910], IR [12, 1910], MS [1910]; TLC [1456].

USE: Activator for peroxygen bleach in laundry detergent for mud-soiled clothing [3371]; Ether with polyoxyethylene glycol, as herbicide [2697]; Foaming improvement of N-acylamino alkanesulfonate detergents by, [2945]; Textile rot proofing by, [873].

BIOLOGICAL ACTIVITY: Inhibition of 17-β-hydroxysteroid dehydrogenase 3 [1908, 1910]; Effect on bacteria (*staphylococcus aureus and tricophyton asteroides*) [3122].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_5$ mol. wt. 456.54

m.p. 151–152° [293], 150.5° [3169], 150–151° [378, 2548], 144–144.5° [448].

Oxime [20803-52-5] $C_{18}H_{29}NO_2$ mol. wt. 291.43

m.p. 77–79° [12]; IR [12].

Semicarbazone [20803-54-7] $C_{19}H_{31}N_3O_2$ mol. wt. 333.47

m.p. 143–143.6° [293], 140–141° [12]; IR [12].

Acetate $C_{20}H_{30}O_3$ mol. wt. 318.46

-Preparation by reaction of acetic anhydride with the title ketone in the presence of sulfuric acid [378].

m.p. 68° [378].

Benzoate $C_{25}H_{32}O_3$ mol. wt. 380.53

-Obtained from Schotten-Baumann reaction [293, 378, 448].

m.p. 109–110° [448], 109–109.8° [293], 108° [378].

Laurate [122214-67-9] $C_{30}H_{50}O_3$ mol. wt. 458.73

-Obtained by reaction of lauric acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3277].

m.p. 76.5–77.5° [3277].

Methyl ether [63829-20-9] $C_{19}H_{30}O_2$ mol. wt. 290.45

-Obtained by reaction of lauroyl chloride with anisole,
*in the presence of aluminium chloride (90 %) [2398];
*in the presence of iodine (50 %) [378];
*under microwaves (90 W; 2 min x 4; 410°) in the presence of graphite (74 %) [1830].
-Also obtained by reaction of lauric acid with anisole,
*in the presence of polyvalent-metal salts of dodecatungstophosphate as effective heterogeneous catalysts for Friedel-Crafts acylation [2870];
*in the presence of montmorillonite-enwrapped titanium as a solid acid catalyst for 48 h at 165° (97 %) [937];
*over zeolite catalysts through Friedel-Crafts acylation [3353].
-Also obtained by reaction of dimethyl sulfate with the title ketone in the presence of alkali [448], (quantitative yield) [378].
-Also obtained by reaction of dodecanoic acid with anisole in the presence of $Cs_{2.5}H_{0.5}PW_{12}O_{40}$ at 110° for 5 h (25 %) [1636].
-Also obtained by reaction of dodecanoic acid with anisole in the presence of $HNTf_2$ in refluxing toluene for 36 h, using a Dean-Stark apparatus (84 %) [1648].
-Also refer to: [175, 378, 416, 1009, 1480, 1963, 2016, 2035, 2252, 2641, 3221].

white powder [937]; plates [2398, 2548];
m.p. 62.5° [1963], 58.5° [378], 57–59° [2548], 57° [2398], 55.5–56.5° [2016], 55–57.5° [3221], 40–45° [448];
^{1}H NMR [937], ^{13}C NMR [937].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{25}H_{34}N_4O_5$ mol. wt. 470.57

m.p. 108–109° [2016].

2-Chloroethyl ether $C_{20}H_{31}ClO_2$ mol. wt. 338.92

-Obtained by reaction of dodecanoyl chloride with 2-chloroethoxybenzene in the presence of aluminium chloride in carbon disulfide for 4 h at 50° (55 %) [476].

shining leaflets [476]; m.p. 72.5° [476].

3-Bromopropyl ether $C_{21}H_{33}BrO_2$ mol. wt. 397.39

-Obtained by reaction of dodecanoyl chloride with 3-bromopropoxybenzene in the presence of aluminium chloride in carbon disulfide for 4 h at 50° (45 %) [476].

m.p. 39–40° [476].

4-Bromobutyl ether $C_{22}H_{35}BrO_2$ mol. wt. 411.42

-Obtained by reaction of dodecanoyl chloride with 4-bromobutoxybenzene in the presence of aluminium chloride in carbon disulfide for 4 h at 50° (33 %) [476].

m.p. 57–58° [476].

2-Hydroxyethyl ether $C_{29}H_{32}O_3$ mol. wt. 320.47

USE: Foaming improvement of N-acylamino alkanesulfonate detergents by, [2945].

N-Dimethylaminoethyl ether $C_{22}H_{37}NO_2$ mol. wt. 347.54

-Obtained by reaction of 4-(2-chloroethoxy)dodecanophenone with dimethylamine in a sealed tube for 2 h at 150° (88.5 %) [476].

free base: $b.p._{0.01}$ 193–197° [476]; m.p. 45–46° [476].
hydrochloride: m.p. 173–175° [476].

N-Dimethylaminopropyl ether $C_{23}H_{39}NO_2$ mol. wt. 361.57

-Obtained by reaction of 4-(3-bromopropoxy)dodecanophenone with dimethylamine in a sealed tube for 2 h at 150° (89 %) [476].

free base: $b.p._{0.1}$ 206° [476]; m.p. 31–32° [476].
hydrochloride: m.p. 186° [476].

N-Dimethylaminobutyl ether $C_{24}H_{41}NO_2$ mol. wt. 375.60

-Obtained by reaction of 4-(4-bromobutoxy)dodecanophenone with dimethylamine in a sealed tube for 2 h at 150° (92 %) [476].

free base: $b.p._{0.005}$ 202° [476].
hydrochloride: m.p. 179° [476].

N-Diethylaminoethyl ether [14392-83-7] $C_{24}H_{41}NO_2$ mol. wt. 375.60

-Obtained by treatment of 4-hydroxydodecanophenone sodium salt in ethanol with diethylaminoethyl chloride in refluxing toluene for 5 h (71 %) [414], (68 %) [415].

free base: $b.p._{0.002}$ 210–220° [414, 415]; $n_D^{21} = 1.5036$ [414, 415].
hydrochloride: m.p. 107–108° [513].

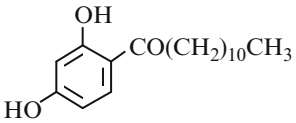
2,3-Epoxypropyl ether [18110-30-0] $C_{21}H_{32}O_3$ mol. wt. 332.48

-Obtained by reaction of epichlorohydrin with p-dodecanoylphenol (0.1 mol) in the presence of 30 % sodium hydroxide between 40 and 50° (59 %) [2669].

m.p. 105° [2669].

1-(2,4-Dihydroxyphenyl)-1-dodecanone

[25632-60-4] $C_{18}H_{28}O_3$ mol. wt. 292.42



Syntheses

-Preparation by reaction of lauric acid with resorcinol,
*in the presence of boron trifluoride for 2 h at 90° (79 %) [2312];
*in the presence of zinc chloride at 150° [2517] or at 125–135° [893].

-Also prepared by reaction of lauronitrile with resorcinol (Hoesch reaction) (20 %) [2928].

-Also obtained by Fries rearrangement of resorcinol dilaurate with aluminium chloride in nitrobenzene for 8 h at 40–50° (24 %) [379].

-Also refer to: [284, 379, 598, 788, 859, 1655, 1700, 2273, 2509, 2790, 2842, 2973, 3077, 3125, 3221].

b.p.$_{.8}$ 260–265° [1700], b.p.$_{.7}$ 243° [3125], b.p.$_{.6–.7}$ 237–239° [893, 2842];
m.p. 84–85.5° [893, 2842], 84° [2312], 82.5–83.5° [3125], 82–83° [379], 81–82° [2273], 79–80° [1700], 77–78° [3221].

USE: Synthesis of substituted polyaniline monomer [788]; Hair conditioning and/or colouring compositions [598]; In prepn. of photog. black coupler [2509]; Polyamide fibers modified with, transparency of, [2790].

4-Nitrophenylhydrazone $C_{24}H_{33}N_3O_4$ mol. wt. 427.54

m.p. 86–87° [859].

2,4-Dinitrophenylhydrazone $C_{24}H_{32}N_4O_6$ mol. wt. 472.54

m.p. 165° [379].

Diacetate [251463-52-2] $C_{22}H_{32}O_5$ mol. wt. 376.49

-Obtained by reaction of acetic anhydride with the title ketone in the presence of pyridine (>80 %) [2517].

white solid [2517]; m.p. 50–51° [2517];
^{1}H NMR [2517], ^{13}C NMR [2517], IR [2517], UV [2517], MS [2517].

Monohydrate $C_{18}H_{28}O_3, H_2O$ mol. wt. 310.43

m.p. 78–79° [3125].

Dimethyl ether $C_{20}H_{32}O_3$ mol. wt. 320.47

m.p. 46° [16].

4-(2-Propenyl) ether $C_{21}H_{32}O_3$ mol. wt. 332.48

USE: Protection against actinic radiations [2959].

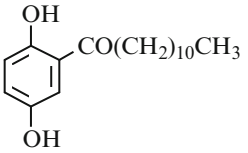
4-(2-Chloro-2-propenyl) ether $C_{21}H_{31}ClO_3$ mol. wt. 366.93

m.p. 57.2–58.3° [2959]; UV [2959].

USE: Protection against actinic radiations [2959].

1-(2,5-Dihydroxyphenyl)-1-dodecanone

[4693-30-5] $C_{18}H_{28}O_3$ mol. wt. 292.42



Syntheses

-Obtained by reaction of lauroyl chloride with hydroquinone in the presence of aluminium chloride in nitrobenzene at r.t. overnight, then heated on a water bath for 3 h [1442].

-Also obtained by Fries rearrangement of hydroquinone dilaurate with aluminium chloride at 150–160° for 5 h [1442].

-Also obtained by reaction of dodecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156].

-Also obtained by treatment of hydroquinone and dodecanoic acid mixture in carbon tetrachloride below 60° with boron trifluoride, kept overnight at r.t., then heated 5 h at 90–95° (58 %) [3204].

-Also obtained by treatment of its dimethyl ether with hydrobromic acid in acetic acid at 0°. The mixture was heated on a stand bath for 6 h under reflux [1442].

-Also obtained by deketalization of 2-dodecanoyl-3-hydroxycyclohex-2-en-1-one with concentrated sulfuric acid in refluxing acetone for 160 min and stand overnight at r.t. [2335].

-Also obtained by reaction of lauroyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in carbon disulfide [159].

-Also refer to: [394, 3204].

light yellow material [2335]; yellow needles [159];
m.p. 101° [1442, 3204], 99° [156, 159];
^{1}H NMR [2335], MS [2335]; TLC [2335]; GLC [2335].

USE: Effect on photographic fogging in multilayered colour films, [394].

Oxime $C_{18}H_{29}NO_3$ mol. wt. 307.43

USE: Effect on photographic fogging in multilayered colour films [394].

Dimethyl ether [98314-46-6] $C_{20}H_{32}O_3$ mol. wt. 320.47

-Obtained by reaction of lauroyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [2859],
*in nitrobenzene at r.t. overnight, the mixture was heated on a water bath for 3 h [1442];
*in tetrachloroethane (76 %) [714].
-Also refer to: [714, 2151].

$b.p._{\cdot 0.2}$ 175–178° [714], $b.p._{1.2}$ 180–185° [1442]; m.p. 27.5° [714];
^1H NMR [2859], MS [2859].

Diethyl ether $C_{22}H_{36}O_3$ mol. wt. 348.53

-Obtained by reaction of lauroyl chloride with hydroquinone diethyl ether in the presence of aluminium chloride in tetrachloroethane (65 %) [714].

$b.p._{\cdot 0.34}$ 180–190° [714]; m.p. 34–35° [714].

2,4-Dinitrophenylhydrazone of the diethyl ether $C_{28}H_{40}N_4O_6$ mol. wt. 528.65

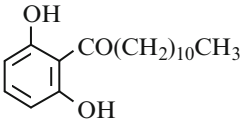
bright red crystals [714]; m.p. 77.5° [714].

Di-dodecyl ether [72047-09-7] $C_{43}H_{78}O_3$ mol. wt. 643.09

-Refer to: [3021–3023].

1-(2,6-Dihydroxyphenyl)-1-dodecanone

[125009-82-7] $C_{18}H_{28}O_3$ mol. wt. 292.42



Syntheses
-Obtained by refluxing a solution of 2-dodecanoyl-3-hydroxycyclohex-2-en-1-one, $Hg(OAc)_2$ and NaOAc in acetic acid under nitrogen for 6.5 h (66 %) [2334].

-Obtaining from 1,3-cyclohexanedione (54 %) [2336].
-Also obtained from methyl 2,6-dimethoxybenzoate [2336].
-Also obtained in three steps, starting from the enolate of 5-hydroxycyclohexane-1,3-dione [3439].
-Also refer to: [2249, 2418].

Isolation from natural sources

-From the exocrine secretions of lace bugs [1563].
-From the exocrine secretions of andromeda lace bug *Stephanitis takeyai* (Hemiptera: Tingidae) [2334].
-A component of the setal exudate of immature andromeda lace bugs (*Stephanitis takeyai* Drake and Maa) [2334, 2336].

-Of the setal exudate of nymphs of the andromeda lace bug, *Stephanitis takeyai* (Hemiptera: Tingidae) [2334].
-From *Stephanitis rhododendrii* [2334].
-In the wood of *Knema austrosiamensis* W. J. J. O. DeWilde (Myristaceae) [1133] or in Ground wood of this same plant [1134].
-From *Horsfieldia irya* seeds [3314].

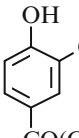
m.p. 86–88° [2334, 2336];
^{1}H NMR [1133, 2334, 2336], IR [2336], UV [2334], MS [1133, 2334, 2336].

USE: Nickel-chelating agent [3080].

BIOLOGICAL ACTIVITY: This compound was equal to aspirin in inhibition of PGE_2 formation with fat body preparations of the American cockroach *(Periplaneta americana)* [1563]; This compound inhibited prostaglandin synthase in two *in vitro systems* [1563]; Inhibition of soybean urease by cyclic β-triketones and fluoride ions [3080].

1-(3,4-Dihydroxyphenyl)-1-dodecanone
(4-Dodecanoylcatechol)

[1158-20-9] $C_{18}H_{28}O_3$ mol. wt. 292.42



Syntheses
-Obtained by treatment of a pyrocatechol and lauric acid mixture,
*with zinc chloride at 135–140° for 2 h (20 %) [1283];
*with zinc chloride and phosphorous oxychloride at 70° for 90 min (83.2 %) [2812].
-Also obtained by reaction of dodecanoyl chloride with pyrocatechol in the presence of aluminium chloride in nitrobenzene, first at 5–7° for 2 h, then at r.t. for 2–3 days (62 %) [1726].
-Also refer to: [283, 985, 3056].

m.p. 105–106° [2812], 97–98° [1283];
^{1}H NMR [1726], UV [985].

USE: Antioxidant [2812].

BIOLOGICAL ACTIVITY: Protective agent against the lethal effects of X-rays [1809].

2,4-Dinitrophenylhydrazone [97153-67-8] $C_{24}H_{32}N_4O_6$ mol. wt. 472.54

bright red needles [2812]; m.p. 216° [2812].

Dimethyl ether [96966-45-9] $C_{20}H_{32}O_3$ mol. wt. 320.47

-Preparation by Friedel-Crafts acylation of veratrole [3056].
-Also obtained by reaction of dodecanoyl chloride with veratrole in the presence of zinc chloride in refluxing carbon disulfide for 6 h and then left overnight (55 %) [2420].
-Also refer to: [1167, 1960, 1963, 3365].

white needles [2420]; b.p.$_1$ 200° [2420];
m.p. 70–71° [2420], 68–69° [1960, 1963], 57° [3056];
^{1}H NMR [1167], ^{13}C NMR [1167], IR [3365].

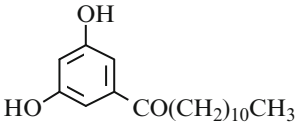
2,4-Dinitrophenylhydrazone of the dimethyl ether

[102947-41-1] $C_{26}H_{36}N_4O_6$ mol. wt. 500.60

m.p. 80–81° [2420].

1-(3,5-Dihydroxyphenyl)-1-dodecanone

[1250871-16-9] $C_{18}H_{28}O_3$ mol. wt. 292.42



Synthesis
-Refer to: [2903].
m.p. 101–103° [2903];
^{1}H NMR [2903], ^{13}C NMR [2903], MS [2903].

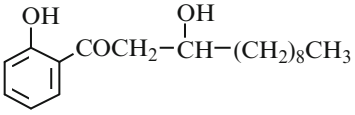
Dimethyl ether [55049-56-4] $C_{20}H_{32}O_3$ mol. wt. 320.47

-Refer to: [1899, 2903].

m.p. 52–53° [2903];
^{1}H NMR [2903], ^{13}C NMR [2903], MS [2903].

3-Hydroxy-1-(2-hydroxyphenyl)-1-dodecanone

[133839-66-4] $C_{18}H_{28}O_3$ mol. wt. 292.42



Synthesis
-Refer to: [3151].

12-Hydroxy-1-(3-hydroxyphenyl)-1-dodecanone

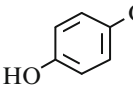
$C_{18}H_{28}O_3$ mol. wt. 292.42

Synthesis
-Obtained by treatment of its tert-butyl dimethylsilyl ether with tetrabutylammonium fluoride in tetrahydrofuran at 0° for 0.5 h (99 %) [1596].

^{1}H NMR [1596], ^{13}C NMR [1596], MS [1596].

12-Hydroxy-1-(4-hydroxyphenyl)-1-dodecanone

$C_{18}H_{28}O_3$ mol. wt. 292.42

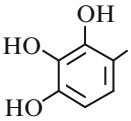


Synthesis
-Obtained by treatment of its tert-butyl dimethylsilyl ether with tetrabutylammonium fluoride in tetrahydrofuran at 0° for 0.5 h (99 %) [1596].

^{1}H NMR [1596], ^{13}C NMR [1596], MS [1596].

1-(2,3,4-Trihydroxyphenyl)-1-dodecanone

[15251-74-8] $C_{18}H_{28}O_4$ mol. wt. 308.42



Syntheses
-Preparation by reaction of lauric acid with pyrogallol,
*in the presence of boron trifluoride,
-in trichloroethylene or carbon tetrachloride for 2–3 h between 65 and 85° (95–98 %) [503];
-without solvent at 55° for 1.5 h [3200];
*in the presence of zinc chloride at 135–140° for 2 h (30 %) [1283];
*in the presence of strongly acidic ion exchanger Amberlyst-15 at 120° for 24 h (38 %) [231].
-Also obtained by reaction of dodecanoyl chloride with pyrogallol,
*without catalyst at 150° for 2 h (5 %) [3200];
*in the presence of aluminium chloride in nitrobenzene, first at 5–7° for 2 h, then at r.t. for 2–3 days (31 %) [1726].
-Also refer to: [859, 2328, 3200].

m.p. 85–86° [3200], 78° [503], 76–77° [1283], 74–75° [859];
^{1}H NMR [231, 1726], ^{13}C NMR [231], UV [3200].

USE: Colour photographic material containing scavenger for oxidized colour developing agent [2328]; Pressure-sensitive copying paper coatings contg for examination papers with hidden texts [1982].

BIOLOGICAL ACTIVITY: Protection against whole-body irradiation [1810].

4-Nitrophenylhydrazone $C_{24}H_{33}N_3O_5$ mol. wt. 443.54

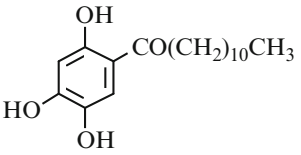
m.p. 182–183° [859].

2,4-Dinitrophenylhydrazone [14725-80-5] $C_{24}H_{32}N_4O_7$ mol. wt. 488.54

m.p. 215–216° (d) [3200]; UV [3200].

1-(2,4,5-Trihydroxyphenyl)-1-dodecanone

[109559-39-9] $C_{18}H_{28}O_4$ mol. wt. 308.42



Syntheses

-Obtained by reaction of lauroyl chloride with 1,2,4-trihydroxybenzene in the presence of aluminium chloride in nitrobenzene [291, 292].

-Also refer to: [1708].

m.p. 119–121° [291, 292].

USE: Antioxidant [1708]; Antioxidant for fats, oils and paraffin waxes [292]; Manuf. of, and oxidative stabilization of fats, oils and paraffin waxes by, [291].

BIOLOGICAL ACTIVITY: Toxicity [1708].

Trimethyl ether [56134-35-1] $C_{21}H_{34}O_4$ mol. wt. 350.50

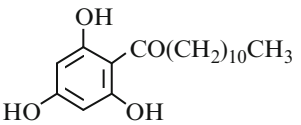
-Preparation by treatment of 2,4,5-trihydroxydodecanophenone with dimethyl sulfate in the presence of potassium carbonate in refluxing acetone for 4 h (88 %) [2752].

-Also refer to: [714].

m.p. 55–56° [2752], 53° [714].

1-(2,4,6-Trihydroxyphenyl)-1-dodecanone

[6790-21-2] $C_{18}H_{28}O_4$ mol. wt. 308.42



Syntheses

-Obtained by reaction of dodecanoyl chloride with phloroglucinol in the presence of boron trifluoride etherate, first at 0°, then at r.t. for 48 h under nitrogen [2786].

-Also obtained by reaction of dodecanoyl chloride with phloroglucinol in the presence of aluminium chloride [2364] in nitrobenzene and carbon disulfide mixture (58 %) [2113].

-Also obtained by reaction of lauronitrile with phloroglucinol (Hoesch reaction) [1441].

-Also obtained by reaction of dodecanoic acid with phloroglucinol in the presence of aluminium chloride and phosphorous oxychloride (40 %) [3202].

-Also obtained by reaction of lauric anhydride with phloroglucinol in tetrahydrofuran in the presence of boron trifluoride etherate at r.t. under nitrogen, for 48 h (78 %) [1975].

-Preparation (25 %) [3202] using to the process [3201].

-Also refer to: [1184, 1694, 1974, 2433, 3202].

Isolation from natural sources

-From the fruits of *Knema glauca* (Myristicaceae) [2562].
-In the wood of *Knema austrosiamensis* W. J. J. O. DeWilde (Myristaceae) [1133] or in Ground wood of this same plant [1134].
-In the seeds of *Horsfieldia iryaghedi* WARB. also named *Myristica horsfieldia* or *Myristica iryaghedhi* (Myristicaceae) [1184, 1694].
-In the bark, leaf and timber of *Horsfieldia iryaghedi* (Myristicaceae) [3111].
-In the seeds of *Myristica fragrans* Houttuyn (nutmegs) [1694].

White amorphous solid [2562], white crystals [3202];
colourless needles [3111], colourless crystalline solid [1184],
colourless plates [1694], colourless solid [1975];
m.p. 134° [2113, 3202], 128–130° [1184], 126–127° [3111], 125–126° [1694], 94–96° [1441].
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [1133, 1694, 1975, 2364, 2562, 3111, 3202], ^{13}C NMR [1975, 2562, 3202], IR [1184, 1694, 2562, 3111, 3202], UV [1694, 2562, 3202],
MS [1133, 1694, 1975, 2562, 3111, 3202];
TLC [1184, 1694, 1975, 3202]; GLC [1694].

BIOLOGICAL ACTIVITY: Simplified YM-26734 inhibitors of secreted phospholipase A_2 group IIA [2364]; Antituberculosis activity against the microbe Mycobacterium tuberculosis [2562]; Antiviral activity against herpes simplex virus type 1 [2562]; Antimycobacterial and antimalarial activities [2562]; Cytotoxicity [2562, 3202]; Antifungal [2113, 3202]; Antibacterial [3202].

Trimethyl ether [888026-39-9] $C_{21}H_{34}O_4$ mol. wt. 350.50

-Refer to: [16, 1974].

m.p. 40° [16]; ^{1}H NMR [1974], ^{13}C NMR [1974].

Triacetate [40220-94-8] $C_{24}H_{34}O_7$ mol. wt. 434.53

-Obtained by reaction of acetic anhydride with 2,4,6-trihydroxydodecanophenone in the presence of pyridine at r.t. for 48 h [1694].

Amorphous [1694]; ^{1}H NMR [1694], IR [1694], MS [1694].

Tris(phenylmethyl) ether [850816-19-2] $C_{39}H_{46}O_4$ mol. wt. 578.79

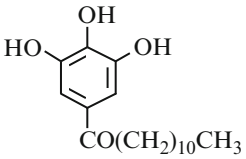
-Preparation by reaction of benzyl bromide with 1-(2,4,6-trihydroxyphenyl)-1-dodecanone in DMF in the presence of potassium carbonate at 40° under a nitrogen atmosphere overnight (63 %) [1975].

USE: DNA polymerase β-inhibiting, and DNA-damaging activity of (+)-myristinin A [1975]; Stereoselective synthesis, abs. stereochem. [1975].

colourless oil [1975];
^{1}H NMR [1975], ^{13}C NMR [1975], MS [1975]; TLC [1975].

1-(3,4,5-Trihydroxyphenyl)-1-dodecanone

[40336-21-8] $C_{18}H_{28}O_4$ mol. wt. 308.42



Synthesis
-Refer to: [1982].

USE: Pressure-sensitive copying paper coatings contg for examination papers with hidden texts [1982].

Trimethyl ether $C_{21}H_{34}O_4$ mol. wt. 350.50

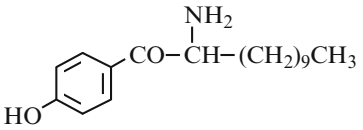
m.p. 65° [160].

4-Nitrophenylhydrazone $C_{27}H_{39}N_3O_5$ mol. wt. 485.62

m.p. 96° [160].

3-Amino-1-(4-hydroxyphenyl)-1-dodecanone

$C_{18}H_{29}NO_2$ mol. wt. 291.43



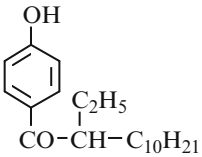
Synthesis
-Refer to: [2253].

Hydrochloride [63424-82-8] $C_{18}H_{29}NO_{2,\ HCl}$ mol. wt. 327.90

m.p. 182–183° [2253]; IR [2253].

2-Ethyl-1-(4-hydroxyphenyl)-1-dodecanone

$C_{20}H_{32}O_2$ mol. wt. 304.47



Synthesis
-Refer to: [956].

Methyl ether [201791-66-4]
$C_{21}H_{34}O_2$ mol. wt. 318.50

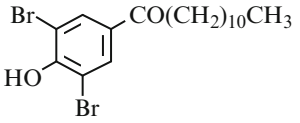
-Obtained from 4-methoxyphenyl cyclopropyl ketone and 1-iododecane (95 %) [956].

^{1}H NMR [956], ^{13}C NMR [956], MS [956]; TLC [956].

1.2 Substituted Hydroxyketones

1-(3,5-Dibromo-4-hydroxyphenyl)-1-dodecanone

[1393654-90-4] $C_{18}H_{26}Br_2O_2$ mol. wt. 434.21

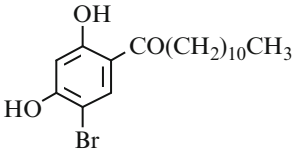


Synthesis
-Obtained by reaction of bromine in acetic acid with the hydroxydodecanone [2339].

BIOLOGICAL ACTIVITY: Enzyme activity, inhibition of, [2339].

1-(5-Bromo-2,4-dihydroxyphenyl)-1-dodecanone

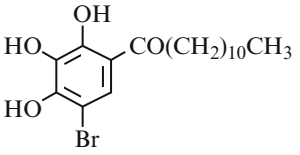
$C_{18}H_{27}BrO_3$ mol. wt. 371.32



Synthesis
-Refer to: [859].
m.p. 84–85° [859].

1-(5-Bromo-2,3,4-trihydroxyphenyl)-1-dodecanone

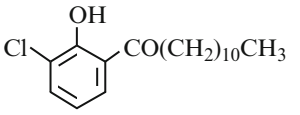
$C_{18}H_{27}BrO_4$ mol. wt. 387.31



Synthesis
-Refer to: [859].
m.p. 84–85° [859].

1-(3-Chloro-2-hydroxyphenyl)-1-dodecanone

$C_{18}H_{27}ClO_2$ mol. wt. 310.86

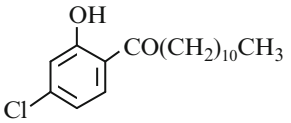


Synthesis
-Refer to: [483].
Oxime [101002-23-7]
$C_{19}H_{28}ClNO_2$ mol. wt. 325.87

USE: Topical preparations comprising at least one aryloxime and bisabolol [483]; As lipoxygenase inhibitor [3077].

1-(4-Chloro-2-hydroxyphenyl)-1-dodecanone

[859310-32-0] $C_{18}H_{27}ClO_2$ mol. wt. 310.86



Syntheses
-Preparation by Fries rearrangement of 3-chlorophenyl laurate with aluminium chloride,
*without solvent at 130° for 2 h (50 %) [2802];
*in nitrobenzene at 25° for 6 h (76 %) [2802].

b.p.$_{.38}$ 240° [2802].

2,4-Dinitrophenylhydrazone $C_{24}H_{31}ClN_4O_5$ mol. wt. 490.99

m.p. 118° [2802].

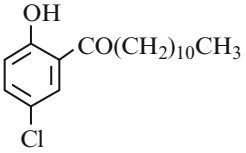
Methyl ether $C_{19}H_{29}ClO_2$ mol. wt. 324.89

-Obtained by methylation of the above ketone in the usual way (77 %) [2802].

b.p.$_{.31}$ 150° [2802].

1-(5-Chloro-2-hydroxyphenyl)-1-dodecanone

[98813-30-9] $C_{18}H_{27}ClO_2$ mol. wt. 310.86



Syntheses
-Obtained by reaction of dodecanoyl chloride with 4-chlorophenol in the presence of aluminium chloride (67.8 %) [2680].
-Also refer to: [483].

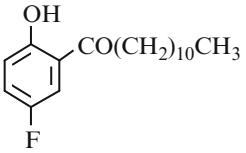
b.p.$_{1}$ 170–173° [2680]; m.p. 74–75° [2680].

Oxime [101002-24-8] $C_{18}H_{28}ClNO_2$ mol. wt. 325.88

USE: Topical preparations comprising at least one aryloxime and bisabolol [483]; As lipoxygenase inhibitor [3077].

1-(5-Fluoro-2-hydroxyphenyl)-1-dodecanone

[1480-47-3] $C_{18}H_{27}FO_2$ mol. wt. 294.41



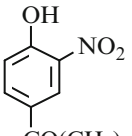
Synthesis
-Obtained by Fries rearrangement of p-fluorophenyl laurate with aluminium chloride for 2 h at 130° (50 %) [1549].
b.p.$_{10}$ 320° [1549].

2,4-Dinitrophenylhydrazone [2341-98-2] $C_{24}H_{31}FN_4O_5$ mol. wt. 474.53

m.p. 105° [1549].

1-(4-Hydroxy-3-nitrophenyl)-1-dodecanone

[70079-24-2] $C_{18}H_{27}NO_4$ mol. wt. 321.42



Syntheses

-Obtained by treatment of 4-dodecanoylphenol with concentrated nitric acid in concentrated sulfuric acid at 0° for 1 h 15 min (91 %) [1222].

-Also refer to: [1221, 1223, 1226].

m.p. 72–73° [1222]; ^{1}H NMR [1222].

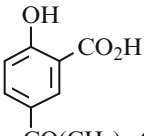
N.B.: Active 4-dodecanoyl-2-nitrophenyl esters of β-alanine, β-alanyl-β-alanine and β-alanyl-β-alanyl-β-alanine were prepared, and tried to polymerize in various solvents [1223].

Methyl ether [76752-90-4] $C_{19}H_{29}NO_4$ mol. wt. 335.44

-Refer to: [1221].

2-Hydroxy-5-dodecanoylbenzoic acid

[78418-03-8] $C_{19}H_{28}O_4$ mol. wt. 320.43



Syntheses

-Obtained by treatment of its methyl ester with 10 % potassium hydroxide in methanol at reflux for 2–2.5 h (64 %) [448].

-Also obtained by saponification of the methyl ester (94 %) [689].

-Also refer to: [1844, 1855, 2439].

b.p.$_{0.5}$ 205–230° [448]; m.p. 121–122° [448], 119–120° [689].

USE: For the preparation of a cosmetic, dermatological or pharmaceutical composition [2885].

Oxime $C_{19}H_{29}NO_4$ mol. wt. 335.44

m.p. 113–116° [448].

Thiosemicarbazone $C_{20}H_{31}N_3O_3S$ mol. wt. 393.55

m.p. 230–232° [448].

Methyl ester [78432-96-9] $C_{20}H_{30}O_4$ mol. wt. 334.46

-Obtained by Fries rearrangement of methyl 2-lauroyloxybenzoate (b.p.$_{0.5}$ 200–205°; m.p. 23–27°) with aluminium chloride in nitrobenzene for 4 h at 60° (82 %) [448].
-Also obtained by reaction of dodecanoyl chloride with methyl salicylate in the presence of aluminium chloride in carbon disulfide first at 5–10°, then at r. t. for 12 h (82 %) [689].

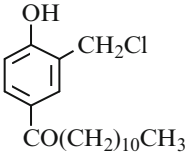
oil [448]; m.p. 70–72° [689].

Ethyl ester $C_{21}H_{32}O_4$ mol. wt. 348.48

b.p.$_{0.5}$ 210–215° [448].

1-[(3-Chloromethyl)-4-hydroxyphenyl]-1-dodecanone

$C_{19}H_{29}ClO_2$ mol. wt. 324.89



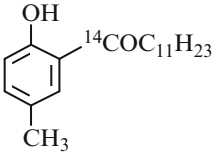
Synthesis
-Refer to: [2252].

Methyl ether $C_{20}H_{31}ClO_2$ mol. wt. 338.92
-Refer to: [2252].

m.p. 41–43° [2252].

1-(2-Hydroxy-5-methylphenyl)-^{14}C-1-dodecanone

$C_{18}{}^{14}CH_{30}O_2$ mol. wt. 292.44

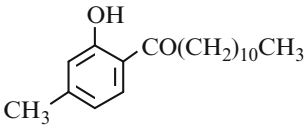


Synthesis
-It was prepared in 2 steps from p-cresol and $CH_3(CH_2)_{10}{}^{14}COCl$ by Friedel-Crafts acylation in the presence of aluminium chloride at 40° to give intermediate ester, which underwent a Fries rearrangement in carbon disulfide (80 %) [474].

HPLC [474], TLC [474].

1-(2-Hydroxy-4-methylphenyl)-1-dodecanone

[72724-26-6] $C_{19}H_{30}O_2$ mol. wt. 290.45



Syntheses

-Preparation by Fries rearrangement of 3-methylphenyl laurate with aluminium chloride without solvent at 140–150° [906].

-Preparation by one-step esterification-Fries rearrangement:

Obtained by heating a mixture of m-cresol and lauric acid with aluminium chloride at 180° for 3 h (esterification). Then, aluminium chloride was added and the mixture heated 2 h again at 180° (70 %) (Fries rearrangement) [1144].

-Also refer to: [17, 92, 1050, 2983, 3013].

m.p. 45–46° [906], 43–44° [3013];
GC [3012, 3013]; polarity [3013].

Nickel complex [80849-31-6].

-Refer to: [1050].

Oxime [40867-42-3] $C_{19}H_{31}NO_2$ mol. wt. 305.46

-Refer to: [17, 2473, 3044].

USE: Copper extn. by, [3044]; Triplet state quenching by, kinetics of [17].

Oxime, nickel complex [29666-10-2]

USE: Antifading agent from, for colour photothermog. image [1071]; Colour photog. material contg. antioxidant and magenta coupler and, with improved image stability [2283]; Photog. stabilizer compns. contg. phenol derivs. and, for magenta images [1050]; Singlet oxygen quenching by, [976]; Antioxidant light stabilizers, for acrylic graft polymers, [3484]; Light stabilizers, for polystyrene, [1251]; Light stabilizers, for titanium dioxide-pigmented polyolefins, [88]; Light stabilizers, for piperidinoanthraquinone dye in epoxy resin film, [86]; Light stabilizers, for polypropylene, mechanism of activity of, [87].

Oxime, nickel complex [40690-25-3]

-Refer to: [451].

USE: Triplet state quenching by, kinetics of [17].

Oxime, palladium complex [41894-24-0]

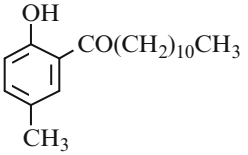
-Energy transfer to ligand-field states of, in aromatic hydrocarbon triplet state quenching [92].

Oxime, cobalt alloys [60202-03-1]

-Catalyst, for oxidation of cycloalkanes to cycloalkanol-cycloalkanone mixtures [426].

1-(2-Hydroxy-5-methylphenyl)-1-dodecanone

[75487-44-4] $C_{19}H_{30}O_2$ mol. wt. 290.45



Syntheses

-Obtained by Fries rearrangement of 4-methylphenyl dodecanoate,

*in the presence of aluminium chloride in nitrobenzene for 2 h at 120° [3434];

*under microwave irradiation for 8 min (89.5–93.4 %) [3434].

-Also obtained by reaction of dodecanoyl chloride with p-cresol in the presence of aluminium chloride [3431], (77 %) [2909] in ethylene chloride at 110–120° for 8 h (71 %) [1769].

-Also refer to: [972, 1355, 1356, 1827, 2078, 2079, 3077, 3432, 3433].

-Refer to: [1827, 2167].

Light yellow solid [2909];
b.p.$_4$ 186–188° [1769]; b.p.$_3$ 190° [2909];
m.p. 43–45° [2909], 37.5–39° [1769];
UV [1827], MS [1827].

USE: Surface activity of Schiff base surfactant [3433].

BIOLOGICAL ACTIVITY: Biotransformation of the lipoxygenase inhibitor (FLM 5011) [1827].

Oxime [50652-76-1] [103582-41-8] (E) $C_{19}H_{31}NO_2$ mol. wt. 305.46

-Refer to: [110, 484–488, 1034, 1769, 1826, 1921, 1927, 2167, 2474, 2475, 2742, 3011, 3149, 3290].

m.p. 95–96.5° [1769];
^{1}H NMR [1769, 1921], ^{13}C NMR [1769], IR [1769, 1921],
UV [1769, 1827, 1921], MS [1769, 1827, 1921].

USE: Compounds comprising active agents, natural products, and vitamins in combination with energy for regulation of mammalian keratinous tissue using skin and/or hair care actives [2078]; Skin and/or hair care compounds comprising Boswellia serrata tree gum and resin xymenynic acid and glycyrrhizinic acid for regulation of mammalian keratinous tissue [2079]; Protective effect of lipoxygenase inhibition during the early septic state [2119]; Topical preparations comprising at least one aryloxime and bisabolol [483]; Solvent extraction of copper (II) [1769, 2520]; In extn. of copper and nickel from sulfate solns. [110].

BIOLOGICAL ACTIVITY: Biotransformation of the lipoxygenase inhibitor (FLM 5011) [1827]; Cytotoxicity [1826]; As lipoxygenase inhibitor [3077]; Also refer to: [2167, 3149].

Oxime, nickel complex [52672-75-0]

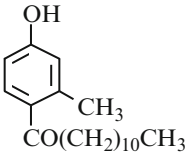
USE: Light stabilizer, for polypropylene, mechanism of action of, [3441].

2,4-Dinitrophenylhydrazone [127699-73-4] $C_{25}H_{34}N_4O_5$ mol. wt. 470.57

m.p. 94–95° [1769].

1-(4-Hydroxy-2-methylphenyl)-1-dodecanone

$C_{19}H_{30}O_2$ mol. wt. 290.45



Synthesis
-Refer to: [2503].

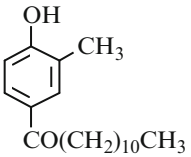
Phenyl ether [791615-80-0]
$C_{25}H_{34}O_2$ mol. wt. 366.54

-Obtained by adding a mixture of m-phenoxytoluene and dodecanoyl chloride to a suspension of aluminium chloride in methylene chloride at 0°, then the mixture stirred for 1.5–2 h at 3–5° (34 %) [2503].

b.p.$_{.3}$ 240–245° [2503]; ^{1}H NMR [2503], IR [2503], MS [2503].

1-(4-Hydroxy-3-methylphenyl)-1-dodecanone

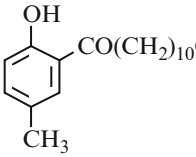
[29665-55-2] $C_{19}H_{30}O_2$ mol. wt. 290.45



Synthesis
-Obtained by Fries rearrangement of phenyl laurate in the presence of aluminium chloride in nitrobenzene [718], according to [380].
m.p. 66–67° [718].

12-Hydroxy-1-(2-hydroxy-5-methylphenyl)-1-dodecanone

$C_{19}H_{30}O_3$ mol. wt. 306.45

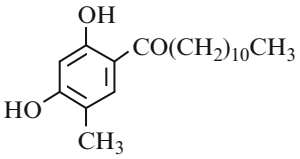


Synthesis
-Refer to: [1827].
UV [1827].

BIOLOGICAL ACTIVITY: Metabolite of 2-hydroxy-5-methylaurophenone oxime in isolated rat hepatocytes.

1-(2,4-Dihydroxy-5-methylphenyl)-1-dodecanone

[95102-14-0] $C_{19}H_{30}O_3$ mol. wt. 306.45



Syntheses
-Refer to: [1595, 2704].

USE: Colour developer, for thermal recording materials [1595].

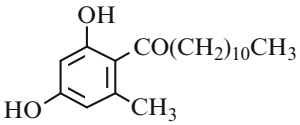
Dimethyl ether $C_{21}H_{34}O_3$ mol. wt. 334.50

-Obtained by reaction of dodecanoyl chloride with 4-methylresorcinol dimethyl ether in the presence of aluminium chloride in 1,2-dichloroethane first at 0°, then 2 h at r.t. (30 %) [11].

m.p. 67–69° [11].

1-(2,4-Dihydroxy-6-methylphenyl)-1-dodecanone
(4-Dodecanoylorcin)

$C_{19}H_{30}O_3$ mol. wt. 306.45

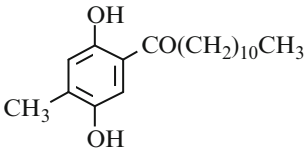


Synthesis
-Obtained by reaction of dodecanoyl chloride with orcinol in the presence of aluminium chloride in nitrobenzene first 3 h at 0°, then at r.t. (20 %) [11].

m.p. 95–97° [11].

1-(2,5-Dihydroxy-4-methylphenyl)-1-dodecanone

$C_{19}H_{30}O_3$ mol. wt. 306.45



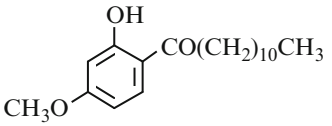
Syntheses
-Refer to: [3021–3023].

Dihexadecyl ether [72046-93-6]
$C_{51}H_{94}O_3$ mol. wt. 755.31
-Refer to: [3021–3023].

USE: Colour photog. stabilizer compn. contg. [3023]; Photog. stabilizer compn. contg. hydroquinone deriv. and, [3021]; Photog. stabilizer compns. contg. for colour photog. materials [3022].

1-(2-Hydroxy-4-methoxyphenyl)-1-dodecanone

[143286-96-8] $C_{19}H_{30}O_3$ mol. wt. 306.45



Syntheses

-Obtained by reaction of methyl bromide with 1-(2,4-dihydroxyphenyl)-1-dodecanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

-Also refer to: [1787, 2273, 2959].

m.p. 50–51° [2273], 48–50° [284]; ^{1}H NMR [284].

USE: Protection against actinic radiations [2959].

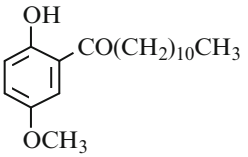
Oxime [143286-65-1] $C_{19}H_{31}NO_3$ mol. wt. 321.46

-Obtained by reaction of hydroxylamine hydrochloride with 1-(2-hydroxy-4-methoxyphenyl)-1-dodecanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 76.5–78.5° [284]; ^{1}H NMR [284].

1-(2-Hydroxy-5-methoxyphenyl)-1-dodecanone

[56134-29-3] $C_{19}H_{30}O_3$ mol. wt. 306.45



Syntheses

-Obtained by reaction of dodecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156] in carbon disulfide [159].

-Also obtained by reaction of dodecanoic acid with hydroquinone monomethyl ether in the presence of boron trifluoride at 60° for 15 h (49 %) [2752].

-Also obtained by reaction of lauroyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in carbon disulfide [159].

-Also obtained by treatment of lauroylhydroquinone with diazomethane [159].

light yellow quartz-like crystals [159];
m.p. 43–44.5° [2752], 42–43° [156, 159].

Oxime [140943-15-3] $C_{19}H_{31}NO_3$ mol. wt. 321.46

-Refer to: [285].

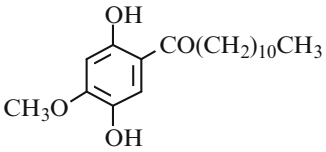
BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

2,4-Dinitrophenylhydrazone $C_{25}H_{34}N_4O_6$ mol. wt. 486.57

m.p. 121–124° [156, 159].

1-(2,5-Dihydroxy-4-methoxyphenyl)-1-dodecanone

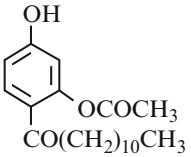
[116577-54-9] $C_{19}H_{30}O_4$ mol. wt. 322.44



Synthesis
-Obtained by deprotection of 2-hydroxy-5-levulinyloxy-4-methoxydodecanophenone (m.p. 55–56°) with a sodium sulfite and sodium metabisulfite mixture in aqueous tetrahydrofuran, acetonitrile or ethanol at 40° for 3 h (95 %) [2345].

1-[2-(Acetyloxy)-4-hydroxyphenyl]-1-dodecanone

[251463-56-6] $C_{20}H_{30}O_4$ mol. wt. 334.46

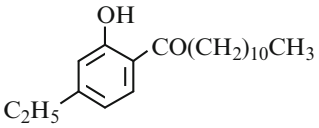


Synthesis
-Obtained by selective deacetylation of 2,4-diacetoxyphenyl undecyl ketone mediated by porcine pancreatic lipase (PPL) in THF at 42–45° for 24 h in the presence of n-butanol (45 %) [2517].

light yellow solid [2517]; m.p. 104° [2517];
^{1}H NMR [2517], ^{13}C NMR [2517], IR [2517], UV [2517], MS [2517].

1-(4-Ethyl-2-hydroxyphenyl)-1-dodecanone

$C_{20}H_{32}O_2$ mol. wt. 304.47



Syntheses
-Obtained by Fries rearrangement of 3-ethylphenyl n-laurate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (75 %) [2801];
*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (73 %) [2801].

b.p.$_{28}$ 230° [2801].

2,4-Dinitrophenylhydrazone $C_{26}H_{36}N_4O_5$ mol. wt. 484.60

m.p. 90° [2801].

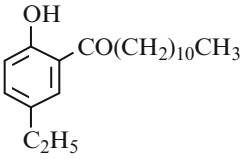
Methyl ether $C_{21}H_{34}O_2$ mol. wt. 318.50

-Obtained by reaction of dimethyl sulfate with 1-(4-ethyl-2-hydroxyphenyl)-1-dodecanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (82 %) [2801].

b.p.$_{35}$ 195° [2801].

1-(5-Ethyl-2-hydroxyphenyl)-1-dodecanone

$C_{20}H_{32}O_2$ mol. wt. 304.47



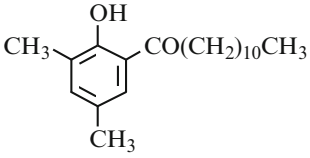
Synthesis
-Obtained by Fries rearrangement of 4-ethylphenyl laurate with aluminium chloride at 100° for 2 h (67 %) [2800].
b.p.$_{19}$ 210° [2800].

2,4-Dinitrophenylhydrazone $C_{26}H_{36}N_4O_5$ mol. wt. 484.60

m.p. 75° [2800].

1-(2-Hydroxy-3,5-dimethylphenyl)-1-dodecanone

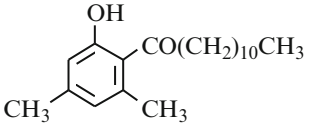
$C_{20}H_{32}O_2$ mol. wt. 304.47



Synthesis
-Refer to: [1831].
Oxime, nickel complexes
-Ultraviolet light inhibitor, spandex fibers contg., [1831].

1-(2-Hydroxy-4,6-dimethylphenyl)-1-dodecanone

[7282-05-5] $C_{20}H_{32}O_2$ mol. wt. 304.47



Syntheses
-Obtained by Fries rearrangement of 3,5-dimethylphenyl n-laurate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (67 %) [2801];
*in the presence of aluminium chloride (2.8 M), first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (60 %) [2801].
-Also obtained by reaction of lauric acid with 3,5-dimethylphenol in the presence of boron trifluoride (56 %) [749].

light yellow oil [749], white crystals [749];
b.p.$_1$ 180–182° [749], b.p.$_2$ 200° [2801]; m.p. 42–44° [749].

4-Nitrophenylhydrazone $C_{26}H_{37}N_3O_3$ mol. wt. 439.60

m.p. 190° [2801].

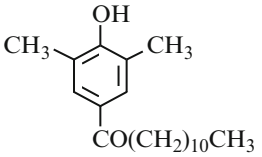
Methyl ether $C_{21}H_{34}O_2$ mol. wt. 318.50

-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxy-4,6-dimethylphenyl)-1-dodecanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (75 %) [2801].

$b.p._{.35}$ 220° [2801].

1-(4-Hydroxy-3,5-dimethylphenyl)-1-dodecanone

[23666-67-3] $C_{20}H_{32}O_2$ mol. wt. 304.47



Syntheses

-Obtained by Fries rearrangement of 2,6-dimethylphenyl laurate (*vic-m-Xylenyl dodecanoate*) ($b.p._{.12}$ 216–218°; m.p. 28–29°) in the presence of aluminium chloride (67 %) [184].

-Also obtained by reaction of dodecanoyl chloride with 2,6-dimethylphenol according to the method described previously [2871], (51 %) [119].

-Also obtained by reaction of lauroyl chloride with 2,6-dimethylphenol at 100° in the presence of aluminium chloride and heating at 120–140° for 1 h (58 %) [1832].

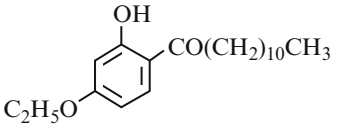
-Also obtained by reaction of dodecanoic acid with 2,6-dimethylphenol in the presence of boron trifluoride [1832].

-Also refer to: [1832].

$b.p._{.0.5}$ 175–185° [1832];
m.p. 52–53° [184], 52–52.5° [119], 50–51° [1832];
^{1}H NMR [119], IR [119].

1-(4-Ethoxy-2-hydroxyphenyl)-1-dodecanone

[49572-23-8] $C_{20}H_{32}O_3$ mol. wt. 320.47



Synthesis

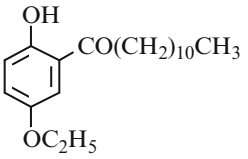
-Refer to: [2273, 2959].

m.p. 50–51° [2273].

USE: Protection against actinic radiations [2959].

1-(5-Ethoxy-2-hydroxyphenyl)-1-dodecanone

[140943-35-7] $C_{20}H_{32}O_3$ mol. wt. 320.47



Synthesis
-Refer to: [285].

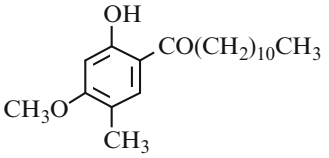
Oxime [140943-21-1]
$C_{20}H_{33}NO_3$ mol. wt. 335.49

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-(2-Hydroxy-4-methoxy-5-methylphenyl)-1-dodecanone

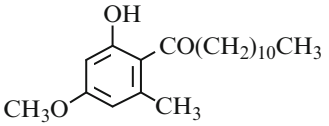
[60488-53-1] $C_{20}H_{32}O_3$ mol. wt. 320.47



Synthesis
-Obtained by selective demethylation of 1-(2,4-dimethoxy-5-methylphenyl)-1-dodecanone with boron trichloride in methylene chloride first at −70°, then 5 min at r.t. (83 %) [11].
m.p. 62–63° [11].

1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1-dodecanone

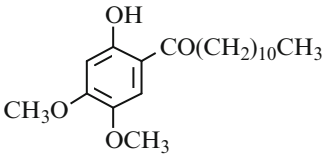
[60488-57-5] $C_{20}H_{32}O_3$ mol. wt. 320.47



Synthesis
-Preparation by partial methylation of 1-(2,4-dihydroxy-6-methylphenyl)-1-dodecanone with methyl iodide in the presence of potassium carbonate in refluxing acetone for 8 h (75 %) [11].
m.p. 58–59° [11].

1-(2-Hydroxy-4,5-dimethoxyphenyl)-1-dodecanone

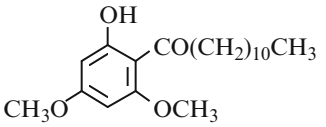
[56134-34-0] $C_{20}H_{32}O_4$ mol. wt. 336.47



Synthesis
-Obtained by reaction of dodecanoic acid with 1,2,4-trimethoxybenzene in the presence of boron trifluoride first at 90–100° for 3 h, then at 60–70° for 15 h (59 %) [2752].
m.p. 75.5–77° [2752].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-dodecanone

[40000-60-0] $C_{20}H_{32}O_4$ mol. wt. 336.47



Syntheses

-Obtained by reaction of dimethyl sulfate with 1-(2,4,6-trihydroxyphenyl)-1-dodecanone in the presence of potassium carbonate in acetone at 50–60° for 1.5 h under nitrogen (46 %) [2786].

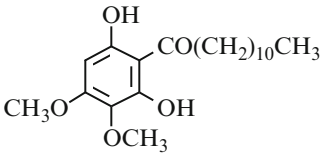
-Also obtained by methylation of dodecanoylphloroglucinol with diazomethane in ethanol at r. t. [1694].

-Also refer to: [2786].

m.p. 80–83° [2786], 79–82° [1694];
^{1}H NMR [2786], ^{13}C NMR [1694, 2786],
IR [1694], MS [1694, 2786].

1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-dodecanone

[134081-97-3] $C_{20}H_{32}O_5$ mol. wt. 352.47



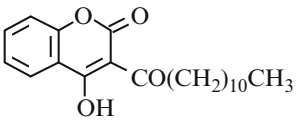
Synthesis

-Preparation by treatment of 1-[6-hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-dodecanone with potassium carbonate in refluxing methanol for 1–3 h (85 %) [1353].

m.p. 73–74° [1353]; ^{1}H NMR [1353].

4-Hydroxy-3-(1-oxododecyl)-2*H*-1-benzopyran-2-one

$C_{21}H_{28}O_4$ mol. wt. 344.45



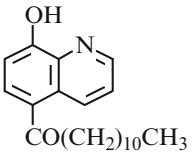
Synthesis

-Obtained by reaction of dodecanoyl chloride with 4-hydroxycoumarin in pyridine containing one drop of piperidine for 12 h on a water bath (57 %) [3174].

m.p. 110° [3174].

1-(8-Hydroxy-5-quinolinyl)-1-dodecanone

[101829-84-9] $C_{21}H_{29}NO_2$ mol. wt. 327.47



Syntheses

-Obtained by reaction of dodecanoyl chloride with 8-hydroxyquinoline in the presence of aluminium chloride [1336],

*in nitrobenzene at 80–85° for 15–16 h (55 %) [1725];

*in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

-Also obtained by treatment of its hydrochloride with a sodium acetate solution [1946].

-Also refer to: [2464].

m.p. 66.8–68.5° [1725], 66–67° [2261], 45–46° [1336], 43° [1946];
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [1725], IR [1725].

USE: Ion-flotation collector [1725]; Ion flotation with, of gallium [1725]; Good fungicide [1336]; Aluminium and gallium complexes, in extn., [2464]; Extn by, aluminium and gallium, [2464]; Extn. by Kelex 100 and, of aluminium and gallium, interface kinetics in relation to, [271].

Hydrochloride $C_{21}H_{29}NO_2$, HCl mol. wt. 363.92

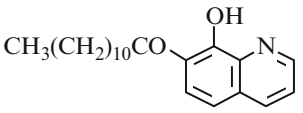
-Obtained by reaction of lauroyl chloride with 8-hydroxyquinoline in the presence of aluminium chloride in nitrobenzene for 12 h at 75–80° [1946].

Methyl ether $C_{22}H_{31}NO_2$ mol. wt. 341.50

-Obtained by treatment of 1-(8-hydroxy-5-quinolinyl)-1-dodecanone with dimethyl sulfate in benzene [1946].

1-(8-Hydroxy-7-quinolinyl)-1-dodecanone

[217815-28-6] $C_{21}H_{29}NO_2$ mol. wt. 327.47



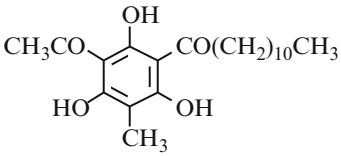
Synthesis

-Obtained by reaction of dodecanoyl chloride with 8-hydroxyquinoline in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

m.p. 56–58° [2261]; ^{1}H NMR [2261].

1-(3-Acetyl-2,4,6-trihydroxy-5-methylphenyl)-1-dodecanone

[1092783-61-3] $C_{21}H_{32}O_5$ mol. wt. 364.48

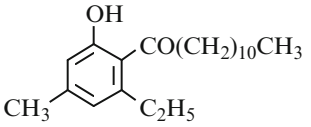


Synthesis
-Obtained by reaction of dodecanoyl chloride with 2,4,6-trihydroxy-3-methylacetophenone in the presence of aluminium chloride [2364].
^{1}H NMR [2364], MS [2364].

BIOLOGICAL ACTIVITY: Simplified YM-26734 inhibitors of secreted phospholipase A_2 group IIA [2364].

1-(2-Ethyl-6-hydroxy-4-methylphenyl)-1-dodecanone

$C_{21}H_{34}O_2$ mol. wt. 318.50



Syntheses
-Preparation by Fries rearrangement of 3-ethyl-5-methyl-phenyl laurate with aluminium chloride,
*without solvent at 130° for 2 h (75 %) [2802];
*in nitrobenzene at 25° for 6 h (78 %) [2802].

b.p.$_{.3}$ 280° [2802].

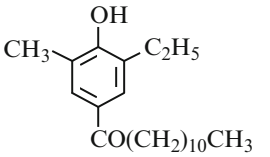
Methyl ether $C_{22}H_{36}O_2$ mol. wt. 332.53

-Obtained by methylation of the above ketone in the usual way (73 %) [2802].

b.p.$_{.23}$ 230° [2802].

1-(3-Ethyl-4-hydroxy-5-methylphenyl)-1-dodecanone

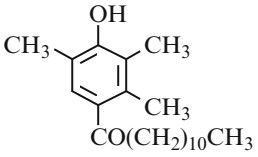
$C_{21}H_{34}O_2$ mol. wt. 318.50



Synthesis
-Obtained by Fries rearrangement of 2-ethyl-6-methylphenyl laurate (b.p.$_{.19}$ 218–220°) in the presence of aluminium chloride (24 %) [184].
m.p. 44.5–45.5° [184].

1-(4-Hydroxy-2,3,5-trimethylphenyl)-1-dodecanone

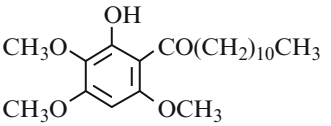
[137832-98-5] $C_{21}H_{34}O_2$ mol. wt. 318.50



Synthesis
-Refer to: [1733].

1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-dodecanone

[134081-66-6] $C_{21}H_{34}O_5$ mol. wt. 366.50



Syntheses

-Obtained by partial selective demethylation of crude 2,3,4,6-tetramethoxydodecanophenone with aluminium chloride in acetonitrile at 50° for 1–2 h (87 %) [1353].

-Also refer to: [1351].

m.p. 62–63° [1353]; ^{1}H NMR [1353].

p-Toluenesulfonic ester [134081-81-5] $C_{28}H_{40}O_7S$ mol. wt. 520.69

-Obtained by reaction of p-toluenesulfonyl chloride with 2-hydroxy-3,4,6-trimethoxy-dodecanophenone in the presence of potassium carbonate in refluxing acetone for 6–14 h (92 %) [1353].

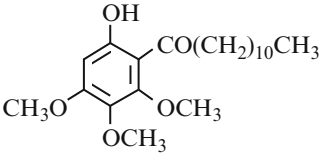
m.p. 85–87° [1353]; ^{1}H NMR [1353].

Methyl ether $C_{22}H_{36}O_5$ mol. wt. 380.52

-Obtained by reaction of dodecanoyl chloride with 1,2,3,5-tetramethoxybenzene in the presence of aluminium chloride in ethyl ether at 0° for 30 min [1353].

1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-dodecanone

[134081-73-5] $C_{21}H_{34}O_5$ mol. wt. 366.50



Syntheses

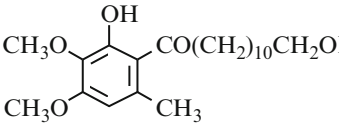
-Obtained by hydrogenation of (6-phenylmethoxy)-2,3,4-trimethoxydodecanophenone over 10 % palladium on charcoal in ethyl acetate/methanol (1:1) until the uptake of hydrogen ceased (91 %) [1353].

-Also refer to: [1351].

m.p. 43.5–44.5° [1353]; ^{1}H NMR [1353].

12-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-dodecanone

[77712-21-1] $C_{21}H_{34}O_5$ mol. wt. 366.50



Synthesis

-Obtained by treatment of its 12-acetyl ester with sodium hydroxide in methanol for 2 h at r.t. (75 %) [1147].

colourless needles [1147]; m.p. 82° [1147];
IR [1147], ^{1}H NMR [1147], MS [1147].

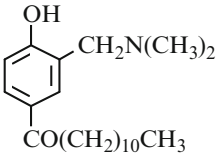
12-Acetyl ester [104966-93-0] $C_{23}H_{36}O_6$ mol. wt. 408.54

-Obtained by Friedel-Crafts reaction of 12-acetoxydodecanoyl chloride with 3,4,5-trimethoxy-toluene in 1,2-dichloroethane in the presence of aluminium chloride (2.1 mol) at 20° for 72 h [1147].

colourless oil [1147];
IR [1147], ^{1}H NMR [1147], MS [1147].

1-[3-(Dimethylaminomethyl)-4-hydroxyphenyl]-1-dodecanone

$C_{21}H_{35}NO_2$ mol. wt. 333.51

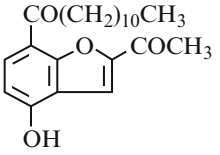


Synthesis
-Refer to: [379].

Methyl ether [63829-15-2]
$C_{22}H_{37}NO_2$ mol. wt. 347.54
-Refer to: [2252].

1-(2-Acetyl-4-hydroxy-7-benzofuranyl)-1-dodecanone

$C_{22}H_{30}O_4$ mol. wt. 358.48



Synthesis
-Refer to: [682].

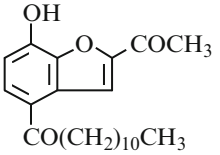
Methyl ether [59445-62-4]
$C_{23}H_{32}O_4$ mol. wt. 372.50

-Obtained by reaction of dodecanoyl chloride with 2-acetyl-4-methoxybenzofuran with aluminium chloride (2.4 mol) in methylene chloride at r.t. for 24 h (82 %) [682].

m.p. 88° [682].

1-(2-Acetyl-7-hydroxy-4-benzofuranyl)-1-dodecanone

$C_{22}H_{30}O_4$ mol. wt. 358.48



Synthesis
-Refer to: [682].

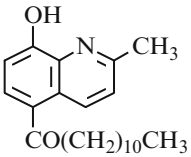
Methyl ether [59445-73-7]
$C_{23}H_{32}O_4$ mol. wt. 372.50

-Obtained by reaction of dodecanoyl chloride with 2-acetyl-7-methoxybenzofuran with aluminium chloride (2.4 mol) in methylene chloride at r.t. for 24 h (83 %) [682].

m.p. 83° [682].

1-(8-Hydroxy-2-methyl-5-quinolinyl)-1-dodecanone

[217815-24-2] $C_{22}H_{31}NO_2$ mol. wt. 341.50



Syntheses

-Obtained by reaction of dodecanoyl chloride with 8-hydroxyquinaldine in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

-Also refer to: [1336].

m.p. 52–54° [1336], 50–52° [2261]; MS [2261].

USE: Good fungicide [1336].

N-Methylcarbamate $C_{24}H_{34}NO_3$ mol. wt. 384.54

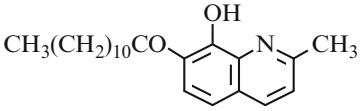
-Refer to: [1335] (36 %).

m.p. 87–90° [1335].

BIOLOGICAL ACTIVITY: Fungicide [1335].

1-(8-Hydroxy-2-methyl-7-quinolinyl)-1-dodecanone

[217815-27-5] $C_{22}H_{31}NO_2$ mol. wt. 341.50



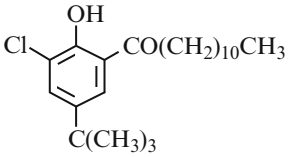
Synthesis

-Obtained by reaction of dodecanoyl chloride with 8-hydroxyquinaldine in the presence of aluminium chloride in nitrobenzene or 1,2-dichloroethane first at 10–30°, then at 70–80° for 20 h [2261].

m.p. 67–68° [2261]; IR [2261], MS [2261].

1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-dodecanone

[102701-83-7] $C_{22}H_{35}ClO_2$ mol. wt. 366.97



Synthesis

-Obtained by Fries rearrangement of 2-chloro-4-tert-butylphenyl laurate with aluminium chloride at 110° (68 %) [3119].

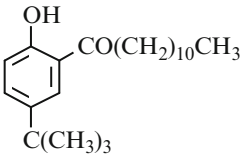
b.p.$_{22}$ 180° [3119].

2,4-Dinitrophenylhydrazone [103330-25-2] $C_{28}H_{39}ClN_4O_5$ mol. wt. 547.09

m.p. 193° [3119].

1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-dodecanone

$C_{22}H_{36}O_2$ mol. wt. 332.53



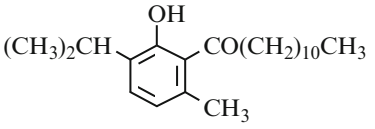
Synthesis
-Refer to: [1050].

Oxime, nickel complex [81321-89-3]

USE: Photog. stabilizer compns. contg. phenol derivs. and, for magenta images [1050].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-dodecanone

$C_{22}H_{36}O_2$ mol. wt. 332.53



Synthesis
-Obtained by Fries rearrangement of thymyl laurate with aluminium chloride at 120° (61 %) [2803].

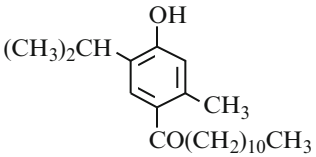
b.p.$_{16}$ 273° [2803].

2,4-Dinitrophenylhydrazone $C_{28}H_{40}N_4O_5$ mol. wt. 512.65

m.p. 151° [2803].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]dodecanone

$C_{22}H_{36}O_2$ mol. wt. 332.53



Synthesis
-Obtained (**XXX**) by treatment of 4-methoxy-2-methyl-5-isopropyldodecanophenone with boiling pyridinium chloride (205–215°) for 5 h (13 %) [2660].

b.p.$_{16}$ 265–267° [2660]; m.p. 59° [2660].

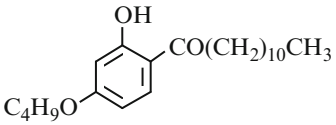
Methyl ether (**XIII**) $C_{23}H_{38}O_2$ mol. wt. 346.55

-Obtained by reaction of lauroyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (52 %) [2660].

b.p.$_{13}$ 245° [2660]; m.p. 29–30° [2660].

1-(4-Butoxy-2-hydroxyphenyl)-1-dodecanone

[143286-97-9] $C_{22}H_{36}O_3$ mol. wt. 348.53



Synthesis
-Obtained by reaction of butyl bromide with 1-(2,4-dihydroxyphenyl)-1-dodecanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 42–43° [284].

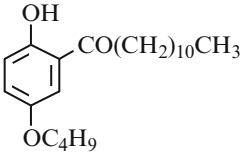
Oxime [143286-66-2] $C_{22}H_{37}NO_3$ mol. wt. 363.54

-Obtained by reaction of hydroxylamine hydrochloride with 1-(4-butoxy-2-hydroxyphenyl)-1-dodecanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 58–62° [284]; ^{1}H NMR [284].

1-(5-Butoxy-2-hydroxyphenyl)-1-dodecanone

[140943-39-1] $C_{22}H_{36}O_3$ mol. wt. 348.53



Synthesis
-Refer to: [285].

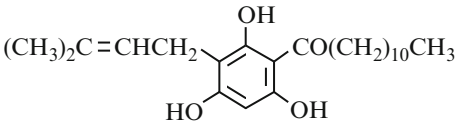
Oxime [140943-25-5]
$C_{22}H_{37}NO_3$ mol. wt. 363.54

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-dodecanone

[872178-00-2] $C_{23}H_{36}O_4$ mol. wt. 376.54



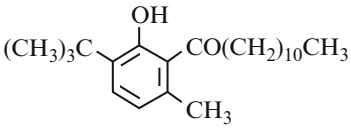
Synthesis
-Obtained by reaction of prenyl bromide with 2,4,6-trihydroxydodecanophenone in the presence of potassium carbonate in refluxing acetone for 5 h (13 %) [3202].

white crystalline solid [3202]; m.p. 114° [3202];
^{1}H NMR [3202], ^{13}C NMR [3202], IR [3202], UV [3202], MS [3202]; TLC [3202].

BIOLOGICAL ACTIVITY: Antibiotic [3202].

1-[3-(1,1-Dimethylethyl)-2-hydroxy-6-methylphenyl]-1-dodecanone

$C_{23}H_{38}O_2$ mol. wt. 346.55



Syntheses

-Obtained by Fries rearrangement of 2-tert-butyl-5-methylphenyl laurate,

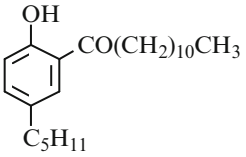
*in the presence of aluminium chloride (1.5 equiv.) in nitrobenzene at 25° for 6 h (72 %) [3118];

*in the presence of aluminium chloride (3 equiv.) at 110° for 2 h (68 %) [3118].

b.p.$_{17}$ 220° [3118].

1-(2-Hydroxy-5-pentylphenyl)-1-dodecanone

[102898-52-2] $C_{23}H_{38}O_2$ mol. wt. 346.55



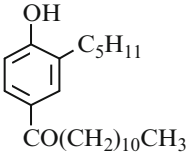
Synthesis

-Obtained by reaction of lauric acid with 4-pentylphenol in the presence of boron trifluoride (66 %) [142].

b.p.$_2$ 189–194° [142]; $n_D^{25} = 1.500$ [142].

1-(4-Hydroxy-3-pentylphenyl)-1-dodecanone

$C_{23}H_{38}O_2$ mol. wt. 346.55



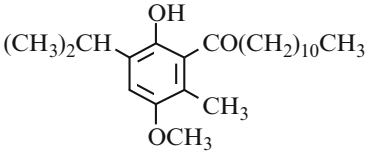
Synthesis

-Obtained by reaction of lauric acid with 2-pentylphenol in the presence of boron trifluoride (66 %) [142].

b.p.$_2$ 189–194° [142].

1-[2-Hydroxy-5-methoxy-6-methyl-3-(1-methylethyl)phenyl]-1-dodecanone

$C_{23}H_{38}O_3$ mol. wt. 362.55



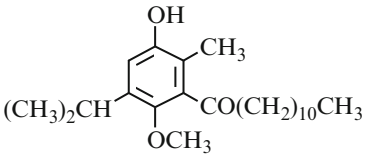
Synthesis

-Obtained by reaction of lauroyl chloride with 2-methyl-5-isopropylhydroquinone dimethyl ether in the presence of aluminium chloride in carbon disulfide, first at 40° for 1 h, then at 0° for 48 h and lastly on the boiling water bath for 3 h (10.5 %) [2663].

colourless crystals [2663]; b.p.$_{18}$ 127–129° [2663]; m.p. 91° [2663].

1-[3-Hydroxy-6-methoxy-2-methyl-5-(1-methylethyl)phenyl]-1-dodecanone

[115211-15-9] $C_{23}H_{38}O_3$ mol. wt. 362.55

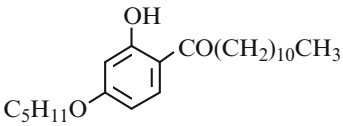


Synthesis
-Obtained by reaction of lauroyl chloride with 2-methyl-5-isopropylhydroquinone dimethyl ether in the presence of aluminium chloride in carbon disulfide, first at 40° for 1 h, then at 0° for 48 h and lastly on the boiling water bath for 3 h (10.5 %) [2663].

colourless crystals [2663]; b.p.$_{18}$ 127–129° [2663]; m.p. 91° [2663]; IR [2663].

1-(2-Hydroxy-4-pentyloxyphenyl)-1-dodecanone

[143286-98-0] $C_{23}H_{38}O_3$ mol. wt. 362.55



Synthesis
-Obtained by reaction of pentyl bromide with 1-(2,4-dihydroxyphenyl)-1-dodecanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 42° [284].

Oxime [143286-67-3] $C_{23}H_{39}NO_3$ mol. wt. 377.57

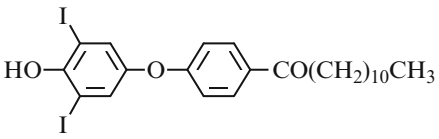
-Obtained by reaction of hydroxylamine hydrochloride with 1-(2-hydroxy-4-pentyloxyphenyl)-1-dodecanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 43° [284]; ^{1}H NMR [284].

4′-[4-Hydroxy-3,5-(diiodo)diphenyl]ether-4-(1-dodecanone)

4′-(4-Hydroxy-3,5-diiodophenoxy)dodecanophenone

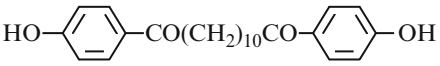
[23951-55-5] $C_{24}H_{30}I_2O_3$ mol. wt. 619.88



Synthesis
-Refer to: [512] (10 %).
colourless needles [512];
m.p. 118° (d) [512].

1,12-Bis(4-hydroxyphenyl)-1,12-dodecanedione

[107259-36-9] $C_{24}H_{30}O_4$ mol. wt. 382.50



Syntheses
-Refer to: [875, 905].

m.p. 177–181° [875].

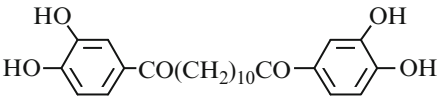
Dimethyl ether [4280-52-8] $C_{26}H_{34}O_4$ mol. wt. 410.55

-Obtained by reaction of dodecanoic acid dichloride with anisole in the presence of aluminium chloride without solvent at <40° (75 %) [905].

m.p. 132–133° [905].

1,12-Bis(3,4-dihydroxyphenyl)-1,12-dodecanedione

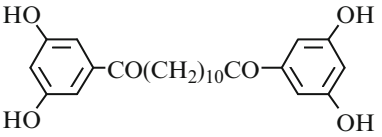
[30151-74-7] $C_{24}H_{30}O_6$ mol. wt. 414.50



Synthesis
-Refer to: [2751].
m.p. 204–208° [2751].

1,12-Bis(3,5-dihydroxyphenyl)-1,12-dodecanedione

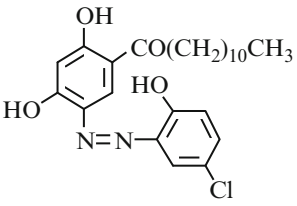
$C_{24}H_{30}O_6$ mol. wt. 414.50



Synthesis
-Refer to: [1316].
m.p. 140–145° [1316].

5-[[(5-Chloro-2-hydroxyphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone

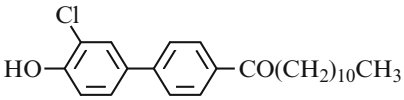
[26993-73-7] $C_{24}H_{31}ClN_2O_4$ mol. wt. 446.97



Synthesis
-Obtained by reaction of 2-amino-4-chlorophenol diazonium salt with 2,4-dihydroxylaurophenone in the presence of sodium hydroxide between 5 and 10° [577].
m.p. 247–248° [577].
Metal complexes Refer to: [577].

1-(3′-Chloro-4′-hydroxy[1,1′-biphenyl]-4-yl)-1-dodecanone

$C_{24}H_{31}ClO_2$ mol. wt. 386.66



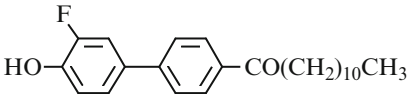
Synthesis
-Refer to: [2107].

6-Methyloctyl ether (S) [112780-57-1] $C_{33}H_{49}ClO_2$ mol. wt. 513.20

-Liq.-crystal compns. contg., for display devices [2107].

1-(3′-Fluoro-4′-hydroxy[1,1′-biphenyl]-4-yl)-1-dodecanone

[112780-73-1] $C_{24}H_{31}FO_2$ mol. wt. 370.51



Synthesis
-Refer to: [2107].
-Liq.-crystal compns. contg., for display devices [2107].

Methyl ether [112780-72-0] $C_{25}H_{33}FO_2$ mol. wt. 384.53

-Liq.-crystal compns. contg., for display devices [2107].

6-Methyloctyl ether (S) [112780-56-0] $C_{33}H_{49}FO_2$ mol. wt. 496.75

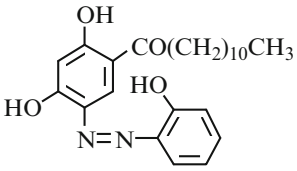
-Liq.-crystal compns. contg., for display devices [2107].

8-Methyldecyl ether (S) [112780-59-3] $C_{35}H_{53}FO_2$ mol. wt. 524.80

-Liq.-crystal compns. contg., for display devices [2107].

5-[[(2-Hydroxyphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone

[27020-17-3] $C_{24}H_{32}N_2O_4$ mol. wt. 412.53

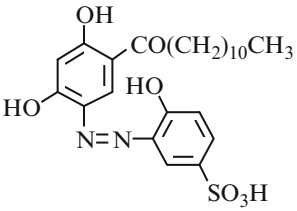


Synthesis
-Obtained by reaction of 2-aminophenol diazonium salt with 2,4-dihydroxylaurophenone in the presence of sodium hydroxide between 5 and 10° [577].
m.p. 185–187° [577].

Metal complexes Refer to: [577].

5-[[(2-Hydroxy-5-sulfonylphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone

$C_{24}H_{32}N_2O_7S$ mol. wt. 492.59



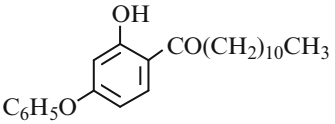
Synthesis

-Obtained by reaction of 2-amino-4-sulfonylphenol diazonium salt with 2,4-dihydroxylaurophenone in the presence of sodium hydroxide between 5 and 10° [578].

Metal complexes -Refer to: [578].

1-(2-Hydroxy-4-phenoxyphenyl)-1-dodecanone

[307000-48-2] $C_{24}H_{32}O_3$ mol. wt. 368.52



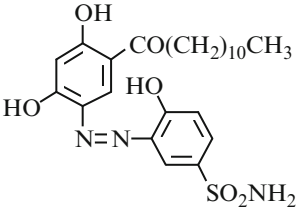
Synthesis

-Refer to: [1345].

BIOLOGICAL ACTIVITY: Antimicrobial [1345].

5-[[(5-Aminosulfonyl-2-hydroxyphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone

[26993-74-8] $C_{24}H_{33}N_3O_6S$ mol. wt. 491.61



Synthesis

-Obtained by reaction of 2-amino-4-aminosulfonylphenol diazonium salt with 2,4-dihydroxylaurophenone in the presence of sodium hydroxide between 5 and 10° [577].

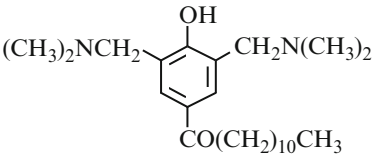
-Also refer to: [576].

m.p. 243–244° [576, 577].

Metal complexes -Refer to: [577].

1-[3,5-Bis(dimethylaminomethyl)-4-hydroxyphenyl]-1-dodecanone

$C_{24}H_{42}N_2O_2$ mol. wt. 390.61

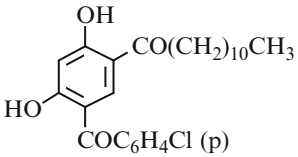


Synthesis

-Refer to: [379].

1-[5-(4-Chlorobenzoyl)-2,4-dihydroxyphenyl]-1-dodecanone

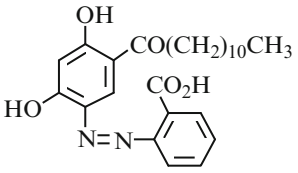
$C_{25}H_{31}ClO_4$ mol. wt. 430.10



Synthesis
-Preparation from 2,4-dihydroxy-4′-chlorobenzophenone [2131].
m.p. 54° [2131].

5-[[(2-Carboxyphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone

[26993-75-9] $C_{25}H_{32}N_2O_5$ mol. wt. 440.54



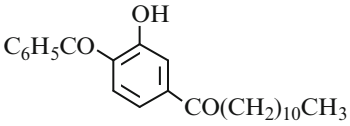
Synthesis
-Obtained by reaction of 2-aminobenzoic acid diazonium salt with 2,4-dihydroxylaurophenone in the presence of sodium hydroxide between 5 and 10° [577].
-Also refer to: [576].
m.p. 163–165° [576, 577].

Metal complexes Refer to: [577].

1-(4-Benzoyl-3-hydroxyphenyl)-1-dodecanone

4′-Benzoyl-3′-hydroxydodecanophenone

$C_{25}H_{32}O_3$ mol. wt. 380.53

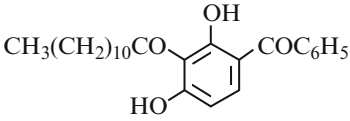


Synthesis
-Refer to: [1925].
UV [1925].

USE: Light stabilization of macromol. compds. [1925].

1-(3-Benzoyl-2,6-dihydroxyphenyl)-1-dodecanone

[14798-38-0] $C_{25}H_{32}O_4$ mol. wt. 396.53



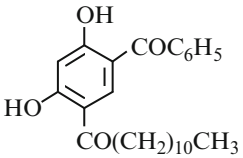
Syntheses
-Obtained by reaction of lauroyl chloride with 2,4-dihydroxybenzophenone in the presence of aluminium chloride in o-dichlorobenzene for 3 h at 120° [134].
-Also obtained by reaction of lauric acid with 2,4-dihydroxybenzophenone in the presence of para-toluenesulfonic acid in refluxing xylene for 20 h [134].
-Also refer to: [133, 1631].

m.p. 80–81° [134].

USE: For stabilizing polyolefins and vinyl halide resins against UV-light and sunlight [134]; As light stabilizer for chlorine-contg. polymers, [133]; Stabilization of vinyl halide resins and polyolefins against photodegradation [133].

1-(5-Benzoyl-2,4-dihydroxyphenyl)-1-dodecanone

[14814-73-4] $C_{25}H_{32}O_4$ mol. wt. 396.53



Syntheses

-Obtained by reaction of lauroyl chloride with 2,4-dihydroxybenzophenone in the presence of aluminium chloride in o-dichlorobenzene for 3 h at 120° [134].

-Also obtained by reaction of lauric acid with 2,4-dihydroxybenzophenone in the presence of para-toluenesulfonic acid in refluxing xylene for 20 h [134].

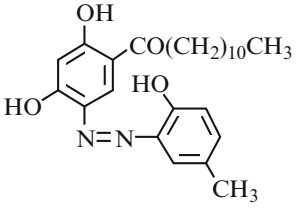
-Also refer to: [133, 1631].

m.p. 80–81° [1631], 59–61° [134].

USE: For stabilizing polyolefins and vinyl halide resins against UV-light and sunlight [134]; As light stabilizer for chlorine-contg. polymers, [133]; Stabilization of vinyl halide resins and polyolefins against photodegradation [133].

5-[[(2-Hydroxy-5-methylphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone

[26993-72-6] $C_{25}H_{34}N_2O_4$ mol. wt. 426.56



Synthesis

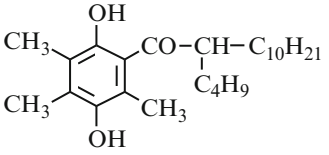
-Obtained by reaction of 2-amino-4-methylphenol diazonium salt with 2,4-dihydroxylaurophenone in the presence of sodium hydroxide between 5 and 10° [577].

m.p. 200–201° [577].

Metal complexes Refer to: [577].

2-Butyl-1-(2,5-dihydroxy-3,4,6-trimethylphenyl)-1-dodecanone

$C_{25}H_{42}O_3$ mol. wt. 390.61



Synthesis

-Refer to: [2352].

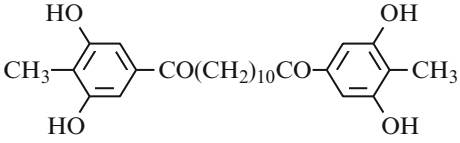
Dibenzyl ether [357172-32-8]

$C_{39}H_{54}O_3$ mol. wt. 570.86

-Refer to: [2352].

1,12-Bis(3,5-dihydroxy-4-methylphenyl)-1,12-dodecanedione

$C_{26}H_{34}O_6$ mol. wt. 442.55



Synthesis

-Refer to: [3132].

Tetramethyl ether [196869-45-1]

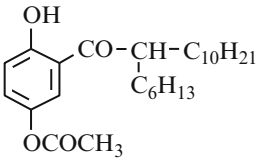
$C_{30}H_{42}O_6$ mol. wt. 498.66

-Synthesis from 3,5-dimethoxy-4-methylbenzaldehyde (70 %) [3132].

colourless crystalline solid [3132];
^{1}H NMR [3132], ^{13}C NMR [3132].

1-[5-(Acetyloxy)-2-hydroxyphenyl]-2-hexyl-1-dodecanone

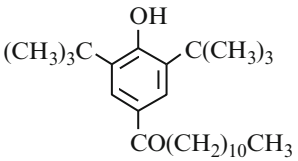
[357172-52-2] $C_{26}H_{42}O_4$ mol. wt. 418.62



Synthesis
-Refer to: [2352].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-dodecanone

[28441-02-3] $C_{26}H_{44}O_2$ mol. wt. 388.63

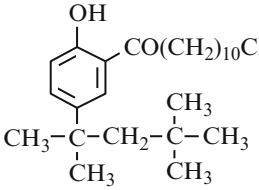


Synthesis
-Preparation by reaction of dodecanoyl chloride with 2,6-di-tert-butylphenol in the presence of aluminium chloride in 1,1,2-trichloroethane at −10 to −20° [951].
m.p. 48–49° [951].

USE: Stabilize plastics, oils, and fats against heat, light, and oxidation [951].

1-[2-Hydroxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-dodecanone

$C_{26}H_{44}O_2$ mol. wt. 388.63



Synthesis
-Refer to: [2282].
Oxime, nickel complex [108111-24-6]
-Refer to: [2280–2282].

USE: Colour photog. emulsions contg. triazolotriazole deriv. magenta coupler and oil-sol. dyes and, for lightfast image formation [2282]; Photog. magenta dye image stabilizer [2284]; Silver halide photog. material contg. [2280, 2281].

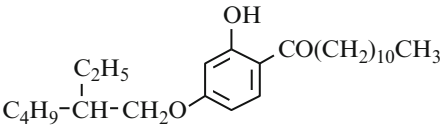
Oxime, nickel complex [110351-70-7].

-Refer to: [1591].

-Singlet oxygen quencher, photog. photosensitive materials contg. [1591].

1-[4-[(2-Ethylhexyl)oxy]-2-hydroxyphenyl]-1-dodecanone

$C_{26}H_{44}O_3$ mol. wt. 404.63



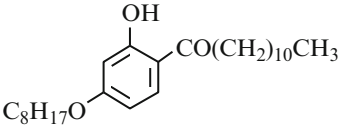
Synthesis
-Refer to: [2282].
Oxime, nickel complex [108111-25-7]

-Refer to: [2282, 2285, 2286].

USE: Colour photog. emulsions contg. triazolotriazole deriv. magenta coupler and oil-sol. dyes and, for lightfast image formation [2282]; Photog. magenta dye image stabilizer [2284]; Photog. stabilizer compns. contg., for magenta dye image stabilization [2286]; Singlet oxygen quencher, colour photog. paper contg. [2285].

1-[2-Hydroxy-4-(octyloxy)phenyl]-1-dodecanone

[101002-34-0] $C_{26}H_{44}O_3$ mol. wt. 404.63
[143287-09-6]



Syntheses
-Obtained by reaction of octyl bromide with 1-(2,4-dihydroxyphenyl)-1-dodecanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

-Refer to: [3077].

m.p. 56–59° [284].

Oxime [101002-21-5] $C_{26}H_{45}NO_3$ mol. wt. 419.65

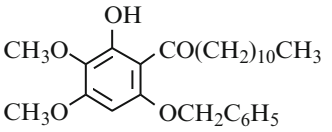
-Obtained by reaction of hydroxylamine hydrochloride with 1-[2-hydroxy-4-(octyloxy)phenyl]-1-dodecanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].
-Also refer to: [2742].

m.p. 60–63° [284, 3077];
^{1}H NMR [284].

USE: Topical preparations comprising at least one aryloxime and bisabolol [483]; As lipoxygenase inhibitor [3077].

1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-dodecanone

[134082-05-6] $C_{27}H_{38}O_5$ mol. wt. 442.60

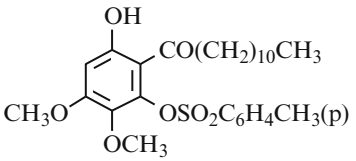


Synthesis
-Obtained by elimination of one phenylmethyl group in 2-position by treatment of 1-(2,6-dibenzyloxy-3,4-dimethoxyphenyl)-1-dodecanone with concentrated hydrochloric acid and acetic acid at r.t. for 2–3 h (82 %) [1353].

m.p. 80.5–81° [1353];
^{1}H NMR [1353].

1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-dodecanone

[134081-89-3] $C_{27}H_{38}O_7S$ mol. wt. 506.66

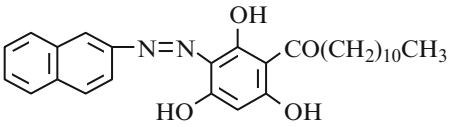


Synthesis
-Obtained by treatment of 1-(2-tosylsulfonyloxy-3,4,6-trimethoxyphenyl)-1-dodecanone with 25 % aluminium bromide in acetonitrile at r.t. for 2–3 h (92 %) [1353].

m.p. 55.5–56° [1353];
^{1}H NMR [1353].

3-[(2-Naphthylazo)-2,4,6-trihydroxyphenyl]-1-dodecanone

$C_{28}H_{34}N_2O_4$ mol. wt. 462.59



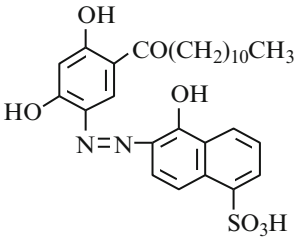
Syntheses
-Obtained by coupling diazotized 2-naphthylamine with 2,4,6-trihydroxy-phenyl undecyl ketone [872].

-Also refer to: [2433].

USE: As water-repellent dye for wood [2433].

5-[[(1-Hydroxy-5-sulfonyl-2-naphthyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone

$C_{28}H_{34}N_2O_7S$ mol. wt. 542.66



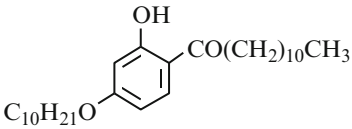
Synthesis

-Obtained by reaction of 2-amino-5-sulfonyl-1-naphthol diazonium salt with 2,4-dihydroxylaurophenone in the presence of sodium hydroxide between 5 and 10° [578].

Metal complexes -Refer to: [578].

1-[4-(Decyloxy)-2-hydroxyphenyl]-1-dodecanone

[143286-99-1] $C_{28}H_{48}O_3$ mol. wt. 432.69



Synthesis

-Obtained by reaction of decyl bromide with 1-(2,4-dihydroxyphenyl)-1-dodecanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 52–60° [284].

Oxime [101002-27-1] $C_{28}H_{49}NO_3$ mol. wt. 447.70

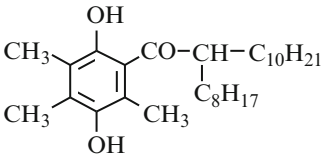
-Obtained by reaction of hydroxylamine hydrochloride with 1-[4-(decyloxy)-2-hydroxyphenyl]-1-dodecanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 64–69° [284, 3077]; ^{1}H NMR [284].

USE: Topical preparations comprising at least one aryloxime and bisabolol [483]; As lipoxygenase inhibitor [3077].

1-(2,5-dihydroxy-3,4,6-trimethylphenyl)-2-octyl-1-dodecanone

[357172-26-0] $C_{29}H_{50}O_3$ mol. wt. 446.71

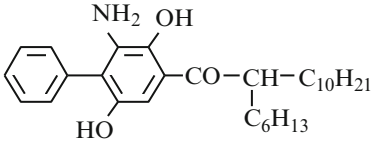


Synthesis

-Refer to: [2352].

1-(2-Amino-3,6-dihydroxy[1,1′-biphenyl]-4-yl)-2-hexyl-1-dodecanone

$C_{30}H_{45}NO_3$ mol. wt. 467.69



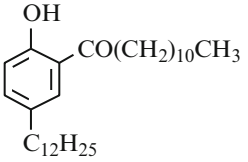
Synthesis
-Refer to: [2352].

Dibutyl ether [375172-48-6]
$C_{38}H_{61}NO_3$ mol. wt. 579.91

-Refer to: [2352].

1-(5-Dodecyl-2-hydroxyphenyl)-1-dodecanone

$C_{30}H_{50}O_2$ mol. wt. 442.73



Synthesis
-Refer to: [3221].

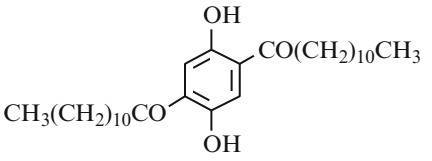
Methyl ether [52066-90-7]
$C_{31}H_{54}O_2$ mol. wt. 458.77

-Refer to: [3221].

m.p. 37.5–39.5° [3221].

1,1′-(2,5-Dihydroxy-1,4-phenylene)bis-1-dodecanone

$C_{30}H_{50}O_4$ mol. wt. 474.72

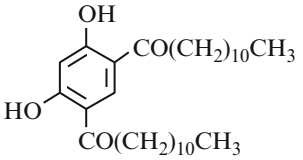


Syntheses
-Obtained by reaction of lauric acid with hydroquinone in the presence of zinc chloride (Nencki reaction) at 130–140° [156] for 2 h (23 %) [1264].

m.p. 68° [1264].

1,1′-(4,6-Dihydroxy-1,3-phenylene)bis-1-dodecanone

[1092783-58-8] $C_{30}H_{50}O_4$ mol. wt. 474.72



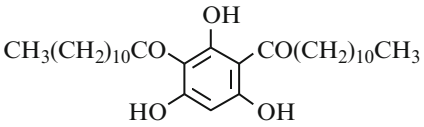
Syntheses
-Preparation by reaction of dodecanoic anhydride with resorcinol in the presence of boron trifluoride etherate [2364].
-Also obtained by reaction of dodecanoic acid with resorcinol in the presence of zinc chloride [2364].

^{1}H NMR [2364], MS [2364].

BIOLOGICAL ACTIVITY: Simplified YM-26734 inhibitors of secreted phospholipase A2 group IIA [2364].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-dodecanone

[144337-28-0] $C_{30}H_{50}O_5$ mol. wt. 490.72



Syntheses
-Obtained by reaction of dodecanoic anhydride with phloroglucinol in the presence of boron trifluoride etherate [2364].

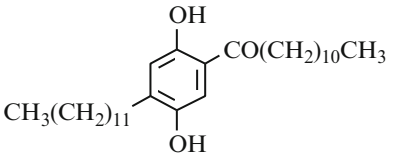
-Also obtained by reaction of dodecanoic acid with phloroglucinol,
*in the presence of zinc chloride [2364];
*in the presence of boron trifluoride etherate at 100° for 2 h (reflux) (60 %) [338].
-Also refer to: [1216].

cream coloured solid [338];
^{1}H NMR [338, 2364], MS [338].

BIOLOGICAL ACTIVITY: Simplified YM-26734 inhibitors of secreted phospholipase A2 group IIA [2364]; As a new class of GPR40 (FFAR1) agonists [338]; As phospholipase A2 inhibitor [1216].

1-(2,5-Dihydroxy-4-dodecylphenyl)-1-dodecanone

[103398-77-2] $C_{30}H_{52}O_3$ mol. wt. 460.74



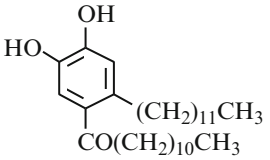
Syntheses
-Obtained by reaction of dodecanoic acid with 2-dodecylhydroquinone in the presence of boron trifluoride in 1,2-dichloroethane at 40–45° for 1.25 h. The mixture was allowed to stand overnight (37 %) [142].

-Also refer to: [1907].

m.p. 88–90° [142, 1907].

1-(2-Dodecyl-4,5-dihydroxyphenyl)-1-dodecanone

$C_{30}H_{52}O_3$ mol. wt. 460.74



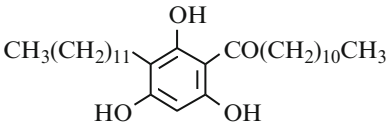
Synthesis
-Refer to: [1167].

Dimethyl ether [930782-40-4]
$C_{32}H_{56}O_3$ mol. wt. 488.80
-Refer to: [1167].

^{1}H NMR [1167], ^{13}C NMR [1167].

1-(3-Dodecyl-2,4,6-trihydroxyphenyl)-1-dodecanone

[1092783-56-6] $C_{30}H_{52}O_4$ mol. wt. 476.74



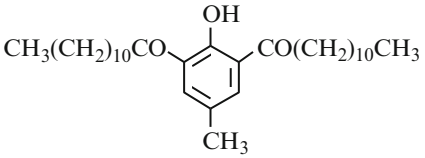
Synthesis
-Preparation by reaction of dodecanoyl chloride with 2-dodecylphloroglucinol in the presence of aluminium chloride [2364].

^{1}H NMR [2364], MS [2364].

BIOLOGICAL ACTIVITY: Simplified YM-26734 inhibitors of secreted phospholipase A_2 group IIA [2364].

1,1′-(2-Hydroxy-5-methyl-1,3-phenylene)bis-1-dodecanone

[1092783-62-4] $C_{31}H_{52}O_3$ mol. wt. 472.75

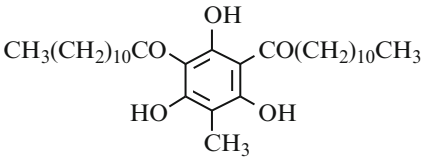


Synthesis
-Obtained by reaction of dodecanoyl chloride with p-cresol in the presence of aluminium chloride [2364].
^{1}H NMR [2364], MS [2364].

BIOLOGICAL ACTIVITY: Simplified YM-26734 inhibitors of secreted phospholipase A_2 group IIA [2364].

1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-dodecanone

[1092783-59-9] $C_{31}H_{52}O_5$ mol. wt. 504.75



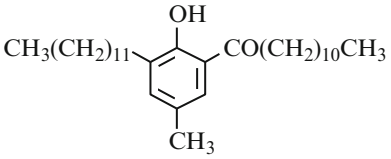
Synthesis
-Obtained by reaction of dodecanoyl chloride with 2-methylphloroglucinol in the presence of aluminium chloride [2364].

^{1}H NMR [2364], MS [2364].

BIOLOGICAL ACTIVITY: Simplified YM-26734 inhibitors of secreted phospholipase A_2 group IIA [2364].

1-(3-Dodecyl-2-hydroxy-5-methylphenyl)-1-dodecanone

$C_{31}H_{54}O_2$ mol. wt. 458.77

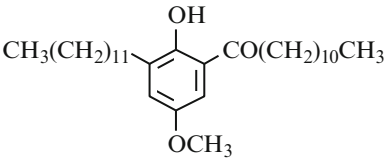


Synthesis
-Refer to: [1831].

Oxime, nickel complexes
-Ultraviolet light inhibitor, spandex fibers contg., [1831].

1-(3-Dodecyl-2-hydroxy-5-methoxyphenyl)-1-dodecanone

[56134-31-7] $C_{31}H_{54}O_3$ mol. wt. 474.77

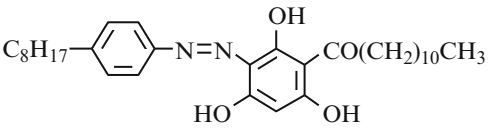


Synthesis
-Obtained by reaction of dodecanoic acid with 2-dodecyl-4-methoxyphenol in the presence of boron trifluoride first at 70–80° for 7 h, then at r.t. for 15 h (52 %) [2752].

m.p. 53–54° [2752].

3-[(4-Octylphenylazo)-2,4,6-trihydroxyphenyl]-1-dodecanone

$C_{32}H_{48}N_2O_4$ mol. wt. 524.74



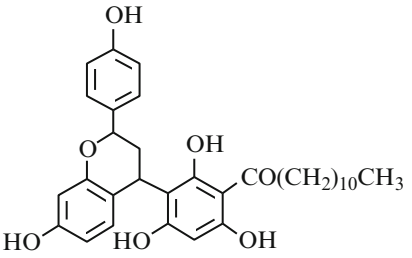
Syntheses
-Obtained by coupling p-octylazobenzene with 2,4,6-trihydroxyphenyl undecyl ketone [872].

-Also refer to: [2433].

USE: As water-repellent dye for wood [2433].

1-[3-[(2*R*,4*S*)-3,4-Dihydro-7-hydroxy-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-4-yl]-2,4,6-trihydroxyphenyl]-1-dodecanone (+)
(Myristinin A)

[145904-69-4] $C_{33}H_{40}O_7$ mol. wt. 548.68



Isolation from natural sources
-From *Myristica cinnamomea* fruits (Myristicaceae) [2726].
-From *Knema elegans* (Myristicaceae) [848].
-From *Horsfielddia amygdaline* [1215].
brown amorphous solid [2726]; colourless amorphous solid [848].

^{1}H NMR [848, 2726], ^{13}C NMR [848, 2726], IR [2726], UV [848, 2726], MS [848, 2726];
$(\alpha)_D^{28} = +39.1°$ (methanol) [2726], $(\alpha)_D^{22} = +45°$ (methanol) [848].

BIOLOGICAL ACTIVITY: Selective COX-2 inhibitor [2726]; Antifungal agent [2726]; Inhibit DNA Polymerase β and Cleave DNA [848]; Cytotoxicity [848].

Pentaacetate $C_{43}H_{50}O_{12}$ mol. wt. 758.86

-Obtained by reaction of acetic anhydride with Myristinin A in the presence of pyridine under argon at 25° for 1.5 h (86 %) [848].

oily product [848]; ^{1}H NMR [848], MS [848].

Myristinin A (+)

[888489-66-5] $C_{33}H_{40}O_7$ mol. wt. 548.68

Isolation from natural sources

-From trunk wood of *Knema elegans* (Warb.) (Myristicaceae) [848].
-From fruits of *Myristica cinnamomea* [2726].

brown amorphous solid [2726];
^{1}H NMR [848, 2726], ^{13}C NMR [848, 2726], IR [2726], UV [848, 2726], MS [848];
Circular dichroism [848];
$(\alpha)_D^{22} = +45°$ (methanol) [848]; $(\alpha)_D^{28} = -280°$ (methanol) [2726].

BIOLOGICAL ACTIVITY: Cytotoxicity [848, 2726]; Genotoxicity [848]; Antifungal [2726]; Inhibition of enzyme activity [848]; Antiinflammatory [2726].

(2R,3R,4R)-2-(4-Hydroxyphenyl)-7-hydroxy-4-(2,4,6-trihydroxy-3-(dodecanoyl)-phenyl)chromane
(Myristinin A)

$C_{33}H_{40}O_7$ mol. wt. 548.68

Isolation from natural sources

-From fruits of *Myristica cinnamomea* [2726].
-Also refer to: [1974, 1975].

^{1}H NMR [1974, 1975, 2726],
^{13}C NMR [1974, 1975, 2726], IR [2726], UV [2726];
$(\alpha)_D^{23} = +57.8°$ (methanol) [1975], $(\alpha)_D^{28} = +39.1°$ (methanol) [2726].

BIOLOGICAL ACTIVITY: Examination of DNA [1975]; Inhibition of enzyme activity [1975]; Cytotoxicity [1975, 2726]; Antiinflammatory [2726]; Antifungal [2726].

Myristinin B and **C** (a mixture of these)

1-[(3*R*)-3-[(2*R*,4*R*)-3,4-Dihydro-7-hydroxy-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-4-yl]-2,4,6-trihydroxyphenyl]-1-dodecanone
(Myristinin B)

[457930-47-1] $C_{33}H_{40}O_7$ mol. wt. 548.68

1-[(3*R*)-3-[(2*S*,4*S*)-3,4-Dihydro-7-hydroxy-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-4-yl]-2,4,6-trihydroxyphenyl]-1-dodecanone
(Myristinin C)

[457926-60-2] $C_{33}H_{40}O_7$ mol. wt. 548.68

Isolation from natural sources

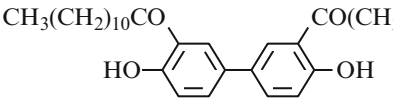
-From *Myristica cinnamomea* fruits (Myristicaceae) [2726].

brown amorphous solid [2726];
^{1}H NMR [2726], ^{13}C NMR [2726], IR [2726], UV [2726], MS [2726];
$(\alpha)_D^{28} = -280°$ (methanol) [2726].

BIOLOGICAL ACTIVITY: Selective COX-2 inhibitors [2726]; Antifungal agents [2726].

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)bis-1-dodecanone

[104440-88-2] $C_{36}H_{54}O_4$ mol. wt. 550.82



Syntheses

-Preparation by Fries rearrangement of 4,4′-biphenyl didodecanoate with aluminium chloride,

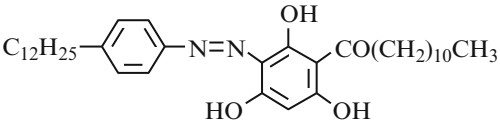
*in the presence of sodium chloride at 140°. The reaction is carried out by adding the ester to the melt, rapidly increasing the temperature to 200° and maintaining it there for 2 min before quick cooling [2091];
*in refluxing chlorobenzene for 24 h (85 %) [2377].

N.B.: The formation of ketonic products by Fries rearrangement of 4,4′-biphenyl didodecanoate with aluminium chloride (1.1 equiv.) according to [2955] could not be demonstrated. Changing the temperature and time used for the reaction also failed to give satisfactory results [2244]. Actually, the quantity of aluminium chloride used is very insufficient.

m.p. 87–88° [2377]; IR [2377].

3-[(4-Dodecylphenylazo)-2,4,6-trihydroxyphenyl]-1-dodecanone
3′-(p-Dodecylphenylazo)-2′,4′,6′-trihydroxydodecanophenone

$C_{36}H_{56}N_2O_4$ mol. wt. 580.85



Syntheses

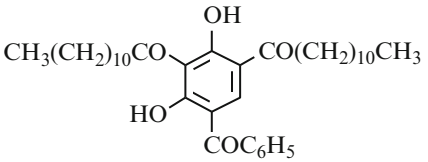
-Obtained by coupling diazotized dodecylaniline with 2,4,6-trihydroxyphenyl undecyl ketone [872].

-Also refer to: [2433].

USE: As water-repellent dye for wood [2433].

1,1′-(5-Benzoyl-2,4-dihydroxy-1,3-phenylene)bis-1-dodecanone

[15041-68-6] $C_{37}H_{54}O_5$ mol. wt. 578.83



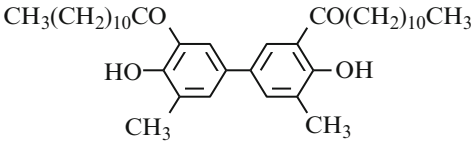
Synthesis
-Obtained by reaction of lauric acid with 2,4-dihydroxybenzophenone in the presence of para-toluenesulfonic acid in refluxing xylene for 20 h [134].
-Also refer to: [133].

m.p. 59–61° [2252], 58–61° [134].

USE: For stabilizing polyolefins and vinyl halide resins against UV-light and sunlight [134]; Stabilization of vinyl halide resins and polyolefins against photodegradation [133].

1,1′-(4,4′-Dihydroxy-5,5′-dimethyl[1,1′-biphenyl]-3,3′-diyl)bis-1-dodecanone

$C_{38}H_{58}O_4$ mol. wt. 578.88

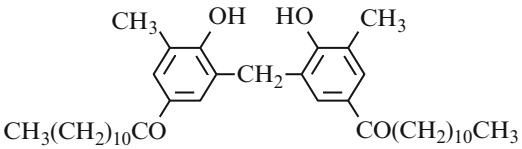


Syntheses
-The formation of ketonic products by Fries rearrangement of 3,3′-dimethyl-4,4′-biphenyl didodecanoate with aluminium chloride (1.1 equiv.) according to [2955] could not be demonstrated.

Changing the temperature and time used for the reaction also failed to give satisfactory results [2244]. Actually, the quantity of aluminium chloride used is very insufficient.

1,1′-[Methylenebis(2-hydroxy-3-methyl-5,1-phenylene)]bis-1-dodecanone

$C_{39}H_{60}O_4$ mol. wt. 592.90

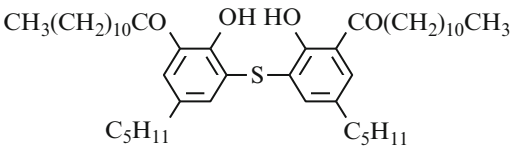


Syntheses
-Obtained by reaction of dodecanoyl chloride with bis(2-hydroxy-3-methylphenyl) methane according to the method described previously [2871], (46 %) [119].

m.p. 95.6–96.8° [119]; ^{1}H NMR [119], IR [119].

1,1′-[Thiobis(2-hydroxy-5-pentyl-3,1-phenylene)]bis-1-dodecanone
3′,3‴-Thiobis[2′-hydroxy-5′-pentyldodecanophenone

$C_{46}H_{74}O_4S$ mol. wt. 723.16



Syntheses
-Refer to: [825, 826].

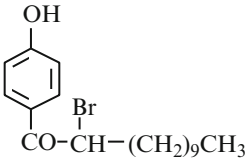
USE: Polycarboxylic acid esters of oxypropylated, [825];
Polycarboxylic acid esters of oxypropylated, in breaking petroleum emulsions, [826].

2 Aromatic Hydroxyketones Derived from Various Bromododecanoic Acids

2.1 Unsubstituted Hydroxyketones

2-Bromo-1-(4-hydroxyphenyl)-1-dodecanone

$C_{18}H_{27}BrO_2$ mol. wt. 355.31



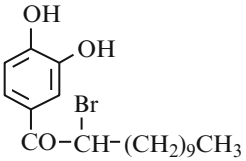
Syntheses
-Refer to: [2252, 2253].
Methyl ether [63424-84-0]
$C_{19}H_{29}BrO_2$ mol. wt. 369.34

-Obtained by reaction of bromine with 4-methoxydodecanophenone,
*in nitrobenzene [2253], (70 %) [2252];
*in carbon tetrachloride at r.t. [378].

m.p. 75–75.5° [378], 72–73° [574, 2252];
^{1}H NMR [2252], IR [2252].

2-Bromo-1-(3,4-dihydroxyphenyl)-1-dodecanone

$C_{18}H_{27}BrO_3$ mol. wt. 371.31



Synthesis
-Refer to: [2252].
Dimethyl ether [63828-97-7]
$C_{20}H_{31}BrO_3$ mol. wt. 399.37

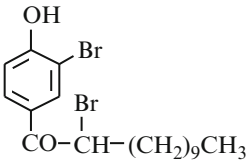
-Obtained by reaction of bromine with 3,4-dimethoxydodecanophenone in nitrobenzene (65 %) [2252].
-Also refer to: [2254].

m.p. 55° [2252]; ^{1}H NMR [2252], IR [2252].

2.2 Substituted Hydroxyketones

2-Bromo-1-(3-bromo-4-hydroxyphenyl)-1-dodecanone

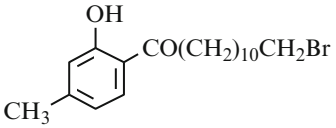
$C_{18}H_{26}Br_2O_2$ mol. wt. 434.21



Synthesis
-Obtained by reaction of bromine with 4-hydroxydodecanophenone in carbon tetrachloride at r.t. [378].
m.p. 77–77.5° [378].

12-Bromo-1-(2-hydroxy-4-methylphenyl)-1-dodecanone

$C_{19}H_{29}BrO_2$ mol. wt. 369.34



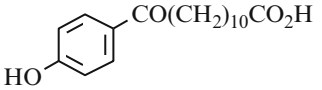
Synthesis
-Obtained by reaction of 12-bromododecanoic acid with m-cresol in the presence of a mixture of graphite and methanesulfonic acid at 120° for 2 h (77 %) [2834].

^{1}H NMR [2834], ^{13}C NMR [2834].

3 Aromatic Hydroxyketone Derived from 12-Oxododecanoic Acid

12-(4-Hydroxyphenyl)-12-oxo-1-dodecanoic acid

[23293-67-6] $C_{18}H_{26}O_4$ mol. wt. 306.40



Synthesis
-Refer to: [1539].
m.p. 92–94° [1539]; IR [1539].

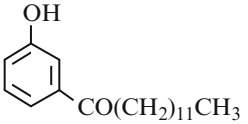
Chapter 11
Tridecanones

1 Aromatic Hydroxyketones Derived from Tridecanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(3-Hydroxyphenyl)-1-tridecanone

[857165-80-1] $C_{19}H_{30}O_2$ mol. wt. 290.45



Syntheses
-Obtained by treatment of its methyl ether with aluminium chloride in benzene by heating on a water bath for 2 h (80 %) [966].
-Also refer to: [967].

b.p.$_{25}$ 165° [966, 967];
n_D^{36} = 1.556 [967].

2,4-Dinitrophenylhydrazone $C_{25}H_{34}N_4O_5$ mol. wt. 470.57

m.p. 100° [967].

Methyl ether [857165-59-4] $C_{20}H_{32}O_2$ mol. wt. 304.47

-Obtained by condensation of dodecylmagnesium bromide with m-methoxybenzamide in ethyl ether. The reaction was carried out at 60° for 48 h under hydrogen atmosphere (60–70 %) [966].
-Also refer to: [967].

b.p.$_{25}$ 210° [966, 967];
n_D^{37} = 1.4405 [967].

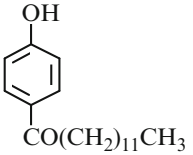
R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_11

2,4-Dinitrophenylhydrazone of the methyl ether $C_{26}H_{36}N_4O_5$ mol. wt. 484.60

m.p. 79° [967].

1-(4-Hydroxyphenyl)-1-tridecanone

[1006710-00-4] $C_{19}H_{30}O_2$ mol. wt. 290.45



Synthesis
-Obtained by reaction of tridecanoyl chloride with phenol [3457].

USE: Application of polyethylene glycol alkylphenyl ether metal acetate for oil recovery [3457].

Methyl ether [55469-24-4] $C_{20}H_{32}O_2$ mol. wt. 304.47

-Obtained by reaction of tridecanoyl chloride with anisole in the presence of graphite in refluxing 1,2-dichloroethane for 8 h (63 %) [1723].
-Also obtained by coupling 1-tridecyne with 4-bromoanisole in the presence of silicon tetrachloride and sodium iodide (Heck reaction) (30 %) [480].
-Also refer to: [152, 481, 1202, 1963].

m.p. 59° [1963];
^{1}H NMR [480], IR [480], MS [480].

USE: Liq. crystal compns. contg., for display devices [152].

2-Chloroethyl ether $C_{21}H_{33}ClO_2$ mol. wt. 352.94

-Obtained by reaction of tridecanoyl chloride with 2-chloroethoxybenzene in the presence of aluminium chloride in carbon disulfide for 4 h at 50° (60 %) [476].

m.p. 77–78° [476].

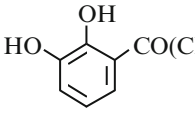
N-Dimethylaminoethyl ether $C_{23}H_{39}NO_2$ mol. wt. 361.57

-Obtained by reaction of 4-(2-chloroethoxy)tridecanophenone with dimethylamine in a sealed tube for 2 h at 150° [476].

free base (oil): $b.p._{0.01}$ 204° [476]; m.p. 55–56° [476].
hydrochloride: (92.5 %) [476].

1-(2,3-Dihydroxyphenyl)-1-tridecanone

[862666-39-5] $C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Obtained by deprotection of its dimethyl ether with boron tribromide in methylene chloride at 0°. Then, the mixture was stirred overnight at r.t. (79 %) [82].

brown solid [82]; m.p. 60° [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

USE: Reactant for preparation of lithium gallium/titanium ketone complexes [82].

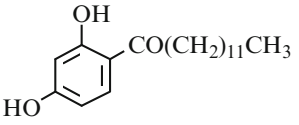
Dimethyl ether [266310-08-1] $C_{21}H_{34}O_3$ mol. wt. 334.50

-Obtained by treatment of 1-(2,3-dimethoxyphenyl)-1-tridecanol in acetone with potassium dichromate in dilute sulfuric acid (Jones reagent) at r.t. for 3 h (53 %) [82].

colourless oil [82];
^{1}H NMR [82], ^{13}C NMR [82], IR [82], MS [82].

1-(2,4-Dihydroxyphenyl)-1-tridecanone

$C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Obtained by reaction of tridecanoic acid with resorcinol in the presence of zinc chloride between 125 and 135° [893].
b.p.$_{11}$ 265–270° [893].

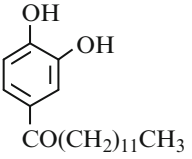
Dimethyl ether $C_{21}H_{34}O_3$ mol. wt. 334.50

-To a stirred suspension of sodium hydride in dry, acid free dimethylacetamide at 10° under nitrogen was added 3,5-dimethoxyphenacylpyridinium perchlorate in dimethylacetamide. The mixture was shaken for 15 min and undecyl iodide added. After keeping overnight at r.t., the mixture was heated for 2 h at 90° and cooled at r.t. Zinc dust and acetic acid were added, the mixture stirred at r.t. for 4 h (34 %) [2603].
-Also refer to: [2627].

needles [2603]; m.p. 53° [2627], 52.5–53° [2603]; IR [2603].

1-(3,4-Dihydroxyphenyl)-1-tridecanone

$C_{19}H_{30}O_3$ mol. wt. 306.45



Synthesis
-Refer to: [256].
Dimethyl ether [930585-36-7]
$C_{21}H_{34}O_3$ mol. wt. 334.50

-Preparation by treatment of 1,2-dimethoxy-4-tridecylbenzene,
*with chromium trioxide in acetic acid, at r.t. for 24 h and at 40° for 16 h (57 %) [256];
*with cerium ammonium nitrate in aqueous acetonitrile for 5 h at 25° (55 %) [256].
-Also refer to: [1960, 1963].

yellow crystals; m.p. 59.5–60° [1960, 1963], 42.2–43.8° [256];
^{1}H NMR [256], ^{13}C NMR [256], IR [256], MS [256].

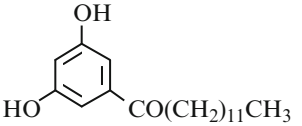
Dibutyl ether [109175-98-6] $C_{26}H_{46}O_3$ mol. wt. 406.65

-Refer to: [1590].

USE: Image stabilizer, photog. film contg. [1590].

1-(3,5-Dihydroxyphenyl)-1-tridecanone

$C_{19}H_{30}O_3$ mol. wt. 306.45



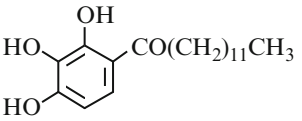
Syntheses
-Refer to: [3340, 3341].
Dimethyl ether [5259-08-5]
$C_{21}H_{34}O_3$ mol. wt. 334.50

-Preparation by reaction of 3,5-dimethoxybenzoyl chloride with n-dodecylmagnesium bromide in ether and toluene mixture at −60° for 2.5 h in the presence of ferric chloride under nitrogen atmosphere (51 %) [2627].
-Also obtained by reaction of dodecylmagnesium bromide with 3,5-dimethoxybenzamide in ether [2876, 2948].
-Refer to: [2603, 3340, 3341].

colourless plates [2627]; m.p. 53° [2627], 52.3–53° [2603];
^{1}H NMR [2627], IR [2627], UV [2627].

1-(2,3,4-Trihydroxyphenyl)-1-tridecanone

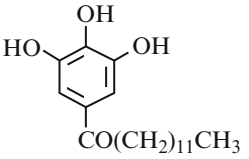
$C_{19}H_{30}O_4$ mol. wt. 322.44



Synthesis
-Obtained by reaction of tridecanoic acid with pyrogallol in the presence of zinc chloride at 140–145° for 4 h [506].
m.p. 84–85° [506].

1-(3,4,5-Trihydroxyphenyl)-1-tridecanone

$C_{19}H_{30}O_4$ mol. wt. 322.44



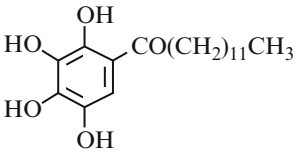
Synthesis
-Refer to: [211].
Trimethyl ether [123059-72-3]
$C_{22}H_{36}O_4$ mol. wt. 364.53

-Obtained by reaction of dodecylmagnesium bromide with 3,4,5-trimethoxybenzoyl chloride in the presence of zinc chloride in benzene at 20° for 12 h (81 %) [211].
-Also refer to: [159].

m.p. 61–62° [159], 57–59° [211]; ^{1}H NMR [211].

1-(2,3,4,5-Tetrahydroxyphenyl)-1-tridecanone

$C_{19}H_{30}O_5$ mol. wt. 338.44



Synthesis
-Refer to: [159].

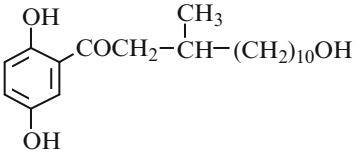
Tetramethyl ether

$C_{23}H_{38}O_5$ mol. wt. 394.55

m.p. 61–62° [159].

13-Hydroxy-3-methyl-1-(2,5-dihydroxyphenyl)-1-tridecanone

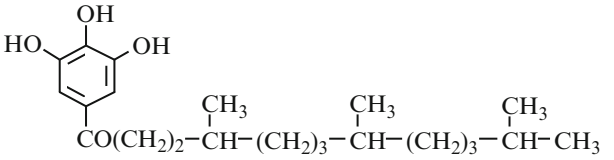
[1254222-61-1] $C_{20}H_{32}O_4$ mol. wt. 336.47



Synthesis
-Refer to: [720].

4,8,12-Trimethyl-1-(3,4,5-trihydroxyphenyl)-1-tridecanone

[278607-60-6] $C_{22}H_{36}O_4$ mol. wt. 364.53



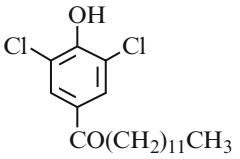
Synthesis
-Refer to: [6].

USE: Potent and selective inhibition of squalene epoxidase [6].

1.2 Substituted Hydroxyketones

1-(3,5-Dichloro-4-hydroxyphenyl)-1-tridecanone

[110581-80-1] $C_{19}H_{26}Cl_2O_2$ mol. wt. 357.32

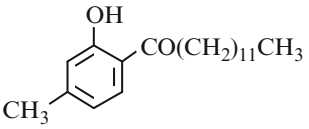


Synthesis
-Refer to: [1463].

USE: Photog. coloration-promoting agent [1463].

1-(2-Hydroxy-4-methylphenyl)-1-tridecanone

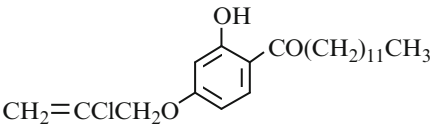
$C_{20}H_{32}O_2$ mol. wt. 304.47



Synthesis
-Refer to: [17].
Oxime, nickel complex [40690-30-0]
-Triplet state quenching by, kinetics of [17].

1-[4-(2-Chloroallyloxy)-2-hydroxyphenyl]-1-tridecanone

$C_{22}H_{33}ClO_3$ mol. wt. 380.95

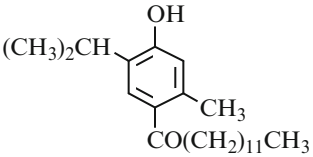


Synthesis
-Refer to: [2959].
Compound with nickel chloride
($NiCl_2$) (1:1), hexahydrate
[19513-15-6] mol. wt. 750.67

USE: As stabilizers (radiation) for propene polymers [2959].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-tridecanone

$C_{23}H_{38}O_2$ mol. wt. 346.55



Synthesis
-Obtained by treatment of 4-methoxy-2-methyl-5-isopropyl-tridecanophenone with boiling pyridinium chloride (205–215°) for 10 h (14 %) [2660].
b.p.$_{11}$ 266–269° [2660]; m.p. 63° [2660].

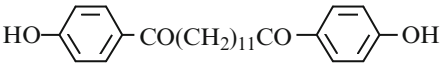
Methyl ether $C_{24}H_{40}O_2$ mol. wt. 360.58

-Preparation by reaction of tridecanoyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (50 %) [2660].

b.p.$_{21}$ 268–270° [2660]; m.p. 34° [2660].

1,13-Bis(4-hydroxyphenyl)-1,13-tridecanedione

[114280-34-1] $C_{25}H_{32}O_4$ mol. wt. 396.53



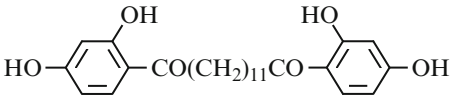
Synthesis
-Refer to: [1337].
m.p. 131–133° [1337].

Acetate [103161-22-4] $C_{29}H_{36}O_6$ mol. wt. 480.60

m.p. 92–92.5° [1337].

1,13-Bis(2,4-dihydroxyphenyl)-1,13-tridecanedione

$C_{25}H_{32}O_6$ mol. wt. 428.53



Synthesis
-Obtained by reaction of 1,13-tridecanedioic acid with resorcinol in the presence of zinc chloride at 140° for 5 h (80 %) [445].

m.p. 146° [445].

Tetraacetate $C_{33}H_{40}O_{10}$ mol. wt. 596.67

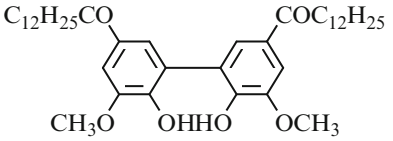
m.p. 57° [445].

Tetramethyl ether [103209-07-0] $C_{29}H_{40}O_6$ mol. wt. 484.63

m.p. 70.5–71° [1337].

1,1′-(6,6′-Dihydroxy-5,5′-dimethoxy[1,1′-biphenyl]-3,3′-diyl)bis-1-tridecanone

[156306-39-7] $C_{40}H_{62}O_6$ mol. wt. 639.02



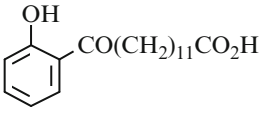
Synthesis
-Manuf. of, with peroxidase, from guaiacyl ketone [1427].

BIOLOGICAL ACTIVITY: Antioxidant and fragrance-keeping effects [1427].

2 Aromatic Hydroxyketone Derived from 13-Oxotridecanoic Acid

13-(2-Hydroxyphenyl)-13-oxo-1-tridecanoic acid

[102166-29-0] $C_{19}H_{28}O_4$ mol. wt. 320.43



Synthesis
-Refer to: [3122].
m.p. 102° [3122].

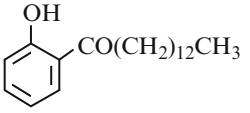
Chapter 12
Tetradecanones

1 Aromatic Hydroxyketones Derived from Tetradecanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-1-tetradecanone

$C_{20}H_{32}O_2$ mol. wt. 304.47



Syntheses

-Obtained by reaction of myristoyl chloride with phenol in the presence of aluminium chloride,
*in tetrachlorethane few hours at 55° (32 %) [2548];
*in nitrobenzene for 3 h at 70° (21 %) [2549];
*in carbon disulfide for 5.5 h at 47° (36 %) [2549].

-Also obtained by Fries rearrangement of phenyl myristate with aluminium chloride in tetrachlorethane for 10 h at 70° (35 %) [2550] or in tetrachloroethane [3169].

-Also obtained by reaction of myristic acid with phenol in the presence of zinc chloride (Nencki reaction) (75 %) [2398].

m.p. 55° [2398], 53.5° [3169], 52–55° [2548].

2,4-Dinitrophenylhydrazone $C_{26}H_{36}N_4O_5$ mol. wt. 484.60

m.p. 92.5° [3169], 92–92.5° [2548].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_12

Methyl ether $C_{21}H_{34}O_2$ mol. wt. 318.50

-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxyphenyl)-1-tetradecanone in the presence of potassium carbonate in boiling acetone for 6 h [2398].

b.p.$_{.66}$ 180–182° [2398].

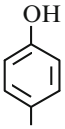
2,3-Epoxypropyl ether [18110-31-1] $C_{23}H_{36}O_3$ mol. wt. 360.54

-Obtained by reaction of epichlorohydrin (0.1 mol) with o-tetradecanoylphenol (0.1 mol) in the presence of 30 % sodium hydroxide between 40 and 50° (63 %) [2669].

b.p.$_{.0.4}$ 230–240° [2669].

1-(4-Hydroxyphenyl)-1-tetradecanone

[2589-75-5] $C_{20}H_{32}O_2$ mol. wt. 304.47



Syntheses

-Obtained by reaction of myristoyl chloride with phenol in the presence of aluminium chloride,

*in tetrachlorethane few hours at 55° (37 %) [2548];

*in nitrobenzene for 3 h at 70° (73 %) [2549];

*in carbon disulfide for 5.5 h at 47° (52 %) [2549] or first at r.t., then heated to boiling for 5 h (poor yield) [1526].

-Also obtained by Fries rearrangement of phenyl myristate with aluminium chloride in tetrachlorethane [3169], for 10 h at 70° (43 %) [2550].

-Also obtained by demethylation of the 4-myristoylanisole [2398].

-Also obtained by reaction of myristic acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3377].

-Also refer to: [873, 1299, 2945, 3371].

m.p. 78–80° [2548, 3377], 77° [2398], 76–78° [3169], 74–74.5° [1526].

USE: Activator for peroxygen bleach in laundry detergent for mud-soiled clothing [3371]; Foaming improvement of N-acylamino alkanesulfonate detergents by, [2945]; Textile rot proofing by, [873].

2,4-Dinitrophenylhydrazone $C_{26}H_{36}N_4O_5$ mol. wt. 484.60

m.p. 142–143° [2548], 141.5° [3169].

Methyl ether [102456-30-4] $C_{21}H_{34}O_2$ mol. wt. 318.50

-Obtained by Friedel-Crafts reaction of myristoyl chloride with anisole (90 %) [2398].

-Also refer to: [2016, 1963].

m.p. 68–68.5° [2016], 67° [1963], 63° [2398].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{27}H_{38}N_4O_5$ mol. wt. 498.62

m.p. 103–104° [2016].

Oxime of the methyl ether $C_{21}H_{35}NO_2$ mol. wt. 333.51

m.p. 66° [2398].

Semicarbazone of the methyl ether $C_{22}H_{37}N_3O_2$ mol. wt. 375.55

m.p. 71° [2398].

Ethyl ether [859947-01-6] $C_{22}H_{36}O_2$ mol. wt. 332.52

-Obtained by reaction of myristyl chloride with phenetole in the presence of aluminium chloride for 2 days at 60–70° (41 %) [1526].

colourless blocks [1526]; m.p. 66–67° [1526].

2-Chloroethyl ether $C_{22}H_{35}ClO_2$ mol. wt. 366.97

-Obtained by reaction of tetradecanoyl chloride with 2-chloroethoxybenzene in the presence of aluminium chloride in carbon disulfide for 4 h at 50° (65 %) [476].

m.p. 68–70° [476].

N-Dimethylaminoethyl ether $C_{24}H_{41}NO_2$ mol. wt. 375.60

-Obtained by reaction of 4-(2-chloroethoxy)tetradecanophenone with dimethylamine in a sealed tube for 2 h at 150° [476].

free base (oil): $b.p._{0.001}$ 202° [476];
hydrochloride (65 %) [476]; m.p. 158° [476].

2,3-Epoxypropyl ether [18110-32-2] $C_{23}H_{36}O_3$ mol. wt. 360.54

-Obtained by reaction of epichlorohydrin (0.1 mol) with p-tetradecanoylphenol (0.1 mol) in the presence of 30 % sodium hydroxide between 40 and 50° (57 %) [2669].

m.p. 111° [2669].

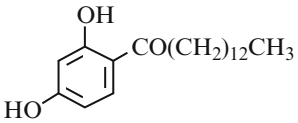
Myristate [119531-08-7] $C_{34}H_{58}O_3$ mol. wt. 514.83

-Obtained by reaction of myristic acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3377].

m.p. 83–83.5° [3377].

1-(2,4-Dihydroxyphenyl)-1-tetradecanone

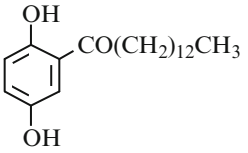
[143286-84-4] $C_{20}H_{32}O_3$ mol. wt. 320.47



Synthesis
-Obtained by reaction of tetradecanoyl chloride with resorcinol in the presence of aluminium chloride in 1,2-dichloroethane at 65° for 5 h [284].

1-(2,5-Dihydroxyphenyl)-1-tetradecanone

$C_{20}H_{32}O_3$ mol. wt. 320.47



Syntheses
-Obtained by reaction of tetradecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156] in carbon disulfide [159].
m.p. 101–103° [156, 159].

Oxime [140943-08-4] $C_{20}H_{33}NO_3$ mol. wt. 335.49

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

Dimethyl ether $C_{22}H_{36}O_3$ mol. wt. 348.52

-Obtained by reaction of myristyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in petroleum ether (quantitative yield) [1526].

plates [1526]; b.p.$_{0.5}$ 209° [714];
m.p. 51–52° [1526], 43° [714].

Diethyl ether $C_{24}H_{40}O_3$ mol. wt. 376.58

-Refer to: [714].

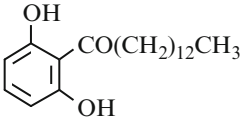
b.p.$_{0.3}$ 204° [714]; m.p. 44.5° [714].

2,4-Dinitrophenylhydrazone of the diethyl ether $C_{30}H_{44}N_4O_6$ mol. wt. 556.70

m.p. 78° [714].

1-(2,6-Dihydroxyphenyl)-1-tetradecanone

[113201-68-6] $C_{20}H_{32}O_3$ mol. wt. 320.47



Syntheses
-Obtaining by aromatization of 2-chloro-2-myristoyl-1,3-cyclohexanedione (70 %) [1816] according to the method [75, 1817].

-Also refer to: [2336].

Isolation from natural sources

-From the fruits of *Knema glauca* (Myristicaceae) [2562].
-From *Myristica dactyloides* (Myristicaceae) [719, 1786, 2336].
-Of the andromeda lace bug *Stephanitis rhododendrii* [2334].
-In the wood bark of *Knema austrosiamensis* W. J. J. O. DeWilde (Myristaceae) [1133] or in Ground wood of this same plant [1134].
-From the fruit rinds of *Myristica malabarica* (Myristicaceae) (0.39 %) [2425].
-From root bark of *Myristica ceylanica* [1307, 1309].
-From the stem bark of *Myristica dactyloides* (Myristicaceae) [1308].
-In plants of the family Myristicaceae [719, 1622].
-Also refer to: [715, 1306, 1504, 3438].

yellow amorphous powder [2562]; pale yellow needles [1786]; gum [1134]; m.p. 93–94° [2336], 91–92° [1306, 1786], 91–91.5° [719]; ^{1}H NMR [719, 1134, 1786, 2336, 2425, 2562], ^{13}C NMR [719, 1786, 2562], IR [719, 1786, 2336, 2562], UV [719, 2562], MS [719, 1134, 1786, 2336, 2425, 2562]; GC [2425].

BIOLOGICAL ACTIVITY: Antituberculosis activity against the microbe Mycobacterium tuberculosis [2562]; Antiviral activity against herpes simplex virus type 1 [2562]; Antimycobacterial and antimalarial activities [2562]; *Myristica dactyloides* is used in native medicine in Sri Lanka and its seeds are used as adulterants to *Myristica fragrans* (nutmeg) [1504]; Elastase of human leukocytes and sputum inhibition by, Brij 35 effect on [715]; Cytotoxicity [2562].

Diacetate [114226-22-1] $C_{24}H_{36}O_5$ mol. wt. 404.55

-Obtained by reaction of acetic anhydride with 1-(2,6-dihydroxyphenyl)-1-tetradecanone in the presence of pyridine at 70° for 12 h [1786].

^{1}H NMR [1786], IR [1786], MS [1786].

Dimethyl ether [114226-23-2] $C_{22}H_{36}O_3$ mol. wt. 348.52

Syntheses

-Obtained by reaction of diazomethane with 1-(2,6-dihydroxyphenyl)-1-tetradecanone in ethyl ether [1786].
-Also obtained by methylation of 1-(2-hydroxy-6-methoxyphenyl)-1-tetradecanone [1786].

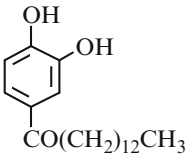
Isolation from natural sources

-From root bark of *Myristica ceylanica* [1307, 1309].

^{1}H NMR [1786], IR [1786], MS [1786].

1-(3,4-Dihydroxyphenyl)-1-tetradecanone
(4-Tetradecanoylcatechol)

$C_{20}H_{32}O_3$ mol. wt. 320.47



Syntheses
-Obtained by treatment of a pyrocatechol and tetradecanoic acid mixture with zinc chloride at 135–140° for 2 h (20 %) [1283].
-Also refer to: [283, 1961].
m.p. 103° [1961], 98–99° [1283].

Dimethyl ether [871901-16-5] $C_{22}H_{36}O_3$ mol. wt. 348.52

-Obtained by reaction of myristyl chloride with veratrole in the presence of aluminium chloride,
*without solvent at 70° (23 %) [1960];
*in petroleum ether at 30–40° for 21–22 h (quantitative yield) [1526].

colourless needles [1526]; $b.p._{0.3–0.5}$ 200–220° [1960];
m.p. 74–75° [1960], 73–75° [1526].

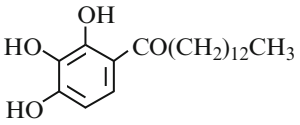
Oxime of the dimethyl ether $C_{22}H_{37}NO_3$ mol. wt. 363.54

-Obtained by treatment of 1-(3,4-dimethoxyphenyl)-1-tetradecanone with hydroxylamine hydrochloride in the presence of potassium acetate in boiling ethanol for 4 h (83 %) [1960].

m.p. 54–55° [1960]

1-[2,3,4-Trihydroxyphenyl]-1-tetradecanone
(4-Tetradecanoylpyrogallol)

$C_{20}H_{32}O_4$ mol. wt. 336.47

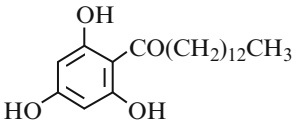


Synthesis
-Obtained by reaction of tetradecanoic acid with pyrogallol in the presence of zinc chloride (Nencki reaction) at 135–140° for 2 h (25 %) [1283].

m.p. 82–84° [1283].

1-[2,4,6-Trihydroxyphenyl]-1-tetradecanone
(4-Tetradecanoylpyrogallol)

[147862-99-5] $C_{20}H_{32}O_4$ mol. wt. 336.47



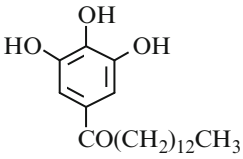
Synthesis
-Refer to: [1133].
Isolation from natural sources

-In the wood of *Knema austrosiamensis* W. J. J. O. DeWilde (Myristaceae) [1133] or in Ground wood of this same plant [1134].

waxy solid [1134]; ^{1}H NMR [1134], MS [1134].

1-[3,4,5-Trihydroxyphenyl]-1-tetradecanone

$C_{20}H_{32}O_4$ mol. wt. 336.47



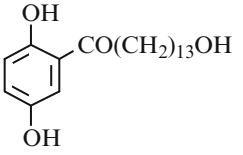
Synthesis
-Refer to: [159].
Trimethyl ether
$C_{23}H_{38}O_4$ mol. wt. 378.55

-Obtained by treatment of ethyl α-(trimethoxybenzoyl)myristate (m.p. 54°) with boiling 1 % ethanolic potassium hydroxide [159].

m.p. 69° [159].

14-Hydroxy-1-(2,5-dihydroxyphenyl)-1-tetradecanone

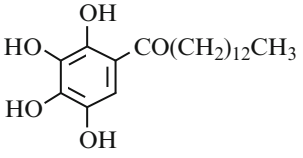
[1254222-90-6] $C_{20}H_{32}O_4$ mol. wt. 336.47



Synthesis
-Refer to: [720].
white crystals [720]; ^{1}H NMR [720].

1-(2,3,4,5-Tetrahydroxyphenyl)-1-tetradecanone

$C_{20}H_{32}O_5$ mol. wt. 352.47

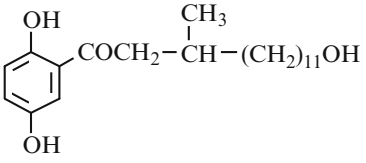


Synthesis
-Refer to: [159] (Japanese paper)
Tetramethyl ether
$C_{24}H_{40}O_5$ mol. wt. 408.57

m.p. 69° [159].

14-Hydroxy-3-methyl-1-(2,5-dihydroxyphenyl)-1-tetradecanone

[1254222-62-2] $C_{21}H_{34}O_4$ mol. wt. 350.50

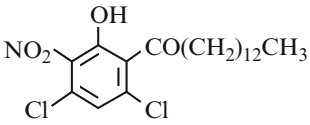


Synthesis
-Refer to: [720].

1.2 Substituted Hydroxyketones

1-(4,6-Dichloro-2-hydroxy-3-nitrophenyl)-1-tetradecanone

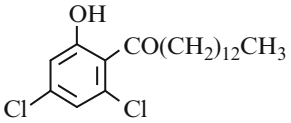
[81515-09-5] $C_{20}H_{30}Cl_2NO_4$ mol. wt. 419.43



Synthesis
-Refer to: [2585].

1-(2,4-Dichloro-6-hydroxyphenyl)-1-tetradecanone

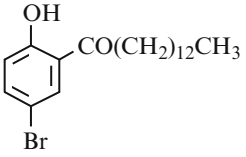
[81515-08-4] $C_{20}H_{30}Cl_2O_2$ mol. wt. 373.36



Synthesis
-Refer to: [2585].

1-(5-Bromo-2-hydroxyphenyl)-1-tetradecanone

$C_{20}H_{31}BrO_2$ mol. wt. 383.37



Synthesis
-Refer to: [468].

Methyl ether

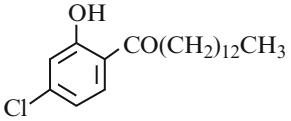
$C_{21}H_{33}BrO_2$ mol. wt. 397.39

-Obtained by reaction of myristoyl chloride with 4-bromoanisole in the presence of aluminium chloride in nitrobenzene first at 20–25° and the mixture kept 2 days at r.t. (36 %) [468].

m.p. 78.5° [468].

1-(4-Chloro-2-hydroxyphenyl)-1-tetradecanone

$C_{20}H_{31}ClO_2$ mol. wt. 338.92



Syntheses
-Preparation by Fries rearrangement of 3-chlorophenyl myristate with aluminium chloride,
*without solvent at 130° for 2 h (45 %) [2802];
*in nitrobenzene at 25° for 6 h (75 %) [2802].

b.p.$_{.32}$ 250° [2802].

2,4-Dinitrophenylhydrazone $C_{26}H_{35}ClN_4O_5$ mol. wt. 519.04

m.p. 114° [2802].

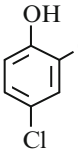
Methyl ether $C_{21}H_{33}ClO_2$ mol. wt. 352.94

-Obtained by methylation of the above ketone in the usual way (75 %) [2802].

$b.p._{.27}$ 127° [2802].

1-(5-Chloro-2-hydroxyphenyl)-1-tetradecanone

[98813-31-1] $C_{20}H_{31}ClO_2$ mol. wt. 338.92

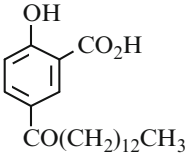


Synthesis
-Obtained by reaction of tetradecanoyl chloride with 4-chlorophenol in the presence of aluminium chloride (73.9 %) [2680].

$b.p._{.1}$ 182–185° [2680]; m.p. 79–80° [2680].

2-Hydroxy-5-tetradecanoylbenzoic acid

[78418-04-9] $C_{21}H_{32}O_4$ mol. wt. 348.48



Synthesis
-Obtained by saponification of the methyl ester (90 %) [689].
m.p. 117–118° [689].

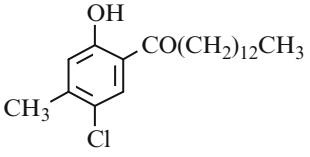
Methyl ester [78417-98-8] $C_{22}H_{34}O_4$ mol. wt. 362.51

-Obtained by reaction of tetradecanoyl chloride with methyl salicylate in the presence of aluminium chloride in carbon disulfide first at 5–10°, then at r.t. for 12 h (70 %) [689].

m.p. 69–70° [689].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-tetradecanone

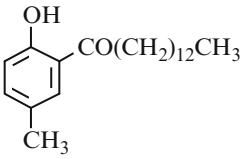
$C_{21}H_{33}ClO_2$ mol. wt. 352.94



Synthesis
-Obtained by reaction of myristic acid with 4-chloro-3-methylphenol in the presence of boron trifluoride for 2–3 h between 65 and 85° (90 %) [503].
m.p. 81° [503].

1-(2-Hydroxy-5-methylphenyl)-1-tetradecanone

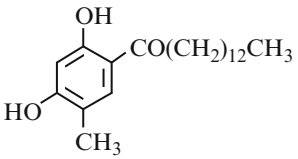
[36946-08-4] $C_{21}H_{34}O_2$ mol. wt. 318.50



Synthesis
-Refer to: [1968].
Dielectric constant [1968].

1-(2,4-Dihydroxy-5-methylphenyl)-1-tetradecanone

[95102-16-2] $C_{21}H_{34}O_3$ mol. wt. 334.50

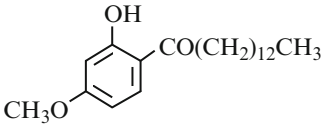


Syntheses
-Refer to: [1595, 2704].

USE: Colour developer, for thermal recording materials [1595].

1-(2-Hydroxy-4-methoxyphenyl)-1-tetradecanone

[143287-00-7] $C_{21}H_{34}O_3$ mol. wt. 334.50



Synthesis
-Obtained by reaction of methyl bromide with 1-(2,4-dihydroxyphenyl)-1-tetradecanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 58–60° [284].

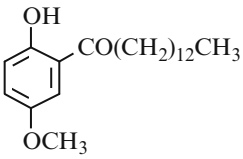
Oxime [143286-68-4] $C_{21}H_{35}NO_3$ mol. wt. 349.51

-Obtained by reaction of hydroxylamine hydrochloride with 1-(2-hydroxy-4-methoxyphenyl)-1-tetradecanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 83–85° [284].

1-(2-Hydroxy-5-methoxyphenyl)-1-tetradecanone

$C_{21}H_{34}O_3$ mol. wt. 334.50



Syntheses
-Obtained by reaction of tetradecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156] in carbon disulfide [159].
m.p. 51–52° [156, 159].

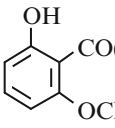
Oxime [140943-16-4] $C_{21}H_{35}NO_3$ mol. wt. 349.51

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-(2-Hydroxy-6-methoxyphenyl)-1-tetradecanone

[114226-24-3] $C_{21}H_{34}O_3$ mol. wt. 334.50

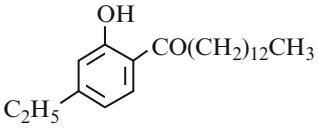


Isolation from natural sources
-From *Myristica dactyloides* (Myristicaceae) [1308, 1786].
-From root bark of *Myristica ceylanica* [1307, 1309].

yellow solid [1786]; m.p. 51–52° [1786];
^{1}H NMR [1786], ^{13}C NMR [1786], IR [1786], MS [1786].

1-(4-Ethyl-2-hydroxyphenyl)-1-tetradecanone

[105701-24-4] $C_{22}H_{36}O_2$ mol. wt. 332.52



Syntheses
-Obtained by Fries rearrangement of 3-ethylphenyl n-myristate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (75 %) [2801];
*in the presence of aluminium chloride (2.8 M),

first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (73 %) [2801].

-Also refer to: [2346].

b.p.$_{29}$ 259° [2801].

2,4-Dinitrophenylhydrazone $C_{28}H_{40}N_4O_5$ mol. wt. 512.64

m.p. 48° [2801].

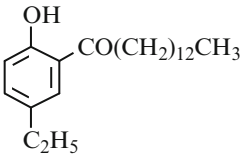
Methyl ether $C_{23}H_{38}O_2$ mol. wt. 346.55

-Obtained by reaction of dimethyl sulfate with 1-(4-ethyl-2-hydroxyphenyl)-1-tetradecanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (86 %) [2801].

m.p. 54° [2801].

1-(5-Ethyl-2-hydroxyphenyl)-1-tetradecanone

$C_{22}H_{36}O_2$ mol. wt. 332.52



Synthesis
-Obtained by Fries rearrangement of 4-ethylphenyl myristate with aluminium chloride at 100° for 2 h (65 %) [2800].
b.p.$_{17}$ 210° [2800].

2,4-Dinitrophenylhydrazone $C_{28}H_{40}N_4O_5$ mol. wt. 512.64

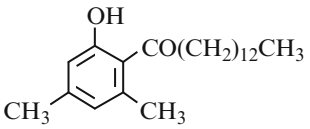
m.p. 66° [2800].

Oxime [105701-23-3] $C_{22}H_{37}NO_2$ mol. wt. 347.54

-Refer to: [2346].

1-(2-Hydroxy-4,6-dimethylphenyl)-1-tetradecanone

[874507-02-5] $C_{22}H_{36}O_2$ mol. wt. 332.52



Syntheses
-Obtained by Fries rearrangement of 3,5-dimethylphenyl n-myristate (1 equiv.),
*in the presence of aluminium chloride (1.3 equiv.) in nitrobenzene at 25° for 6 h (56 %) [2801];
*in the presence of aluminium chloride (2.8 M),

first in refluxing carbon disulfide for 2 h, then for 2 h at 130° after solvent elimination (50 %) [2801].

b.p.$_{.2}$ 220° [2801].

4-Nitrophenylhydrazone $C_{28}H_{41}N_3O_3$ mol. wt. 467.65

m.p. 195° [2801].

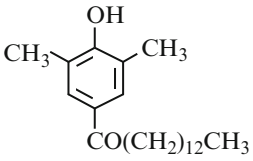
Methyl ether $C_{23}H_{38}O_2$ mol. wt. 346.55

-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxy-4,6-dimethylphenyl)-1-tetradecanone in the presence of 10 % sodium hydroxide, first at r.t., then by heating on the water bath for 5 h (74 %) [2801].

b.p.$_{.45}$ 230° [2801].

1-(4-Hydroxy-3,5-dimethylphenyl)-1-tetradecanone

$C_{22}H_{36}O_2$ mol. wt. 332.52



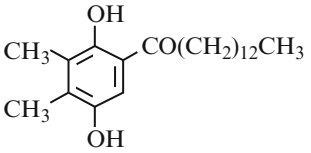
Synthesis
-Refer to: [718].
Methyl ether [29665-49-4]
$C_{23}H_{38}O_2$ mol. wt. 346.55

-Obtained by Fries rearrangement of 2,6-dimethylphenyl tetradecanoate in the presence of aluminium chloride in nitrobenzene [718], according to [380].

m.p. 40–41° [718].

1-(2,5-Dihydroxy-3,4-dimethylphenyl)-1-tetradecanone

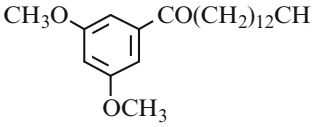
[76402-07-8] $C_{22}H_{36}O_3$ mol. wt. 348.52



Synthesis
-Refer to: [748].

1-(3,5-Dimethoxyphenyl)-1-tetradecanone

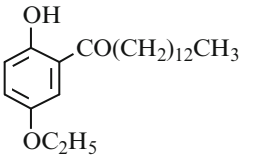
$C_{22}H_{36}O_3$ mol. wt. 348.52



Synthesis
-Refer to: [497].
m.p. 60–61° [497].

1-(5-Ethoxy-2-hydroxyphenyl)-1-tetradecanone

[140943-36-8] $C_{22}H_{36}O_3$ mol. wt. 348.52



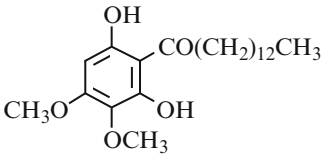
Synthesis
-Refer to: [285].
Oxime [140943-22-2]
$C_{22}H_{37}NO_3$ mol. wt. 363.54

-Refer to: [285].

BIOLOGICAL ACTIVITY: As lipoxygenase and cyclooxygenase inhibitor [285].

1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-tetradecanone

[134081-98-4] $C_{22}H_{36}O_5$ mol. wt. 380.52



Synthesis
-Preparation by treatment of 1-[6-hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-tetradecanone with potassium carbonate in refluxing methanol for 1–3 h (82 %) [1353].

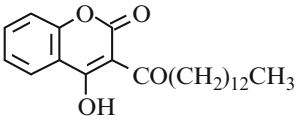
m.p. 79–80° [1353]; ^{1}H NMR [1353].

Dibenzyl ether $C_{36}H_{48}O_5$ mol. wt. 560.77

-Refer to: [1353].

4-Hydroxy-3-(1-oxotetradecyl)-2*H*-1-benzopyran-2-one

[20924-71-4] $C_{23}H_{32}O_4$ mol. wt. 372.50



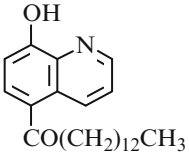
Syntheses
-Obtained by reaction of tetradecanoyl chloride with 4-hydroxycoumarin in pyridine containing one drop of piperidine for 12 h on a water bath (57 %) [3174].

-Also refer to: [3143].

m.p. 110.5° [3174].

1-(8-Hydroxy-5-quinolinyl)-1-tetradecanone

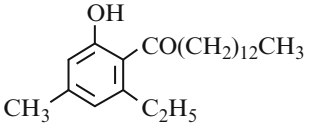
[158905-44-3] $C_{23}H_{33}NO_2$ mol. wt. 355.52



Syntheses
-Preparation by Fries rearrangement of 8-hydroxyquinolinyl myristate using aluminium chloride as catalyst [992].
-Also refer to: [993].

1-(2-Ethyl-6-hydroxy-4-methylphenyl)-1-tetradecanone

$C_{23}H_{38}O_2$ mol. wt. 346.55



Syntheses
-Preparation by Fries rearrangement of 3-ethyl-5-methyl-phenyl myristate with aluminium chloride,
*without solvent at 130° for 2 h (75 %) [2802];
*in nitrobenzene at 25° for 6 h (77 %) [2802].

m.p. 37° [2802].

Methyl ether $C_{24}H_{40}O_2$ mol. wt. 360.58

-Obtained by methylation of the above ketone in the usual way (74 %) [2802].

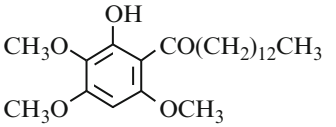
m.p. 58° [2802].

2,4-Dinitrophenylhydrazone $C_{29}H_{42}N_4O_5$ mol. wt. 526.68

m.p. 110° [2802].

1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-tetradecanone

[134081-67-7] $C_{23}H_{38}O_5$ mol. wt. 394.55



Syntheses

-Obtained by partial selective demethylation of crude 2,3,4,6-tetramethoxytetradecanophenone with aluminium chloride in acetonitrile at 50° for 1–2 h (82 %) [1353].

-Also refer to: [1351].

m.p. 66–68° [1353]; ^{1}H NMR [1353].

p-Toluenesulfonic ester [134081-82-6] $C_{30}H_{44}O_7S$ mol. wt. 548.74

-Obtained by reaction of p-toluenesulfonyl chloride with 2-hydroxy-3,4,6-trimethoxy-tetradecanophenone in the presence of potassium carbonate in refluxing acetone for 6–14 h (92 %) [1353].

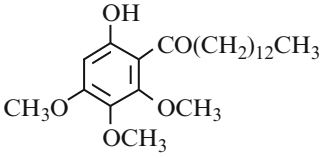
m.p. 58.5–60° [1353]; ^{1}H NMR [1353].

Methyl ether $C_{24}H_{40}O_5$ mol. wt. 408.57

-Obtained by reaction of tetradecanoyl chloride with 1,2,3,5-tetramethoxybenzene in the presence of aluminium chloride in ethyl ether at 0° for 30 min [1353].

1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-tetradecanone

[134081-74-6] $C_{23}H_{38}O_5$ mol. wt. 394.55



Syntheses

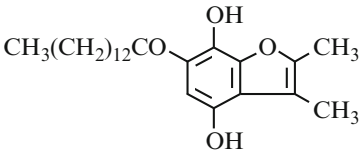
-Obtained by hydrogenation of (6-phenylmethoxy)-2,3,4-trimethoxytetradecanophenone over 10 % palladium on charcoal in ethyl acetate/methanol (1:1) until the uptake of hydrogen ceased (90 %) [1353].

-Also refer to: [1351].

m.p. 52.5–54° [1353]; ^{1}H NMR [1353].

1-(4,7-Dihydroxy-2,3-dimethyl-6-benzofuranyl)-1-tetradecanone

$C_{24}H_{36}O_4$ mol. wt. 388.02



Synthesis
-Refer to: [1040].

Dimethyl ether [49710-85-2]
$C_{26}H_{40}O_4$ mol. wt. 416.60

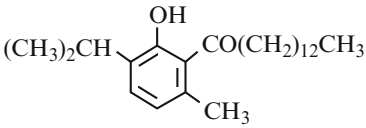
-Obtained by acylation of 4,7-dimethoxy-2,3-dimethylbenzofuran in the presence of stannic chloride in benzene (74 %) [1040].

m.p. 70° [1040]; LD_{50} [1040].

USE: Prepn. and radio protective activity of, [1040].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-tetradecanone

$C_{24}H_{40}O_2$ mol. wt. 360.58



Synthesis
-Obtained by Fries rearrangement of thymyl myristate with aluminium chloride at 120° (83 %) [2803].

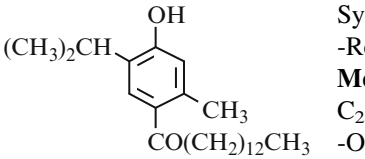
$b.p._{.2}$ 223° [2803].

2,4-Dinitrophenylhydrazone $C_{30}H_{44}N_4O_5$ mol. wt. 540.70

m.p. 143° [2803].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-tetradecanone

$C_{24}H_{40}O_2$ mol. wt. 360.58



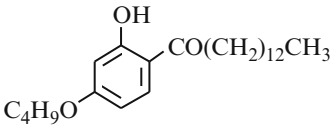
Synthesis
-Refer to: [2660].

Methyl ether (**XV**)
$C_{25}H_{42}O_2$ mol. wt. 374.61
-Obtained by reaction of myristyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (44 %) [2660].

$b.p._{.1}$ 265° [2660]; m.p. 41° [2660].

1-(4-Butoxy-2-hydroxyphenyl)-1-tetradecanone

[143287-01-8] $C_{24}H_{40}O_3$ mol. wt. 376.58



Synthesis
-Obtained by reaction of butyl bromide with 1-(2,4-dihydroxyphenyl)-1-tetradecanone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 45–62° [284].

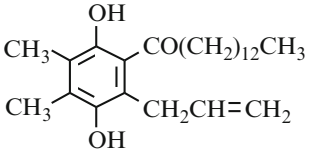
Oxime [143286-69-5] $C_{24}H_{41}NO_3$ mol. wt. 391.59

-Obtained by reaction of hydroxylamine hydrochloride with 1-(4-butoxy-2-hydroxyphenyl)-1-tetradecanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 69–72° [284].

1-[2,5-Dihydroxy-3,4-dimethyl-6-(2-propenyl)phenyl]-1-tetradecanone

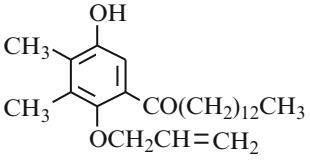
[76402-09-0] $C_{25}H_{40}O_3$ mol. wt. 388.58



Synthesis
-Obtained by allylic rearrangement of 1-[5-hydroxy-3,4-dimethyl-2-(2-propenyloxy)phenyl]-1-tetradecanone [748].

1-[5-Hydroxy-3,4-dimethyl-2-(2-propenyloxy)phenyl]-1-tetradecanone

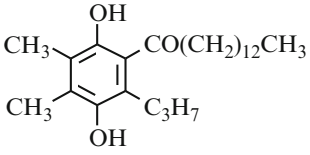
[76402-08-9] $C_{25}H_{40}O_3$ mol. wt. 388.58



Synthesis
-Refer to: [748].

1-(2,5-Dihydroxy-3,4-dimethyl-6-propylphenyl)-1-tetradecanone

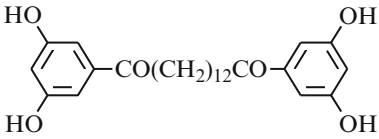
[76402-10-3] $C_{25}H_{42}O_3$ mol. wt. 390.61



Synthesis
-Refer to: [748].

1,14-Bis(3,5-dihydroxyphenyl)-1,14-tetradecanedione

$C_{26}H_{34}O_6$ mol. wt. 442.55



Synthesis
-Refer to: [2569].
m.p. 140–145° [1316].

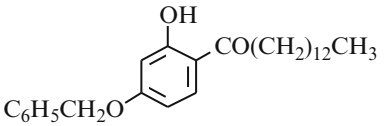
Tetramethyl ether [21390-01-2] $C_{30}H_{42}O_6$ mol. wt. 498.66

-Preparation: To a stirred suspension of sodium hydride in dimethylacetamide (DMA) at 10° under nitrogen was added 3,5-dimethoxyphenacylpyridinium perchlorate in DMA. The mixture was stirred for 0.5 h and treated with 1,10-diiodododecane. After keeping overnight at 5°, the mixture was heated for 6 h at 80° and finally at r.t. for 4 h with zinc dust and acetic acid (26 %) [2569].

colourless plates [2569]; m.p. 88–89° [2569];
^{1}H NMR [2569], IR [2569], UV [2569], MS [2569].

1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-tetradecanone

[143287-06-3] $C_{27}H_{38}O_3$ mol. wt. 410.60



Synthesis
-Obtained by reaction of benzyl chloride with 2,4-dihydroxytetradecanophenone in the presence of potassium carbonate in refluxing acetone for 20 h [284].

m.p. 64–68° [284].

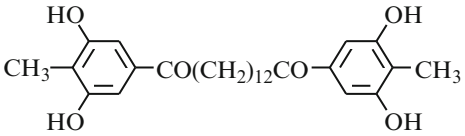
Oxime [143286-83-3] $C_{27}H_{39}NO_3$ mol. wt. 425.60

-Obtained by reaction of hydroxylamine hydrochloride with 1-[2-hydroxy-4-(phenylmethoxy)-phenyl]-1-tetradecanone in the presence of potassium acetate in refluxing ethanol for 3 h [284].

m.p. 75–78° [284].

1,14-Bis(3,5-dihydroxy-4-methylphenyl)-1,14-tetradecanedione

$C_{28}H_{38}O_6$ mol. wt. 470.61



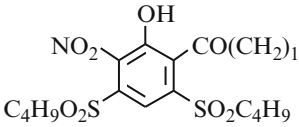
Synthesis
-Refer to: [3132].
Tetramethyl ether [21390-11-4]
$C_{32}H_{46}O_6$ mol. wt. 526.71

-Synthesis from 3,5-dimethoxy-4-methylbenzaldehyde (75 %) [3132].
-Also refer to: [2569].

colourless crystalline solid [3132]; m.p. 122° [2569];
^{1}H NMR [2569, 3132], ^{13}C NMR [3132], IR [2569],
UV [2569], MS [2569].

1-[4,6-Bis(butylsulfonyl)-2-hydroxy-3-nitrophenyl]-1-tetradecanone

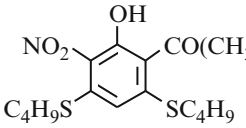
[81515-11-9] $C_{28}H_{43}NO_8S_2$ mol. wt. 571.75



Synthesis
-Refer to: [2585].

1-[4,6-Bis(butylthio)-2-hydroxy-3-nitrophenyl]-1-tetradecanone

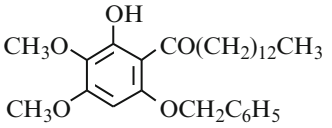
[81515-10-8] $C_{28}H_{47}NO_4S_2$ mol. wt. 525.82



Synthesis
-Refer to: [2585].

1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-tetradecanone

[134082-06-7] $C_{29}H_{42}O_5$ mol. wt. 470.65



Synthesis
-Obtained by elimination of one phenylmethyl group in 2-position by treatment of 1-(2,6-dibenzyloxy-3,4-dimethoxyphenyl)-1-tetradecanone with concentrated hydrochloric acid and acetic acid at r.t. for 2–3 h (82 %) [1353].

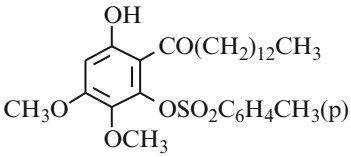
m.p. 80.5–82.5° [1353]; ^{1}H NMR [1353].

Methyl ether $C_{30}H_{44}O_5$ mol. wt. 484.68

-Refer to: [1353].

1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-tetradecanone

[134081-90-6] $C_{29}H_{42}O_7S$ mol. wt. 534.71



Synthesis
-Obtained by treatment of 1-(2-tosyloxy-3,4,6-trimethoxyphenyl)-1-tetradecanone with 25 % aluminium bromide in acetonitrile at r.t. for 2–3 h (78 %) [1353].

m.p. 59–61° [1353]; ^{1}H NMR [1353].

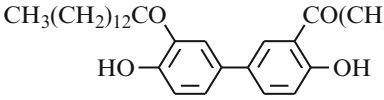
Methyl ether [134081-82-6] $C_{30}H_{44}O_7S$ mol. wt. 548.74

-Refer to: [1353].

m.p. 58.5–60° [1353]; ^{1}H NMR [1353].

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-tetradecanone

$C_{40}H_{62}O_4$ mol. wt. 606.93



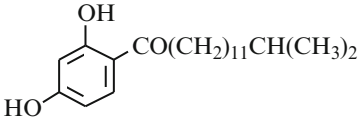
Synthesis
-Preparation by Fries rearrangement of 4,4′-biphenyl ditetradecanoate with aluminium chloride in the refluxing chlorobenzene for 24 h (72 %) [2091].

m.p. 87–88° [2091].

2 Aromatic Hydroxyketones Derived from 13-Methyltetradecanoic Acids

13-Methyl-(2,4-dihydroxyphenyl)-1-tetradecanone

[354585-20-9] $C_{21}H_{34}O_3$ mol. wt. 334.50



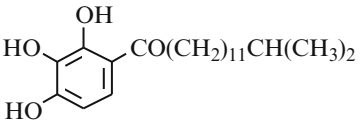
Syntheses
-Refer to: [3385, 3386, 3388].
m.p. 87° [3388].

USE: Process of preparing compounds with particular structure and anticancer activity [3385]; As anticancer and immunostimulation agent [3386]; Cytotoxic [3388].

BIOLOGICAL ACTIVITY: Cytotoxicity [3388].

13-Methyl-1-(2,3,4-trihydroxyphenyl)-1-tetradecanone

[354585-22-1] $C_{21}H_{34}O_4$ mol. wt. 350.50

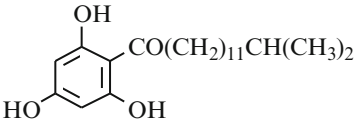


Synthesis
-Refer to: [3386].

USE: As anticancer and immunostimulation agent [3386].

13-Methyl-1-(2,4,6-trihydroxyphenyl)-1-tetradecanone

[354585-21-0] $C_{21}H_{34}O_4$ mol. wt. 350.50



Synthesis
-Refer to: [3386].

USE: As anticancer and immunostimulation agent [3386].

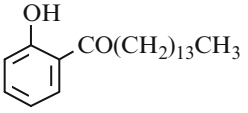
Chapter 13
Pentadecanones

1 Aromatic Hydroxyketones Derived from Pentadecanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-1-pentadecanone

[100486-17-7] $C_{21}H_{34}O_2$ mol. wt. 318.50



Syntheses

-Obtained by reaction of pentadecanoyl chloride with phenol in the presence of aluminium chloride,

*in ethylene dichloride for 16 h at 85° (44 %) [948];

*in nitrobenzene for 6 h at 60–70° (25 %) [1900].

-Also obtained by Fries rearrangement of phenyl pentadecanoate with aluminium chloride for 1 h at 150° (20 %) [1273].

m.p. 51.2–51.6° [1273], 51–51.5° [948], 42.5–43.5° [1900];
^{1}H NMR [948], IR [948], MS [948].

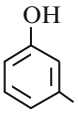
2,4-Dinitrophenylhydrazone $C_{27}H_{38}N_4O_5$ mol. wt. 498.62

m.p. 91.4–92.8° [1273].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_13

1-(3-Hydroxyphenyl)-1-pentadecanone

$C_{21}H_{34}O_2$ mol. wt. 318.50



Synthesis
-Refer to: [1067].

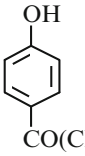
Methyl ether

$C_{22}H_{36}O_2$ mol. wt. 332.53

-Refer to: [1067]; m.p. 34–35° [1067].

1-(4-Hydroxyphenyl)-1-pentadecanone

[110662-32-3] $C_{21}H_{34}O_2$ mol. wt. 318.50



Syntheses
-Obtained by Fries rearrangement of phenyl pentadecanoate with aluminium chloride for 1 h at 150° [1273];
-Also obtained by reaction of pentadecanoyl chloride with phenol in the presence of aluminium chloride in nitrobenzene for 6 h at 60–70° (68 %) [1900].

-Also refer to: [948].

b.p.$_{10}$ 230° [1273]; m.p. 72.8–73.5° [1900].

2,4-Dinitrophenylhydrazone $C_{27}H_{38}N_4O_5$ mol. wt. 498.62

m.p. 140–141° [1273].

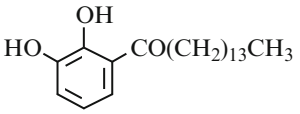
Methyl ether $C_{22}H_{36}O_2$ mol. wt. 332.53

-Refer to: [943, 1963].

m.p. 65–66° [1963]; $d_{80.5} = 0.8981$ [943]; $n_D^{80.5} = 1,47605$ [943].

1-(2,3-Dihydroxyphenyl)-1-pentadecanone

[1346860-11-4] $C_{21}H_{34}O_3$ mol. wt. 334.50



Synthesis
-Obtained by demethylation of the dimethyl ether [1935].
-Also refer to: [1935].

BIOLOGICAL ACTIVITY: Induction of neurite outgrowth [1935].

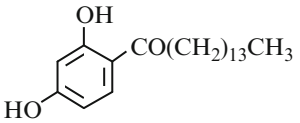
Dimethyl ether [1346860-08-9] $C_{23}H_{38}O_3$ mol. wt. 362.55

-Refer to: [1935].

BIOLOGICAL ACTIVITY: Induction of neurite outgrowth [1935].

1-(2,4-Dihydroxyphenyl)-1-pentadecanone

[100486-26-8] $C_{21}H_{34}O_3$ mol. wt. 334.50



Syntheses

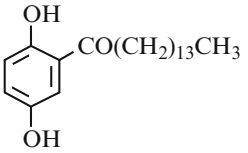
-Obtained by reaction of pentadecanoyl chloride with resorcinol in the presence of aluminium chloride in ethylene dichloride for 16 h at 85° (56 %) [948].

-Also obtained by reaction of pentadecanoic acid with resorcinol in the presence of zinc chloride for 3 h at 140–150° (55 %) [1900].

pale yellow crystals [1900];
m.p. 91.2–91.8° [1900]; ^{1}H NMR [948], MS [948].

1-(2,5-Dihydroxyphenyl)-1-pentadecanone

$C_{21}H_{34}O_3$ mol. wt. 334.50



Synthesis

-Refer to: [3274].

Dimethyl ether [855605-97-9]

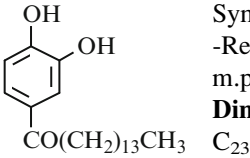
$C_{23}H_{38}O_3$ mol. wt. 362.55

-Preparation by reaction of pentadecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride in tetrachloroethane first at 0° for 3 h, then at 4° for 72 h (90.5 %) [3274].

white plates [3274];
b.p.$_{0.5}$ 205–207° [3274]; m.p. 37.5–38.5° [3274].

1-(3,4-Dihydroxyphenyl)-1-pentadecanone

$C_{21}H_{34}O_3$ mol. wt. 334.50



Synthesis

-Refer to: [1960].

m.p. 100° [1961].

Dimethyl ether

$C_{23}H_{38}O_3$ mol. wt. 362.55

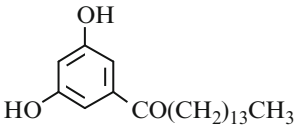
-Obtained by reaction of pentadecanoyl chloride with veratrole in the presence of aluminium chloride without solvent at 70° (22 %) [1960].

-Also obtained by condensation of veratrole with n-pentadecanoic acid in the presence of zinc chloride or aluminium chloride [1961].

b.p.$_{0.3}$ 220° [1960]; m.p. 64–65° [1960], 51–52° [1961].

1-(3,5-Dihydroxyphenyl)-1-pentadecanone

[124210-61-3] $C_{21}H_{34}O_3$ mol. wt. 334.50



Synthesis
-Obtained by demethylation of its dimethyl ether with boron tribromide in methylene chloride, first at −20°, then at r.t. overnight (34 %) [140].

Isolation from natural sources

-From the roots and stems of *Ardisia virens* Kurz (Myrsinaceae) [607].

colourless amorphous powder [140];
^{1}H NMR [140], IR [140], MS [140].

BIOLOGICAL ACTIVITY: Cytotoxicity [140].

Dimethyl ether [124210-60-2] $C_{23}H_{38}O_3$ mol. wt. 362.55

-Obtained by adding PPC/Al_2O_3 to a solution of 1-(3,5-dimethoxyphenyl)-1-pentadecanol in benzene, then the mixture obtained was stirred for 2 h (92 %) [140].

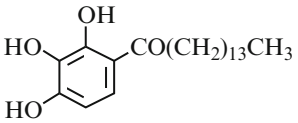
colourless needles [140];
m.p. 61.5–62.5° [1068, 1069], 61–62° [140];
IR [140], UV [140], MS [140].

USE: Direct prepn. of benzylic manganese reagents from benzyl halides, sulfonates, and phosphates, their reactions and applications in org. synthesis [2978].

BIOLOGICAL ACTIVITY: Cytotoxicity [140].

1-(2,3,4-Trihydroxyphenyl)-1-pentadecanone

$C_{21}H_{34}O_4$ mol. wt. 350.50

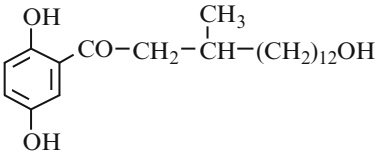


Synthesis
-Obtained by reaction of pentadecanoic acid with pyrogallol in the presence of zinc chloride (Nencki reaction) at 140–145° for 4 h [506].

lustrous colourless leaflets [506]; m.p. 87–88° [506].

15-Hydroxy-3-methyl-1-(2,5-dihydroxy)phenyl]-1-pentadecanone

[1254222-60-0] $C_{22}H_{36}O_4$ mol. wt. 364.53



Synthesis
-Refer to: [720].
yellow crystals [720]; ^{1}H NMR [720], ^{13}C NMR [720].

BIOLOGICAL ACTIVITY: Inhibition of nitrite production [720]; Inhibition of tumor necrosis factor-α (TNF-α) production [720].

Oxime [1254222-72-4] $C_{22}H_{37}NO_4$ mol. wt. 379.54

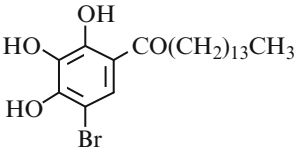
white crystals [720]; ^{1}H NMR [720].

BIOLOGICAL ACTIVITY: Inhibition of nitrite production [720].

1.2 Substituted Hydroxyketones

1-(5-Bromo-2,3,4-trihydroxyphenyl)-1-pentadecanone

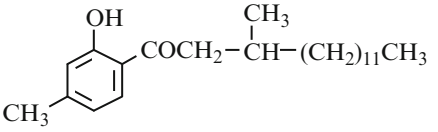
$C_{21}H_{33}BrO_4$ mol. wt. 429.39



Synthesis
-Obtained by reaction of bromine with 4-pentadecanoyl-pyrogallol in acetic acid [506].
m.p. 89–90° [506].

1-(2-Hydroxy-4-methylphenyl)-3-methyl-1-pentadecanone

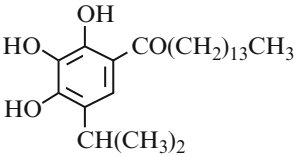
$C_{23}H_{38}O_2$ mol. wt. 346.55



Synthesis
-Refer to: [1903].
b.p.$_{0.1}$ 162–176° [1903].

1-[2,3,4-Trihydroxy-5-(1-methylethyl)phenyl]-1-pentadecanone

[877877-96-8] $C_{24}H_{40}O_4$ mol. wt. 392.58

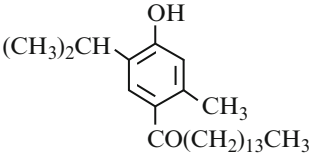


Synthesis
-Refer to: [3267].
^{1}H NMR [3267], ^{13}C NMR [3267].

BIOLOGICAL ACTIVITY: As inhibitors of antiapoptotic Bcl-2 [3267].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-pentadecanone

$C_{25}H_{42}O_2$ mol. wt. 374.61



Synthesis
-Obtained by treatment of 4-methoxy-2-methyl-5-isopropylpentadecanone with boiling pyridinium chloride (205–215°) for 7.5 h (23 %) [2660].

b.p.$_{11}$ 276–279° [2660]; m.p. 41° [2660].

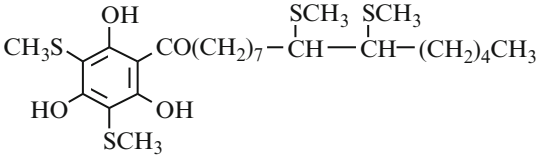
Methyl ether $C_{26}H_{44}O_2$ mol. wt. 388.63.

-Preparation by reaction of pentadecanoyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (44 %) [2660].

b.p.$_{19}$ 280–283° [2660]; m.p. 44° [2660].

1-[3,5-(Dithiomethyl)-2,4,6-trihydroxyphenyl]-9,10-(dithiomethyl)-1-pentadecanone

$C_{25}H_{42}O_4S_4$ mol. wt. 534.87

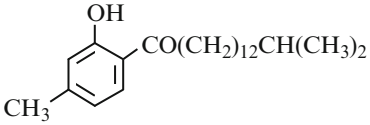


Synthesis
-Refer to: [1133].
MS [1133].

2 Aromatic Hydroxyketones Derived from 14-Methylpentadecanoic Acid

1-(2-Hydroxy-4-methylphenyl)-14-methyl-1-pentadecanone

[57080-94-1] $C_{23}H_{38}O_2$ mol. wt. 346.55



Synthesis
-Refer to: [1903].

Oxime [57125-28-7]
$C_{23}H_{39}NO_2$ mol. wt. 361.57

-Refer to: [1903].

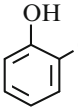
Chapter 14
Hexadecanones

1 Aromatic Hydroxyketones Derived from Hexadecanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-1-hexadecanone

[2589-84-6] $C_{22}H_{36}O_2$ mol. wt. 332.53



Syntheses
-Obtained by reaction of palmitoyl chloride with phenol in the presence of aluminium chloride,
*in tetrachlorethane few hours at 25° (26 %) [2548];
*in nitrobenzene for 3 h at 70° (22 %) [2549];
*in carbon disulfide for 5.5 h at 47° (47 %) [2549].
-Also obtained by Fries rearrangement of phenyl palmitate with aluminium chloride [1456],
*in tetrachlorethane for 10 h at 70° (15 %) [2550];
*without solvent for 1 h at 150° (20 %) [1273].
-Also obtained by reaction of palmitic acid with phenol,
*in the presence of zinc chloride (Nencki reaction) (75 %) [2398];
*in the presence of boron trifluoride first at 60°, then at 80–90° [2598].
-Also refer to: [873, 1225].

m.p. 58° [2398], 57–58° [1273], 54–56° [2548], 54–55° [2598];
TLC [1456].

USE: Textile rot proofing by, [873].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_14

Oxime $C_{22}H_{37}NO_2$ mol. wt. 347.54

m.p. 87° [2598].

2,4-Dinitrophenylhydrazone $C_{28}H_{40}N_4O_5$ mol. wt. 512.65

m.p. 96–97° [1273], 94–95° [2548], 93° [2598].

2,4-Dinitrophenylhydrazone, nickel complex [116803-89-5]

USE: Metal complex discolouration inhibitor, silver halide photog. material contg. [2976].

Acetate $C_{24}H_{38}O_3$ mol. wt. 374.56

m.p. 52° [2598].

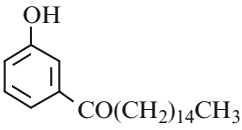
Methyl ether $C_{23}H_{38}O_2$ mol. wt. 346.55

-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxyphenyl)-1-hexadecanone in the presence of potassium carbonate in boiling acetone for 6 h [2398].

colourless liquid [2398]; b.p.$_{30}$ 190° [2398]; m.p. 38° [2398].

1-(3-Hydroxyphenyl)-1-hexadecanone

[63442-87-5] $C_{22}H_{36}O_2$ mol. wt. 332.53



Syntheses
-Refer to: [1984, 1985].
m.p. 56° [1984]; IR [1984].

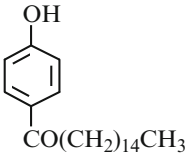
Methyl ether [63442-84-2] $C_{23}H_{38}O_2$ mol. wt. 346.55

-Refer to: [1984, 1985].

m.p. 42° [1984]; IR [1984].

1-(4-Hydroxyphenyl)-1-hexadecanone

[2589-76-6] $C_{22}H_{36}O_2$ mol. wt. 332.53



Syntheses
-Obtained by reaction of palmitoyl chloride with phenol in the presence of aluminium chloride,
*in tetrachlorethane few hours at 25° (29 %) [2548];
*in nitrobenzene for 3 h at 70° (67 %) [2549];
*in carbon disulfide for 5.5 h at 47° (51 %) [2549].

-Also obtained by Fries rearrangement of phenyl palmitate with aluminium chloride [1456],
*in tetrachlorethane for 10 h at 70° (20 %) [2550];
*without solvent for 1 h at 150° (30 %) [1273];
*in the presence of aluminium chloride in refluxing carbon disulfide for 5 h. Then, the mixture was kept at 80–90° for 2 h and at 140–150° for 1 h after solvent elimination [1222].
-Also obtained by demethylation of 4-palmitoylanisole with hydrobromic acid in acetic acid [2398].
-Also obtained by fusion of its methyl ether with potassium hydroxide [1757].
-Also obtained by dealkylation of its ethyl ether with aluminium chloride in carbon disulfide for 8 h at 60–70° [191].
-Also obtained by reaction of palmitic acid with phenol in the presence,
*of boron trifluoride for 2–3 h between 65 and 85° (96–98 %) [503] or first at 60°, then at 80–90° [2598];
*of activated acid clay catalyst at 190° for 2 h [3277].
-Also refer to: [873, 1057, 1116, 1225, 1299, 3424].

m.p. 85° [2398], 84.5–86° [3277], 84.5–85° [1273, 2548], 84–85° [2598], 81–82° [3424], 80° [503], 78° [191];
^{1}H NMR [3424]; Cryoscopic study [182]; TLC [1456].

USE: Textile rot proofing by, [873].

Oxime $C_{22}H_{37}NO_2$ mol. wt. 347.54

m.p. 95° [2598].

2,4-Dinitrophenylhydrazone $C_{28}H_{40}N_4O_5$ mol. wt. 512.65

m.p. 142.3–143.5° [1273], 141–142° [2548], 141° [2598].

iso-Nicotinylhydrazone [103159-09-7] $C_{28}H_{41}N_3O_2$ mol. wt. 451.65

m.p. 153° [520, 521].

USE: In chemotherapy of leprosy [520, 521].

Methyl ether [102898-55-5] $C_{23}H_{38}O_2$ mol. wt. 346.55

-Obtained by reaction of palmitoyl chloride with anisole in the presence of aluminium chloride (90 %) [2398] at 70° on a water bath for 3 days (69 %) [1757] or for 2 h (50 %) [15].
-Also obtained by reaction of palmitoyl chloride with anisole in the presence of zinc in toluene at 70° for 5 h (91 %) [2064].
-Also obtained by reaction of palmitic acid with anisole,
*in the presence of chloracetyl anhydride (80 %) [3178];

*on the solid surface of alumina in the presence of trifluoroacetic anhydride for 180 min at r.t. (92 %) [2563].
-Also refer to: [643, 1104, 1756, 1758, 1963, 2016].

b.p.$_{15}$ 279–280° [1756–1758];
m.p. 75° [3178], 72.5° [2016], 72–73° [1963], 71–71.5° [15], 70.5° [1756–1758], 70° [1104, 2398];
^{1}H NMR [2064, 2563], IR [2064, 2563], MS [2064];
$n_D^{80.5} = 1.47605$ [643].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{29}H_{34}N_4O_5$ mol. wt. 518.61

m.p. 97–98° [2016].

Ethyl ether [416846-26-9] $C_{24}H_{40}O_2$ mol. wt. 360.58

-Obtained by Friedel-Crafts reaction of palmitoyl chloride with phenetole in the presence of aluminium chloride [191, 1757].
-Also refer to: [1756, 1758].

b.p.$_{15}$ 288–289° [1756–1758];
m.p. 69° [1756–1758].

2-Chloroethyl ether $C_{24}H_{39}ClO_2$ mol. wt. 395.03

-Obtained by reaction of hexadecanoyl chloride with 2-chloroethoxybenzene in the presence of aluminium chloride in carbon disulfide for 4 h at 50° (75 %) [476].

m.p. 70–71° [476].

N-Dimethylaminoethyl ether $C_{26}H_{45}NO_2$ mol. wt. 403.65

-Obtained by reaction of 4-(2-chloroethoxy)hexadecanophenone with dimethylamine in a sealed tube for 2 h at 150° [476].

free base: b.p.$_{0.3}$ 210° [476]; m.p. 41–42°[476].
hydrochloride (49 %) [476]; m.p. 150° [476].

2,3-Epoxypropoxy ether [18211-88-6] $C_{25}H_{40}O_3$ mol. wt. 388.58

-Obtained by reaction of epichlorohydrin (0.1 mol) with p-hexadecanoylphenol (0.1 mol) in the presence of 30 % sodium hydroxide between 40 and 50° (51 %) [2669].

m.p. 110° [2669].

Acetate $C_{24}H_{38}O_3$ mol. wt. 374.56

m.p. 79° [2598].

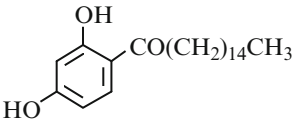
Palmitate [120857-41-2] $C_{38}H_{66}O_3$ mol. wt. 570.94

-Obtained by reaction of palmitic acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3277].

m.p. 87–88° [3277].

1-(2,4-Dihydroxyphenyl)-1-hexadecanone

[40372-79-0] $C_{22}H_{36}O_3$ mol. wt. 348.53



Syntheses

-Obtained by reaction of palmitic acid with resorcinol,

*in the presence of boron trifluoride for 2–3 h between 65 and 85° (95–98 %) [503] or first at 60°, then at 80–90° [2598];

*in the presence of zinc chloride [16].

-Also refer to: [859, 1296, 1757, 2973].

m.p. 95–95.5° [2598], 95° [503], 94–95° [16], 89–90° [859].

USE: Protection against whole-body irradiation [1810]; Emulsifying agent, in waterproofing of leather [1296]; Protection against X-rays [1811].

Na salt [41729-72-0] $C_{22}H_{34}Na_2O_3$ mol. wt. 392.48

USE: Emulsifying agent, in waterproofing of leather [1296].

Oxime $C_{22}H_{37}NO_3$ mol. wt. 363.54

m.p. 158° [2598].

4-Nitrophenylhydrazone $C_{28}H_{41}N_3O_4$ mol. wt. 483.64

m.p. 94–95° [859].

Dimethyl ether $C_{24}H_{40}O_3$ mol. wt. 376.58

-Obtained by Friedel-Crafts reaction of palmitoyl chloride (2 parts) with resorcinol dimethyl ether (3 parts) in the presence of aluminium chloride (2 parts) by heating the mixture from 40° to 100° [1757].

-Also refer to: [16].

b.p.$_{15}$ 289–290° [1757]; m.p. 63.5° [1757], 61° [16].

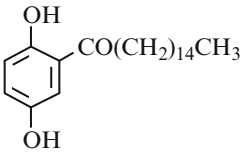
Diacetate [96968-05-7] $C_{26}H_{40}O_5$ mol. wt. 432.60

-Refer to: [2517].

m.p. 73–74° [2598].

1-(2,5-Dihydroxyphenyl)-1-hexadecanone
(2-Palmitoylhydroquinone)

[95807-67-3] $C_{22}H_{36}O_3$ mol. wt. 348.53



Syntheses
-Obtained by reaction of palmitic acid with hydroquinone in the presence of boron trifluoride,
*in 1,2-dichloroethane (50 %) [142];
*without solvent first at 60°, then at 80–90° [2598].

-Also obtained by reaction of hexadecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156] in carbon disulfide [159].
-Also refer to: [393, 2090, 2151].

m.p. 106–107° [142], 106° [2598], 103–104° [156, 159].

USE: Probing the redox activity of T-lymphocytes deposited at electrode surfaces with voltammetric methods (as a redox mediator) [393]; Redox Chemistry of Ca-Transporter 2-palmitoylhydroquinone in an Artificial Thin Organic Film Membrane [2090].

Oxime $C_{22}H_{37}NO_3$ mol. wt. 363.54

m.p. 102° [2598].

Dimethyl ether [180133-49-7] $C_{24}H_{40}O_3$ mol. wt. 376.58

-Obtained by reaction of hexadecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [2859],
*in carbon disulfide (78 %) [1633];
*in tetrachloroethane (69 %) [714].
-Also refer to: [1632].

$b.p._{\cdot 0.18}$ 205° [714];
m.p. 51.5° [714], 44° [1632, 1633];
^{1}H NMR [2859]; MS [2859].

Phenylhydrazone of the dimethyl ether $C_{30}H_{46}N_2O_2$ mol. wt. 466.71

m.p. 64° [1633].

Diethyl ether $C_{26}H_{44}O_3$ mol. wt. 404.63

-Obtained by reaction of palmitoyl chloride with hydroquinone diethyl ether in the presence of aluminium chloride in tetrachloroethane [714].

2,4-Dinitrophenylhydrazone of the diethyl ether C32H48N4O6 mol. wt. 584.76

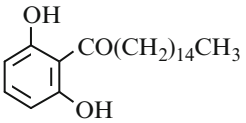
bright red crystals [714]; m.p. 75° [714].

Diacetate $C_{26}H_{40}O_5$ mol. wt. 432.60

m.p. 77° [2598].

1-(2,6-Dihydroxyphenyl)-1-hexadecanone

[96820-25-6] $C_{22}H_{36}O_3$ mol. wt. 348.53



Syntheses

-Preparation in 4 steps from 1,3-cyclohexanedione by acylation with hexadecanoyl chloride, rearrangement, chlorination by tert-butyl hypochlorite, and aromatization (90 %) [1816], according to the method [75, 1817].

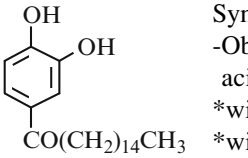
Isolation from natural sources

-From fruits of *Virola elongata* (Myristicaceae) [1622, 1623].
-In plants of the family Myristicaceae [719].

amorphous solid [1622];
^{1}H NMR [1622], ^{13}C NMR [1622], IR [1622], MS [1622].

1-(3,4-Dihydroxyphenyl)-1-hexadecanone
(4-Hexadecanoylcatechol)

[54535-83-0] $C_{22}H_{36}O_3$ mol. wt. 348.53



Syntheses

-Obtained by treatment of a pyrocatechol and hexadecanoic acid mixture,
*with zinc chloride [1961] at 135–140° for 2 h (10 %) [1283];
*with boron trifluoride first at 60°, then at 80–90° [2598].

-Also refer to: [283, 3159].

m.p. 101–102° [2598], 99–100° [1283].

Oxime $C_{22}H_{37}NO_3$ mol. wt. 363.54

m.p. 103° [2598].

2,4-Dinitrophenylhydrazone $C_{28}H_{40}N_4O_5$ mol. wt. 512.65

m.p. 225° [2598].

Dimethyl ether [855956-25-1] $C_{24}H_{40}O_3$ mol. wt. 376.58

-Obtained by Friedel-Crafts reaction of palmitoyl chloride with veratrole in the presence of aluminium chloride [2574],
*without solvent at 70° (24 %) [1960];
*in carbon disulfide [1526].
-Also refer to: [1960].

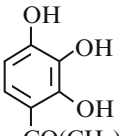
b.p.$_{0.5}$ 230° [1960];
m.p. 79–80° [1960], 78–79° [1526], 72–72.5° [2574].

Diacetate $C_{26}H_{40}O_5$ mol. wt. 432.60

m.p. 72–73° [2598].

1-(2,3,4-Trihydroxyphenyl)-1-hexadecanone
(4-Hexadecanoylpyrogallol)

[40366-12-9] $C_{22}H_{36}O_4$ mol. wt. 364.53



Syntheses
-Obtained by reaction of palmitic acid with pyrogallol,
*in the presence of boron trifluoride for 2–3 h between 65 and 85° (95–98 %) [503];
*in the presence of zinc chloride (Nencki reaction) at 135–140° for 2 h (30 %) [1283].

-Also refer to: [859, 1296, 2327].

m.p. 92° [503], 89–90° [1283], 84–85° [859].

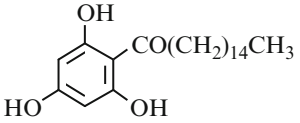
USE: Colour photog. development-promoting agent, for rapid development without benzyl alc. [2327]; Emulsifying agent, in waterproofing of leather [1296].

2,4-Dinitrophenylhydrazone $C_{28}H_{40}N_4O_7$ mol. wt. 544.65

m.p. 171–172° [859].

1-(2,4,6-Trihydroxyphenyl)-1-hexadecanone

[82461-11-8] $C_{22}H_{36}O_4$ mol. wt. 364.53



Syntheses
-Obtained by reaction of hexadecanoic (palmitic) acid with phloroglucinol in the presence of aluminium chloride and phosphorous oxychloride (16 %) [3202].

Isolation from natural sources

-From fruits of *Virola elongata* (Myristicaceae) [1623].
-From the related brown algae *Zonaria farlowii*, *Zonaria diesingiana* and *Lobophora papenfussii* (9 %) (Dictyotaceae) [1103, 3202].

white crystals [3202]; m.p. 129° [3202];
^{1}H NMR [1103, 3202], ^{13}C NMR [1103, 3202],
IR [1103, 3202], UV [1103, 3202], MS [1103, 3202]; TLC [3202].

Triacetate [82460-91-1] $C_{28}H_{42}O_7$ mol. wt. 490.64

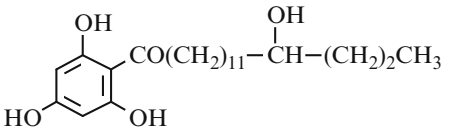
-Obtained by reaction of acetic anhydride with 1-(2,4,6-trihydroxyphenyl)-1-hexadecanone in the presence of pyridine at r.t. overnight (near quantitative yield) [1103].

^{1}H NMR [1103], IR [1103].

BIOLOGICAL ACTIVITY: Antibiotic [3202].

13-Hydroxy-1-(2,4,6-Trihydroxyphenyl)-1-hexadecanone
(Byssomeruliol C)

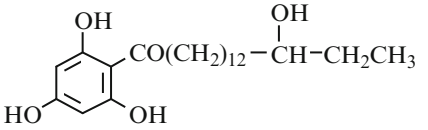
[83162-76-9] $C_{22}H_{36}O_5$ mol. wt. 380.52



Isolation from natural sources
-From fruit bodies and mycelia of *Byssomerulius Corium* [1931].

14-Hydroxy-1-(2,4,6-Trihydroxyphenyl)-1-hexadecanone
(Byssomeruliol D)

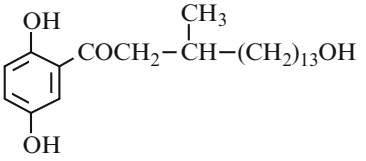
[83162-77-0] $C_{22}H_{36}O_5$ mol. wt. 380.52



Isolation from natural sources
-From fruit bodies and mycelia of *Byssomerulius Corium* [1931].

16-Hydroxy-3-methyl-1-(2,5-dihydroxyphenyl)-1-hexadecanone

[1254222-63-3] $C_{23}H_{38}O_4$ mol. wt. 378.55

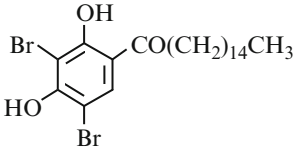


Synthesis
-Refer to: [720].
Oxime [1254222-75-7]
$C_{23}H_{39}NO_4$ mol. wt. 393.57

1.2 Substituted Hydroxyketones

1-(3,5-Dibromo-2,4-dihydroxyphenyl)-1-hexadecanone
(2,6-Dibromo-4-palmitylresorcinol)

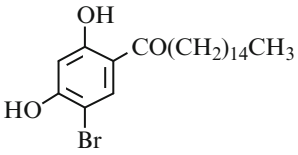
$C_{22}H_{34}Br_2O_3$ mol. wt. 506.32



Synthesis
-Obtained by reaction of bromine with 4-palmitylresorcinol in acetic acid at 37–38° for few min [507].
colourless leaflets [507]; m.p. 104° [507].

1-(5-Bromo-2,4-dihydroxyphenyl)-1-hexadecanone

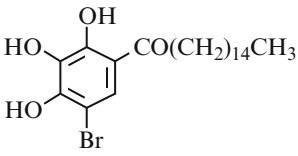
$C_{22}H_{35}BrO_3$ mol. wt. 427.42



Synthesis
-Refer to: [859].
needles [859];
m.p. 92–93° [859].

1-(5-Bromo-2,3,4-trihydroxyphenyl)-1-hexadecanone

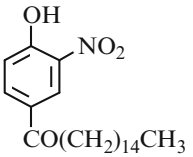
$C_{22}H_{35}BrO_4$ mol. wt. 443.42



Syntheses
-Obtained by reaction of bromine with 4-palmitoyl-pyrogallol in acetic acid [506].
-Also refer to: [859].
needles [859]; m.p. 87–88° [859], 89–90° [506].

1-(4-Hydroxy-3-nitrophenyl)-1-hexadecanone

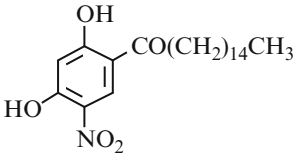
[70079-28-6] $C_{22}H_{35}NO_4$ mol. wt. 377.52



Syntheses
-Obtained by Fries rearrangement of o-nitrophenyl hexadecanoate [1222].
-Also refer to: [1224, 1315].
m.p. 85–86° [1222].

1-(2,4-Dihydroxy-5-nitrophenyl)-1-hexadecanone

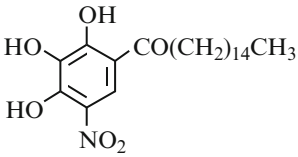
$C_{22}H_{35}NO_5$ mol. wt. 393.52



Synthesis
-Refer to: [859].
pale yellow needles [859];
m.p. 97–98° [859].

1-(2,3,4-Trihydroxy-5-nitrophenyl)-1-hexadecanone

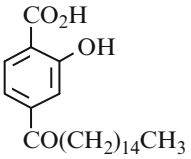
$C_{22}H_{35}NO_6$ mol. wt. 409.52



Synthesis
-Refer to: [859].
m.p. 92–93° [859].

4-Hexadecanoylsalicylic acid

[40372-78-9] $C_{23}H_{36}O_4$ mol. wt. 376.54

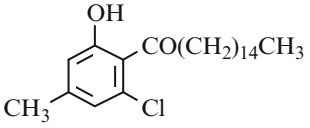


Synthesis
-Refer to: [1296].

USE: Emulsifying agent, in waterproofing of leather [1296].

1-(2-Chloro-6-hydroxy-4-methylphenyl)-1-hexadecanone

[24490-29-7] $C_{23}H_{37}ClO_2$ mol. wt. 381.00

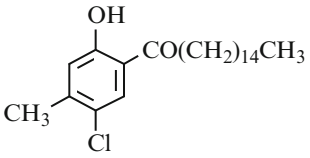


Synthesis
-Refer to: [3138].

USE: Fluorescence of, hyperchromic shifts in, [3138].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-hexadecanone

$C_{23}H_{37}ClO_2$ mol. wt. 381.00

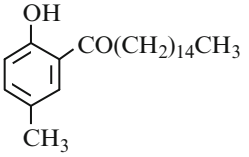


Syntheses
-Obtained by reaction of palmitic acid with 4-chloro-3-methylphenol in the presence of boron trifluoride for 2–3 h between 65 to 85° (90 %) [503].
-Also refer to: [3138].

m.p. 86° [503]; fluorescence spectral data [3138].

1-(2-Hydroxy-5-methylphenyl)-1-hexadecanone

$C_{23}H_{38}O_2$ mol. wt. 346.55



Syntheses
-Obtained by reaction of palmitic acid with p-cresol in the presence of boron trifluoride for 2–3 h between 65 and 85° (90–95 %) [503].
-Also refer to: [879].

m.p. 61° [503]; ^{1}H NMR [879], IR [879].

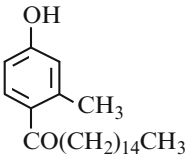
Oxime of the methyl ether [101396-06-9] $C_{24}H_{41}NO_2$ mol. wt. 375.60

m.p. 51–52° [879].

USE: Palladium extn. and purifn. with, [3191].

1-(4-Hydroxy-2-methylphenyl)-1-hexadecanone

$C_{23}H_{38}O_2$ mol. wt. 346.55



Synthesis
-Refer to: [2503].

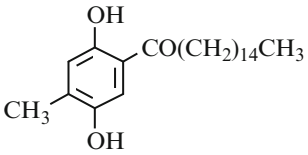
Phenyl ether [791615-81-1]
$C_{29}H_{42}O_2$ mol. wt. 422.65

-Obtained by adding a mixture of m-phenoxytoluene and hexadecanoyl chloride to a suspension of aluminium chloride in methylene chloride at 0°, then the mixture stirred for 1.5–2 h at 3–5° (31 %) [2503].

b.p.$_3$ 261–263° [2503]; m.p. 30–31° [2503];
^{1}H NMR [2503], IR [2503], MS [2503].

1-(2,5-Dihydroxy-4-methylphenyl)-1-hexadecanone

[21182-64-9] $C_{23}H_{38}O_3$ mol. wt. 362.55



Syntheses
-Obtained by reaction of hexadecanoic acid with 2-methyl-hydroquinone in the presence of boron trifluoride,
*in 1,2-dichloroethane at 40–45° for 1.25 h. The mixture was allowed to stand overnight (69 %) [142];
*in *sym*-tetrachloroethane at r.t. overnight, then on a steam bath for 8 h (68.5 %) [3106].

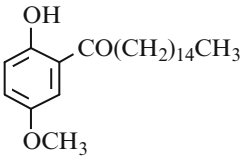
-Also obtained by reaction of hexadecanoyl chloride with 2,5-dimethoxytoluene in the presence of aluminium chloride in refluxing carbon disulfide for 10 h. Demethylation was accompanied in the course of the reaction (quantitative yield) [2370].
-Also refer to: [748, 750, 3106].

yellow plates [2370];
m.p. 94–94.5° [142, 3106], 93.5° [2370]; IR [2370].

USE: As photographic antistain agent [3106]; Improvements in heat-sensitive copy materials [750].

1-(2-Hydroxy-5-methoxyphenyl)-1-hexadecanone

[102898-63-5] $C_{23}H_{38}O_3$ mol. wt. 362.55



Syntheses

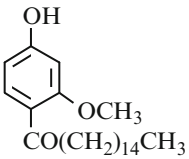
-Obtained by reaction of hexadecanoic acid with p-methoxyphenol in the presence of boron trifluoride in tetrachloroethane for 4 h. The reaction mixture was allowed to stand overnight at r.t. and was then heated on a steam bath for about 3 h (47 %) [142].

-Also obtained by reaction of hexadecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156], in carbon disulfide [159].

m.p. 59–60.5° [156, 159], 57.5–59° [142].

1-(4-Hydroxy-2-methoxyphenyl)-1-hexadecanone

$C_{23}H_{38}O_3$ mol. wt. 362.55



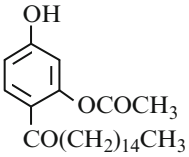
Syntheses

-Refer to: [14, 16, 1756, 1758].

m.p. 66° [14, 16].

1-[2-(Acetyloxy)-4-hydroxyphenyl]-1-hexadecanone

[251463-57-7] $C_{24}H_{38}O_4$ mol. wt. 390.56



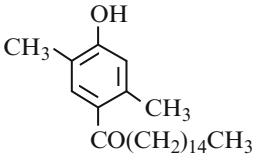
Synthesis

-Obtained by selective deacetylation of 2,4-diacetoxyphenyl pentadecyl ketone mediated by porcine pancreatic lipase (PPL) in THF at 42–45° for 24 h in the presence of n-butanol (60 %) [2517].

white solid [2517]; m.p. 105° [2517];
^{1}H NMR [2517], ^{13}C NMR [2517], IR [2517], UV [2517], MS [2517].

1-(4-Hydroxy-2,5-dimethylphenyl)-1-hexadecanone

[95185-68-5] $C_{24}H_{40}O_2$ mol. wt. 360.58

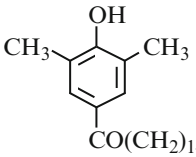


Synthesis

-Refer to: [2704].

1-(4-Hydroxy-3,5-dimethylphenyl)-1-hexadecanone

$C_{24}H_{40}O_2$ mol. wt. 360.58



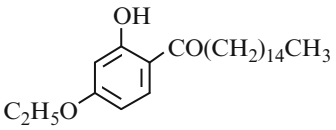
Syntheses

-Obtained by reaction of hexadecanoyl chloride with 2,6-dimethylphenol in the presence of aluminium chloride [1832].

-Also obtained by reaction of hexadecanoic acid with 2,6-dimethylphenol in the presence of boron trifluoride [1832].

1-(4-Ethoxy-2-hydroxyphenyl)-1-hexadecanone

[19347-52-5] $C_{24}H_{40}O_3$ mol. wt. 376.58



Syntheses

-Obtained by reaction of hexadecanoyl chloride with m-diethoxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°.

The temperature was then raised to 80° and stirring was continued at that temperature for 5 h (78 %) [1194, 1195].

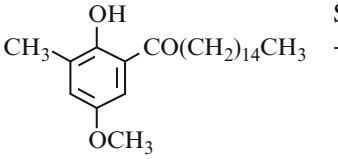
-Also obtained by treating hexadecanoyl chloride with resorcinol diethyl ether under Friedel-Crafts reaction conditions [1197, 1198].

m.p. 66–66.3° [1194, 1195]; UV [1194, 1195].

USE: UV absorber [1194]; Light-stabilizer of polymeric materials [1194].

1-(2-Hydroxy-5-methoxy-3-methylphenyl)-1-hexadecanone

[103168-03-2] $C_{24}H_{40}O_3$ mol. wt. 376.58



Syntheses

-Obtained by reaction of hexadecanoic acid with 4-methoxy-2-methylphenol in the presence of boron trifluoride in tetrachloroethane for 6 h. The reaction mixture was allowed to stand overnight at r.t. and was then heated on a steam bath for about 5 h (37 %) [142].

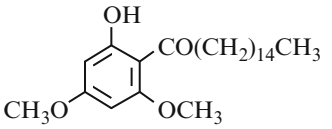
-Also refer to: [1907, 3106].

b.p.$_1$ 205–215° [3106]; m.p. 66–67° [142, 3106].

USE: As photographic antistain agent [3106].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-hexadecanone

[82460-89-7] $C_{24}H_{40}O_4$ mol. wt. 392.58



Synthesis

-Preparation by reaction of excess diazomethane with 1-(2,4,6-trihydroxyphenyl)-1-hexadecanone in ethyl ether for 10 h at 25° (quantitative yield) [1103].

^{1}H NMR [1103], IR [1103].

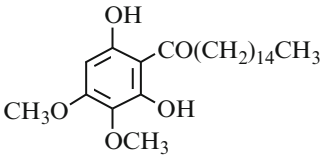
Acetate [82460-90-0] $C_{26}H_{42}O_5$ mol. wt. 434.62

-Obtained by reaction of acetic anhydride with 1-(2-hydroxy-4,6-dimethoxyphenyl)-1-hexadecanone in the presence of pyridine at r.t. overnight (near quantitative yield) [1103].

^{1}H NMR [1103], IR [1103].

1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-hexadecanone

[134081-99-5] $C_{24}H_{40}O_5$ mol. wt. 408.58



Synthesis

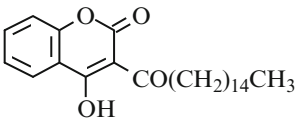
-Preparation by treatment of 1-[6-hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy) phenyl]-1-hexadecanone with potassium carbonate in refluxing methanol for 1–3 h (89 %) [1353].

m.p. 83.5–85° [1353]; ^{1}H NMR [1353].

4-Hydroxy-3-(1-oxohexadecyl)-2*H*-1-benzopyran-2-one

4-Hydroxy-3-palmitoyl-2*H*-chromen-2-one

[74965-90-5] $C_{25}H_{36}O_4$ mol. wt. 400.56



Syntheses

-To the PTFE reaction vessel, 4-hydroxycoumarin, a catalytic amount of piperidine, and pyridine (1 ml/mmol) were added. After the solution was cooled to 0°, palmitoyl chloride (1.6 equiv.) was slowly added through a septum.

The mixture was sonicated (21 kHz, 40 W/cm^2) for about 1.5 h under nitrogen at 38°, and monitored by TLC [746].

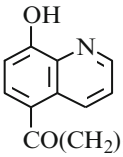
-Also obtained by reaction of hexadecanoyl chloride with 4-hydroxycoumarin in pyridine containing one drop of piperidine for 12 h on a water bath (61 %) [3174].

white powder [746]; m.p. 111° [3174], 103–104° [746];
^{1}H NMR [746], IR [746], MS [746]; TLC [746].

BIOLOGICAL ACTIVITY: Antibacterial [746].

1-(8-Hydroxy-5-quinolinyl)-1-hexadecanone

[103045-61-0] $C_{25}H_{37}NO_2$ mol. wt. 383.57



Syntheses

-Obtained by neutralizing an aqueous suspension of its hydrobromide with alkali [938].

-Preparation by Fries rearrangement of 8-hydroxyquinolinyl palmitate using aluminium chloride as catalyst [992].

-Also refer to: [892, 993–996, 3108].

USE: Preconcentration and speciation of chromium (III) in waters by using 5-palmitoyl-8-hydroxyquinoline immobilized on a nonpolar adsorbent [995]; Amebicidal action of, [3108].

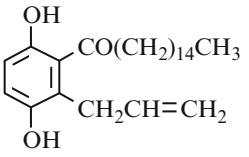
Hydrobromide $C_{25}H_{37}NO_2$, HBr mol. wt. 464.48

-Obtained by reaction of palmitoyl chloride with 8-quinolinol in the presence of aluminium chloride in nitrobenzene first at 75° for 16 h, then at r.t. for 20 h. Then, the acetone solution was saturated with hydrogen bromide (11 %) [938].

m.p. 223° [938].

1-[3,6-Dihydroxy-2-(2-propenyl)phenyl]-1-hexadecanone
1-(3,6-Dihydroxy-2-allylphenyl)-1-hexadecanone

[98357-90-5] $C_{25}H_{40}O_3$ mol. wt. 388.58



Syntheses

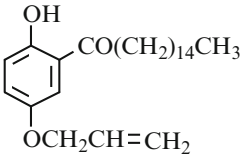
-Obtained by Claisen rearrangement of 1-[2-hydroxy-5-(allyloxy)phenyl]-1-hexadecanone, first at 170° and in fine at 223° under nitrogen (63 %) [142].

-Also refer to: [2151].

m.p. 77.5–78.5° [142].

1-[2-Hydroxy-5-(2-propenyloxy)phenyl]-1-hexadecanone
1-[2-Hydroxy-5-(allyloxy)phenyl]-1-hexadecanone

[98357-89-2] $C_{25}H_{40}O_3$ mol. wt. 388.58



Syntheses

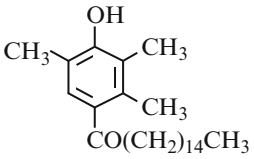
-Obtained by reaction of allyl bromide with 2-palmitoylhydroquinone in the presence of potassium carbonate in refluxing acetone for 8 h, then at r.t. overnight (62 %) [142].

-Also refer to: [2151].

m.p. 58–59° [142].

1-(4-Hydroxy-2,3,5-trimethylphenyl)-1-hexadecanone

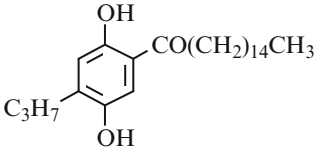
[137833-03-5] $C_{25}H_{42}O_2$ mol. wt. 374.61



Synthesis
-Refer to: [1733].

1-(2,5-Dihydroxy-4-propylphenyl)-1-hexadecanone

[115486-55-0] $C_{25}H_{42}O_3$ mol. wt. 390.61

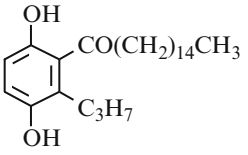


Synthesis
-Obtained by reaction of hexadecanoic acid with 2-propyl-hydroquinone in the presence of boron trifluoride in 1,2-dichloroethane at 40–45° for 1.25 h. The mixture was allowed to stand overnight (56 %) [142].

m.p. 76.5–77.5° [142].

1-(3,6-Dihydroxy-2-propylphenyl)-1-hexadecanone

$C_{25}H_{42}O_3$ mol. wt. 390.61

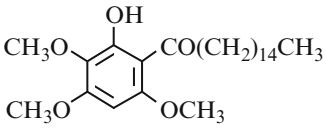


Synthesis
-Obtained by hydrogenation of 3-allyl-2-palmitoyl-hydroquinone in ethanol in the presence of Raney nickel under 2.7 atm. of hydrogen. The reduction was complete in few min at r.t. (96 %) [142].

cream-coloured crystalline powder [142]; m.p. 67–68° [142].

1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-hexadecanone

[134081-68-8] $C_{25}H_{42}O_5$ mol. wt. 422.61



Syntheses
-Obtained by partial selective demethylation of crude 2,3,4,6-tetramethoxyhexadecanophenone with aluminium chloride in acetonitrile at 50° for 1–2 h (85 %) [1353].
-Also refer to: [1351].

m.p. 74–75° [1353]; ^{1}H NMR [1353].

p-Toluenesulfonic ester [134081-83-7] $C_{32}H_{48}O_7S$ mol. wt. 576.79

-Obtained by reaction of p-toluenesulfonyl chloride with 2-hydroxy-3,4,6-trimethoxy-hexadecanophenone in the presence of potassium carbonate in refluxing acetone for 6 to 14 h (96 %) [1353].

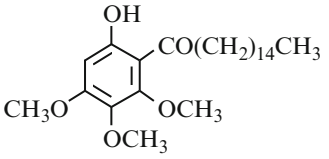
m.p. 65.5–67.5° [1353]; ^{1}H NMR [1353].

Methyl ether $C_{26}H_{44}O_5$ mol. wt. 436.63

-Obtained by reaction of hexadecanoyl chloride with 1,2,3,5-tetramethoxybenzene in the presence of aluminium chloride in ethyl ether at 0° for 30 min [1353].

1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-hexadecanone

[134081-75-7] $C_{25}H_{42}O_5$ mol. wt. 422.61



Syntheses

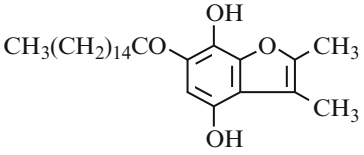
-Obtained by hydrogenation of (6-phenylmethoxy)-2,3,4-trimethoxyhexadecanophenone over 10 % palladium on charcoal in ethyl acetate/methanol (1:1) until the uptake of hydrogen ceased (91 %) [1353].

-Also refer to: [1351].

m.p. 59–60.5° [1353]; ^{1}H NMR [1353].

1-(4,7-Dihydroxy-2,3-dimethyl-6-benzofuranyl)-1-hexadecanone

$C_{26}H_{40}O_4$ mol. wt. 416.60



Synthesis

-Refer to: [1040].

Dimethyl ether [49710-86-3]

$C_{28}H_{44}O_4$ mol. wt. 444.65

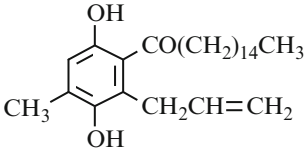
-Obtained by acylation of 4,7-dimethoxy-2,3-dimethylbenzofuran in the presence of stannic chloride in benzene (73 %) [1040].

m.p. 72° [1040]; LD_{50} [1040].

USE: Prepn. and radioprotective activity of, [1040].

1-[3,6-Dihydroxy-4-methyl-2-(2-propenyl)phenyl]-1-hexadecanone

[76402-13-6] $C_{26}H_{42}O_3$ mol. wt. 402.61

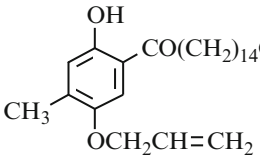


Synthesis

-Obtained by Claisen rearrangement of 1-[2-hydroxy-4-methyl-5-(2-propenyloxy)phenyl]-1-hexadecanone [748].

1-[2-Hydroxy-4-methyl-5-(2-propenyloxy)phenyl]-1-hexadecanone

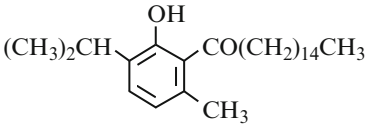
[76402-12-5] $C_{26}H_{42}O_3$ mol. wt. 402.61



Synthesis
-Refer to: [748].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-hexadecanone

$C_{26}H_{44}O_2$ mol. wt. 388.63

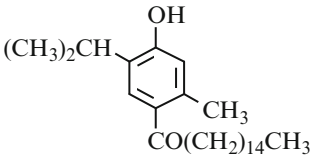


Synthesis
-Obtained by reaction of hexadecanoic acid with thymol in the presence of aluminium chloride on heating at reflux for 12 h (81 %) [2960].

b.p.$_{13}$ 130–132° [2960]; m.p. 46° [2960].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-hexadecanone

$C_{26}H_{44}O_2$ mol. wt. 388.63



Synthesis
-Refer to: [2660].

Methyl ether (XVII)

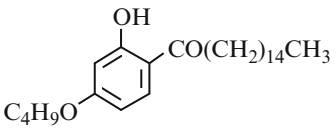
$C_{27}H_{46}O_2$ mol. wt. 402.66

-Obtained by reaction of palmityl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (55 %) [2660].

b.p.$_{0.7}$ 235–240° [2660], b.p.$_{15}$ 280° [2660]; m.p. 51° [2660].

1-(4-Butoxy-2-hydroxyphenyl)-1-hexadecanone

[24313-92-6] $C_{26}H_{44}O_3$ mol. wt. 404.63



Synthesis
-Obtained by reaction of hexadecanoyl chloride with m-dibutoxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°.

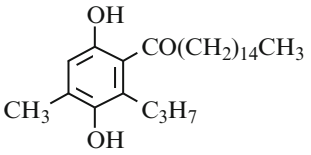
The temperature was then raised to 80° and stirring was continued at that temperature for 5 h (79 %) [1194, 1195].

m.p. 48–49° [1194, 1195]; UV [1194, 1195].

USE: UV absorber [1194]; Light-stabilizer of polymeric materials [1194].

1-(3,6-Dihydroxy-4-methyl-2-propylphenyl)-1-hexadecanone

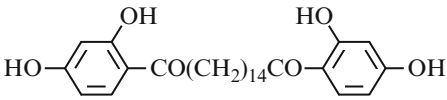
[76402-14-7] $C_{26}H_{44}O_3$ mol. wt. 404.63



Synthesis
-Refer to: [748].

1,16-Bis(2,4-dihydroxyphenyl)-1,16-hexadecanedione

$C_{28}H_{38}O_6$ mol. wt. 470.61

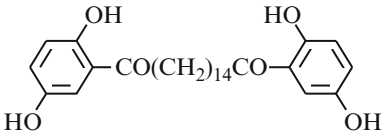


Synthesis
-Obtained by reaction of 1,16-hexadecanedioic acid with resorcinol in the presence of zinc chloride at 140° for 5 h [445].

m.p. 162° [445].

1,16-Bis(2,5-dihydroxyphenyl)-1,16-hexadecanedione

$C_{28}H_{38}O_6$ mol. wt. 470.61



Synthesis
-Refer to: [3417].

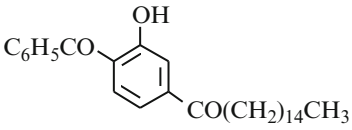
Tetramethyl ether [21772-21-4]
$C_{32}H_{46}O_6$ mol. wt. 526.71

-Obtained by reaction of thapsic acid dichloride with p-dimethoxybenzene in the presence of aluminium chloride in tetrachlorethane for 7 h at 100° (61 %) [3417].

yellow needles [3417]; m.p. 78° [3417]; IR [3417].

1-(4-Benzoyl-3-hydroxyphenyl)-1-hexadecanone
4′-Benzoyl-3′-hydroxyhexadecanophenone

$C_{29}H_{40}O_3$ mol. wt. 436.63

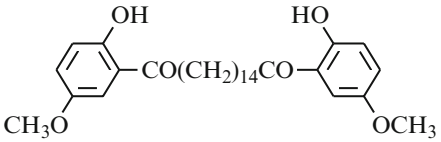


Synthesis
-Refer to: [1925].
UV [1925].

USE: Light stabilization of macromol. compds. [1925].

1,16-Bis(2-hydroxy-5-methoxyphenyl)-1,16-hexadecanedione

[21772-22-5] $C_{30}H_{42}O_6$ mol. wt. 498.66



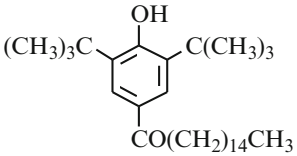
Synthesis

-Obtained by reaction of thapsic acid dichloride (1 mol) with p-dimethoxybenzene (2.5 mol) in the presence of aluminium chloride (8 mol) in tetrachlorethane for 7 h at 100° (main product) [3417].

colourless needles [3417]; m.p. 157° [3417]; IR [3417].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-hexadecanone

[28441-03-4] $C_{30}H_{52}O_2$ mol. wt. 444.74



Syntheses

-Preparation by reaction of hexadecanoyl chloride with 2,6-di-tert-butylphenol in the presence of aluminium chloride [2145] in 1,2,2-trichloroethane at −10 to −20° [951].

m.p. 57–58° [951].

O-Methyloxime [169888-16-8] $C_{31}H_{54}NO_2$ mol. wt. 472.78

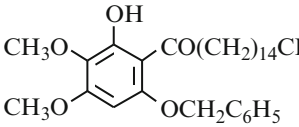
-Refer to: [1408]; ESR [1408].

O-d3-Methyloxime $C_{31}H_{52}D_3NO_2$ mol. wt. 476.76

m.p. 37° [1408].

1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-hexadecanone

[134082-07-8] $C_{31}H_{46}O_5$ mol. wt. 498.70



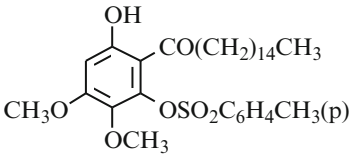
Synthesis

-Obtained by elimination of one phenylmethyl group in 2-position by treatment of 1-(2,6-dibenzyloxy-3,4-dimethoxyphenyl)-1-hexadecanone with concentrated hydrochloric acid and acetic acid at r.t. for 2–3 h (82 %) [1353].

m.p. 79–81° [1353]; ^{1}H NMR [1353].

1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-hexadecanone

[134081-91-7] $C_{31}H_{46}O_7S$ mol. wt. 562.77

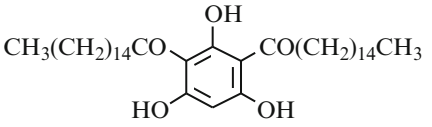


Synthesis
-Obtained by treatment of 1-(2-tosyloxy-3,4,6-trimethoxyphenyl)-1-hexadecanone with 25 % aluminium bromide in acetonitrile at r.t. for 2–3 h (90 %) [1353].

m.p. 54–56° [1353]; ^{1}H NMR [1353].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-hexadecanone

[1103524-17-9] $C_{38}H_{66}O_5$ mol. wt. 602.94

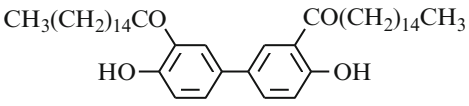


Synthesis
-Obtained by reaction of hexadecanoic acid with phloroglucinol in the presence of boron trifluoride etherate at 100° for 2 h (50–75 %) [338].

BIOLOGICAL ACTIVITY: As a new class of GPR40 (FFAR1) agonists [338].

1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-hexadecanone

$C_{44}H_{70}O_4$ mol. wt. 663.04



Synthesis
-Preparation by Fries rearrangement of 4,4′-biphenyl dihexadecanoate with aluminium chloride in refluxing chlorobenzene for 24 h (76 %) [2091].

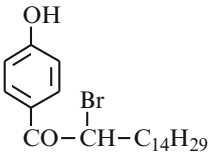
m.p. 90–91° [2091].

2 Aromatic Hydroxyketones Derived from Bromohexadecanoic Acids

2.1 Unsubstituted Hydroxyketones

2-Bromo-1-(4-hydroxyphenyl)-1-hexadecanone

$C_{22}H_{35}BrO_2$ mol. wt. 411.42



Synthesis
-Refer to: [1104].

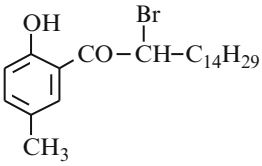
Methyl ether $C_{23}H_{37}BrO_2$ mol. wt. 425.45
-Obtained by reaction of bromine (1 equiv.) with 4-methoxyhexanophenone in carbon tetrachloride [1104].

m.p. 79–80° [1104].

2.2 Substituted Hydroxyketone

2-Bromo-1-(2-hydroxy-5-methylphenyl)-1-hexadecanone

$C_{23}H_{37}BrO_2$ mol. wt. 425.45

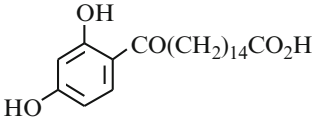


Synthesis
-Refer to: [190].
m.p. 46–47° [190].

3 Aromatic Hydroxyketones Derived from 16-Oxohexadecanoic Acids

16-(2,4-Dihydroxyphenyl)-16-oxo-1-hexadecanoic acid

[720675-30-9] $C_{22}H_{34}O_5$ mol. wt. 378.51



Synthesis
-Obtained by reaction of thapsic acid (tetradecamethylene-dicarbonic acid) with resorcinol in the presence of zinc chloride at 140° for 5 h (40 %) [445].

m.p. 113–115° [445].

Methyl ester [720676-31-3] $C_{23}H_{36}O_5$ mol. wt. 392.54

b.p.$_{0.2}$ 260–270° [445]; m.p. 89–90° [445].

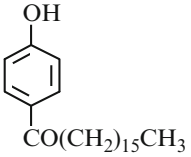
Chapter 15
Heptadecanones

1 Aromatic Hydroxyketones Derived from Heptadecanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(4-Hydroxyphenyl)-1-heptadecanone

[135649-79-5] $C_{23}H_{38}O_2$ mol. wt. 346.55



Syntheses
-Refer to: [3027, 3376].

USE: Electroluminescent device [3376].

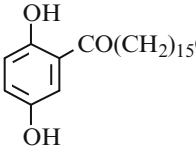
Methyl ether $C_{24}H_{40}O_2$ mol. wt. 360.58

-Refer to: [1963].

m.p. 70.5° [1963].

1-(2,5-Dihydroxyphenyl)-1-heptadecanone

[26639-19-0] $C_{23}H_{38}O_3$ mol. wt. 362.55



Syntheses
-Refer to: [1481, 1820].

USE: Diffusion of, in photographic emulsions, [1481].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_15

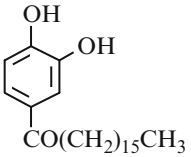
Dimethyl ether [103044-77-5] $C_{25}H_{42}O_3$ mol. wt. 390.61

-Obtained by condensation of heptadecanoyl chloride with hydroquinone dimethyl ether [1820].

colourless prisms [1820]; m.p. 45–46° [1820]; IR [1820].

1-(3,4-Dihydroxyphenyl)-1-heptadecanone

$C_{23}H_{38}O_3$ mol. wt. 362.55



Syntheses
-Refer to: [1175, 1962].
m.p. 100–103° [1962].
Dimethyl ether [186454-86-4]
$C_{25}H_{42}O_3$ mol. wt. 390.61

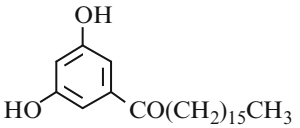
-Obtained by reaction of n-hexadecylmagnesium bromide with 3,4-dimethoxybenzaldehyde in tetrahydrofuran under a stream of nitrogen. Then, the reaction mixture was refluxed gently for 20 h (39 %) [1175].

m.p. 67–68° [1960, 1963];
^{1}H NMR [1175], ^{13}C NMR [1175], MS [1175].

BIOLOGICAL ACTIVITY: Cytotoxicity [1175].

1-(3,5-Dihydroxyphenyl)-1-heptadecanone

$C_{23}H_{38}O_3$ mol. wt. 362.55

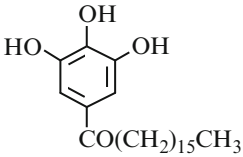


Syntheses
-Refer to: [3340, 3341].
Dimethyl ether [1186123-07-8]
$C_{25}H_{42}O_3$ mol. wt. 390.61

USE: Preparation of benzoquinone natural product derivs. primin, AC-7-1, pallasone B, ardisianone A, irisquinone, dietrichequinone [3340]; Preparation of primin, AC-7, pallasone B, ardisianone A, irisquinone [3341].

1-(3,4,5-Trihydroxyphenyl)-1-heptadecanone

$C_{23}H_{38}O_4$ mol. wt. 378.55



Synthesis
-Refer to: [158].
Trimethyl ether [855955-03-2]
$C_{26}H_{44}O_4$ mol. wt. 420.63

-Obtained by treatment of ethyl 2-(3,4,5-trimethoxybenzoyl)-2-pentadecylethanoate (m.p. 61.5–62°) with potassium hydroxide in boiling ethanol for 3 h (87 %) [158].

needles [158]; m.p. 72–72.5° [158].

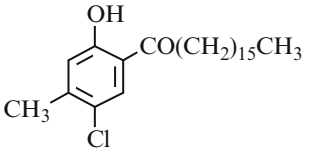
4-Nitrophenylhydrazone of the trimethyl ether $C_{32}H_{49}N_3O_5$ mol. wt. 555.76

yellow plates [158]; m.p. 111–112° [158].

1.2 Substituted Hydroxyketones

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-heptadecanone

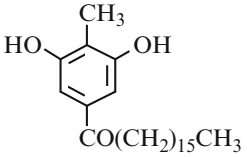
$C_{24}H_{39}ClO_2$ mol. wt. 395.03



Synthesis
-Refer to: [3138].
fluorescence [3138].

1-(3,5-Dihydroxy-4-methylphenyl)-1-heptadecanone

$C_{24}H_{40}O_3$ mol. wt. 376.58



Synthesis
-Refer to: [158].
Dimethyl ether [855891-01-9]
$C_{26}H_{44}O_3$ mol. wt. 404.63

-Obtained by treatment of ethyl 2-(3,5-dimethoxy-4-methylbenzoyl)-2-pentadecylethanoate (m.p. 64–65°) with potassium hydroxide in boiling ethanol for 3 h (71 %) [158].

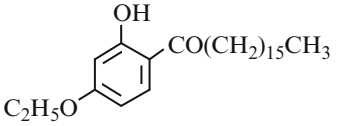
needles [158]; m.p. 76–77° [158].

4-Nitrophenylhydrazone of the dimethyl ether $C_{32}H_{49}N_3O_4$ mol. wt. 539.76

yellow plates [158]; m.p. 88–88.5° [158].

1-(4-Ethoxy-2-hydroxyphenyl)-1-heptadecanone

$C_{25}H_{42}O_3$ mol. wt. 390.61

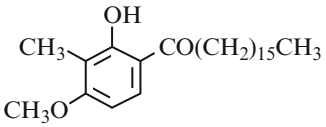


Synthesis
-Refer to: [1834].
Oxime [33488-77-6]
$C_{25}H_{43}NO_3$ mol. wt. 405.62

USE: Extraction agents, in copper manuf. [1834].

1-(2-Hydroxy-4-methoxy-3-methylphenyl)-1-heptadecanone

[855890-85-6] $C_{25}H_{42}O_3$ mol. wt. 390.61



Synthesis
-Obtained by Friedel-Crafts acylation of 2,6-dimethoxy-toluene with heptadecanoyl chloride in the presence of aluminium chloride in carbon disulfide (70 %) [158].

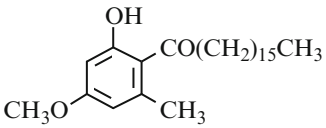
m.p. 74.5–75.5° [158].

4-Nitrophenylhydrazone $C_{31}H_{47}N_3O_4$ mol. wt. 525.73

m.p. 95–96° [1421], 98–99° [158].

1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1-heptadecanone

[855890-69-6] $C_{25}H_{42}O_3$ mol. wt. 390.61



Synthesis
-Obtained by Friedel-Crafts acylation of 3,5-dimethoxy-toluene with heptadecanoyl chloride in the presence of aluminium chloride in carbon disulfide cooled in an ice bath. Then, the mixture let stand 2 h, heated 4 h at 60°, left overnight [158].

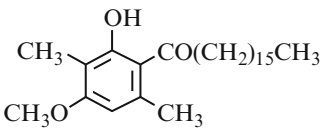
m.p. 71–72° [158].

4-Nitrophenylhydrazone $C_{31}H_{47}N_3O_4$ mol. wt. 525.73

m.p. 114–115° [158], 123–124° [158].

1-(2-Hydroxy-4-methoxy-3,6-dimethylphenyl)-1-heptadecanone

[855954-88-0] $C_{26}H_{44}O_3$ mol. wt. 404.63



Synthesis
-Obtained by Friedel-Crafts acylation of 1,3-dimethoxy-2,5-dimethylbenzene with heptadecanoyl chloride in the presence of aluminium chloride in carbon disulfide (42 %) [158].

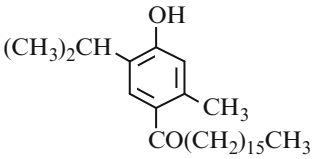
m.p. 57–58° [158].

4-Nitrophenylhydrazone $C_{32}H_{49}N_3O_4$ mol. wt. 539.76

m.p. 94–95° [158].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-heptadecanone

$C_{27}H_{46}O_2$ mol. wt. 402.65



Synthesis
-Refer to: [2660].

Methyl ether (XVIII)

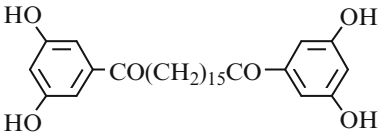
$C_{28}H_{48}O_2$ mol. wt. 416.69

-Obtained by reaction of margaryl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (30 %) [2660].

b.p.$_{19}$ 303–305° [2660]; m.p. 55° [2660].

1,17-Bis-(3,5-dihydroxyphenyl)-1,17-heptadecanedione

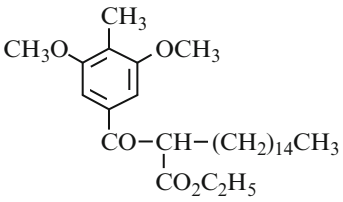
$C_{29}H_{40}O_6$ mol. wt. 484.63



Synthesis
-Refer to: [1316].

Ethyl 2-(3,5-Dimethoxy-4-methylbenzoyl)heptadecanoate

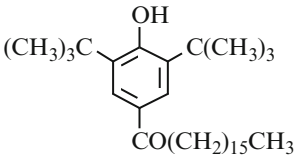
[855892-35-2] $C_{29}H_{48}O_5$ mol. wt. 476.70



Synthesis
-Refer to: [1326].
m.p. 64–65° [1421].

1-(3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl)-1-heptadecanone

[645336-90-9] $C_{31}H_{54}O_2$ mol. wt. 458.77



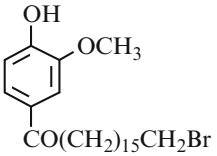
Synthesis
-Refer to: [1027].

USE: Stabilizer, dynamically-vulcanized blends of polyamide and silicone elastomers with high elongation and tensile strength [1027].

2 Aromatic Hydroxyketones Derived from 17-Bromoheptadecanoic Acid

17-Bromo-1-(4-hydroxy-3-methoxyphenyl)-1-heptadecanone

[13149-48-9] $C_{24}H_{39}BrO_3$ mol. wt. 455.48



Synthesis

-Obtained by reaction of 17-bromoheptadecanoic acid with guaiacol in the presence of boron trifluoride at 70° for 2.5 h (73.5 %) [2750].

m.p. 77–78° [2750].

Allyl ether [13149-49-0] $C_{27}H_{43}BrO_3$ mol. wt. 495.54

-Obtained by reaction of allyl bromide with the title ketone in the presence of potassium carbonate in refluxing acetone for 9 h (84 %) [2750].

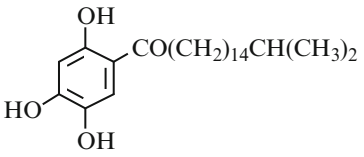
m.p. 81–84° [2750].

3 Aromatic Hydroxyketones Derived from 16-Methylheptadecanoic Acid

1-(2,4,5-Trihydroxyphenyl)-16-methyl-1-heptadecanone

1-(2,4,5-Trihydroxyphenyl)-1-isooctadecanone

[123687-72-9] $C_{24}H_{40}O_4$ mol. wt. 392.58



Synthesis

-Refer to: [2328] (Japanese patent).

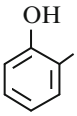
Chapter 16
Octadecanones

1 Aromatic Hydroxyketones Derived from Octadecanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-9-octadecyn-1-one
2′-Hydroxyphenyl heptadecyn-9, one-1

$C_{24}H_{36}O_2$ mol. wt. 356.55



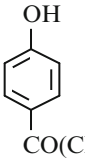
Synthesis
-Obtained by Fries rearrangement of phenyl stearolate with aluminium chloride at 115–120° for 2 h (43 %) [200].

2,4-Dinitrophenylhydrazone [23803-76-1] $C_{30}H_{40}N_4O_5$ mol. wt. 536.67

m.p. 185° [200].

1-(4-Hydroxyphenyl)-9-octadecyn-1-one
4′-Hydroxyphenyl heptadecyn-9, one-1

[23842-91-3] $C_{24}H_{36}O_2$ mol. wt. 356.55



Synthesis
-Obtained by Fries rearrangement of phenyl stearolate with aluminium chloride at 115–120° for 2 h (4 %) [200].
b.p.$_8$ 263° [200].

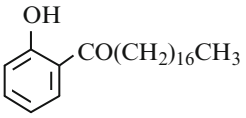
R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_16

2,4-Dinitrophenylhydrazone [23803-77-2] $C_{30}H_{40}N_4O_5$ mol. wt. 536.67

m.p. 225° [200].

1-(2-Hydroxyphenyl)-1-octadecanone

[2589-85-7] $C_{24}H_{40}O_2$ mol. wt. 360.58



Syntheses

-Obtained by reaction of stearoyl chloride with phenol in the presence of aluminium chloride,
*in tetrachlorethane few hours at 55° (28 %) [2548];
*in nitrobenzene for 3 h at 70° (21 %) [2549];
*in carbon disulfide for 5.5 h at 47° (42 %) [2549].
-Also obtained by Fries rearrangement of phenyl stearate with aluminium chloride [1456] in tetrachlorethane for 10 h at 70° (18 %) [2550] or without solvent at 150° for 1 h [293].
-Also obtained by reaction of stearic acid with phenol in the presence of zinc chloride heated together on stand bath for 6 h [2398].
-Formation of, in stearic acid reactions with phenol, geochem. origin of alkyl aroms. in coal in relation to, [897].
-Also obtained by reaction of hydrogenated olive oil with phenol in the presence of boron trifluoride for 1.5–2 h at 9–5° [2599].
-Also refer to: [873, 2035].

$b.p._{0.2}$ 164–182° [2035]; $b.p._1$ 210–245° [2599];
m.p. 66–67° [293, 2398], 64–66° [2548], 60–64° [2550], 56–58° [2599]; TLC [1456].

Isolation from natural sources

-From karite or olive oils [2599].

USE: Textile rot proofing by, [873].

2,4-Dinitrophenylhydrazone $C_{30}H_{44}N_4O_5$ mol. wt. 540.70

m.p. 97.4–97.8° [293], 96–97° [2548].

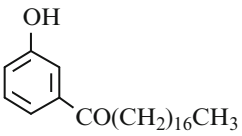
Methyl ether $C_{25}H_{42}O_2$ mol. wt. 374.61

-Obtained by reaction of dimethyl sulfate with 1-(2-hydroxyphenyl)-1-octadecanone in the presence of potassium carbonate in boiling acetone for 6 h [2398].

m.p. 42° [2398].

1-(3-Hydroxyphenyl)-1-octadecanone

[63442-88-6] $C_{24}H_{40}O_2$ mol. wt. 360.58



Syntheses
-Refer to: [1984, 1985].
m.p. 62° [1984]; IR [1984].

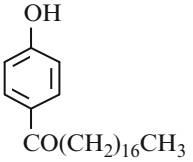
Methyl ether [63442-85-3] $C_{25}H_{42}O_2$ mol. wt. 374.61

-Refer to: [1984, 1985].

m.p. 48° [1984]; IR [1984].

1-(4-Hydroxyphenyl)-1-octadecanone

[2589-77-7] $C_{24}H_{40}O_2$ mol. wt. 360.58



Syntheses
-Obtained by reaction of stearoyl chloride with phenol in the presence of aluminium chloride,
*in tetrachlorethane few hours at 55° (28 %) [2548];
*in nitrobenzene for 3 h at 70° (67 %) [2549];
*in carbon disulfide for 5.5 h at 47° (54 %) [2549].

-Also obtained by Fries rearrangement of phenyl stearate,
*with aluminium chloride [1456] in nitrobenzene at 38° for 2 days (62 %) [414], in tetrachlorethane for 10 h at 70° (21 %) [2550] or without solvent at 150° for 1 h [293].
*in the presence of aluminium chloride in refluxing carbon disulfide for 5 h. Then, the mixture was kept at 80–90° for 2 h and at 140–150° for 1 h after solvent elimination [1222].
-Also obtained by reaction of stearic acid with phenol in the presence,
*of boron trifluoride for 2–3 h between 65 and 85° (70 %) [503];
*of activated acid clay catalyst at 190° for 2 h [3277].
-Also obtained by demethylation of 4-stearoylanisole with hydrobromic acid in acetic acid [2398].
-Also obtained by reaction of hydrogenated olive oil with phenol in the presence of boron trifluoride for 1.5–2 h at 5° [2599].
-Also refer to: [873, 1299, 1357, 1963, 1985, 2035, 2790, 2791].

b.p.$_{0.2}$ 209–212° [2035]; b.p.$_1$ 245–265° [2599]; b.p.$_{15}$ 320° [293];
m.p. 90–90.5° [293], 90° [2398], 89° [503], 87–89° [2548], 87–87.5° [3277], 84–87° [2550], 80–82° [2599], 76° [414].
TLC [1456].

Isolation from natural sources

-From karite or olive oils [2599].

USE: Polyamide fibers modified with, transparency of, [2790]; Nylon 6 monofilaments contg. transparency of, morphol. in relation to, [2791]; Textile rot proofing by, [873].

2,4-Dinitrophenylhydrazone $C_{30}H_{44}N_4O_5$ mol. wt. 540.70

m.p. 142–142.2° [293], 139.5–140° [2548].

Semicarbazone $C_{25}H_{43}N_3O_2$ mol. wt. 417.64

m.p. 133.4–134.7° [293].

Benzoate $C_{31}H_{44}O_3$ mol. wt. 464.69

prisms [293]; m.p. 113.2–113.6° [293].

Stearate [122492-61-9] $C_{42}H_{74}O_3$ mol. wt. 627.05

-Obtained by reaction of stearic acid with phenol in the presence of activated acid clay catalyst at 190° for 2 h [3277].

m.p. 90–91° [3277].

Methyl ether [95869-30-0] $C_{25}H_{42}O_2$ mol. wt. 374.61

-Preparation by reaction of stearoyl chloride with anisole in the presence of aluminium chloride in nitrobenzene at r.t. overnight (90 %) [2398].
-Also obtained by treatment of anisole with octadecanoic anhydride or octadecanoyl chloride in the presence of sulfated zirconia [867].
-Synthesis of acylanisoles with Y zeolite catalyst [1941].
-Zeolite-catalysed Friedel-Crafts acylation of anisole [3264].
-Also refer to: [89, 1963, 2016, 2761 (59 %)].

m.p. 77–78° [2016], 77–77.5° [1963], 75° [2398, 2761].

2,4-Dinitrophenylhydrazone of the methyl ether $C_{31}H_{46}N_4O_5$ mol. wt. 554.73

m.p. 98–99° [2016].

USE: Films (unimol.) of, on D-cellobiose and quinol, [89].

2-Chloroethyl ether $C_{26}H_{43}ClO_2$ mol. wt. 423.08

-Obtained by reaction of octadecanoyl chloride with 2-chloroethoxybenzene in the presence of aluminium chloride in carbon disulfide for 4 h at 50° (76 %) [476].

m.p. 74–75° [476].

N-Dimethylaminoethyl ether $C_{28}H_{49}NO_2$ mol. wt. 431.70

-Obtained by reaction of 4-(2-chloroethoxy)octadecanophenone with dimethylamine in a sealed tube for 2 h at 150° [476].

free base: $b.p._{0.3}$ 228° [476]; m.p. 42–43°[476].
hydrochloride: (69 %) [476]; m.p. 171° [476].

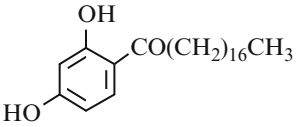
N-Diethylaminoethyl ether [14392-84-8] $C_{30}H_{53}NO_2$ mol. wt. 459.76

-Preparation from 4-hydroxyoctadecanophenone, which is metalated and condensed with $ClCH_2CH_2N(C_2H_5)_2$ (65 %) [414].

fumarate [414]; m.p. 71–72° [414].

1-(2,4-Dihydroxyphenyl)-1-octadecanone
(4-Stearylresorcinol)

[21093-22-1] $C_{24}H_{40}O_3$ mol. wt. 376.58



Syntheses
-Obtained by reaction of stearic acid with resorcinol,
*in the presence of boron trifluoride for 2–3 h between 65 and 85° (95–98 %) [503];
*in the presence of zinc chloride (86–87 %) [2273], at 125–130° for 2 h [249].

-Also obtained by the Hoesch method (83 %) [2673].
-Also refer to: [16, 507, 859, 1272, 1412, 2247, 2673, 2959].

shiny colourless needles [507];
m.p. 99° [249, 503, 507], 98–99° [1412], 97° [2673], 96.5–97.5° [2247], 89–90° [859], 68–69° [2273].
N.B.: One of the reported melting point is obviously wrong.
IR [1412], UV [1412].

USE: Protection against actinic radiations [2959].

4-Nitrophenylhydrazone $C_{30}H_{45}N_3O_4$ mol. wt. 511.71

m.p. 95–96° [859].

4-(2-Propenyl) ether $C_{27}H_{44}O_3$ mol. wt. 416.64

USE: Protection against actinic radiations [2959].

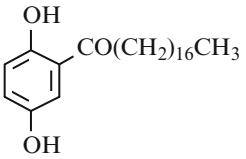
4-(2-Chloro-2-propenyl) ether $C_{27}H_{43}ClO_3$ mol. wt. 451.08

m.p. 57.2–58.3° [2959]; UV [2959].

USE: Protection against actinic radiations [2959].

1-(2,5-Dihydroxyphenyl)-1-octadecanone

[4693-29-2] $C_{24}H_{40}O_3$ mol. wt. 376.58



Syntheses

-Obtained by reaction of stearic acid with hydroquinone in the presence of boron trifluoride etherate at 140° for 2 h (85 %) [142, 1992].

-Also obtained by treatment of 2-hydroxy-5-methoxy-stearophenone with aluminium chloride [2226].

-Also obtained by reaction of octadecanoic acid with p-methoxyphenol in the presence of boron trifluoride without solvent for 5 h at 95–100° (11 %) [3184].

-Also obtained by treatment of hydroquinone and octadecanoic acid mixture in carbon tetrachloride below 60° with boron trifluoride, kept overnight at r.t., then heated 5 h at 90–95° (65 %) [3204].

-Also obtained by reaction of octadecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156] in carbon disulfide [159].

-Also obtained by reaction of octadecanoic acid with p-methoxyphenol in the presence of boron trifluoride without solvent for 5 h at 95–100° (20 %) [3184], (11 %) [3185].

-Also refer to: [335, 394, 2251, 2349–2351, 3185].

m.p. 108–110° [142, 1992], 107–108° [3184, 3185], 106–108.5° [156, 159], 106° [3204].

USE: Photographic colour fog inhibitor [2349]; Photog. film contg., for inhibition of reaction of colour developer oxidn. product with colour-forming compds. [2350]; Colour photog. fog inhibitor, [2351]; Effect on photographic fogging in multilayered colour films [394].

Dimethyl ether [103048-59-5] $C_{26}H_{44}O_3$ mol. wt. 404.63

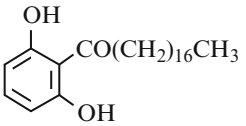
-Obtained by reaction of octadecanoic acid chloride with hydroquinone dimethyl ether [1820] in tetrachloroethane in the presence of aluminium chloride (80 %) [1638].

-Also refer to: [714, 1637].

m.p. 56–56.5° [1820], 46° [714]; IR [1820].

1-(2,6-Dihydroxyphenyl)-1-octadecanone

[921758-91-0] $C_{24}H_{40}O_3$ mol. wt. 376.58



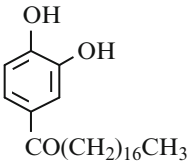
Synthesis

-Refer to: [2320].

USE: Black and white photothermog. material and image forming method using fluorescent intensifying screen [2320].

1-(3,4-Dihydroxyphenyl)-1-octadecanone
(4-Octadecanoylcatechol) (4-Stearoylpyrocatechol)

[1177-44-2] $C_{24}H_{40}O_3$ mol. wt. 376.58



Syntheses
-Obtained by Fries rearrangement of pyrocatechol distearate (m.p. 83–85°) with aluminium chloride for 1 h at 110° [2646].
-Also obtained by treatment of a pyrocatechol and octadecanoic acid mixture with zinc chloride at 135–140° for 2 h (10 %) [1283].

-Also obtained by acylating pyrocatechol with octadecanoic acid at 100° for 3 h in the presence of boron trifluoride (85 %) [1605].
-Also obtained by reaction of octadecanoyl chloride with pyrocatechol in the presence of aluminium chloride in nitrobenzene, first at 5–7° for 2 h, then at r.t. for 2–3 days (66 %) [1726].
-Also refer to: [653, 985, 1521, 1604].

grey crystals [1605];
m.p. 100–101° [1283], 97–99° [1604, 1605], 70° [2646].
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [1604, 1605, 1726], IR [1604, 1605], UV [985].

USE: As antioxidant for propene polymers [985].

Dimethyl ether [501361-68-8] $C_{26}H_{44}O_3$ mol. wt. 404.63

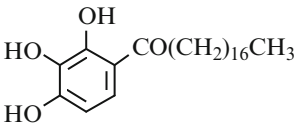
-Refer to: [1960, 1963].

m.p. 82–83° [1960, 1963].

USE: Formation of self-assembled monolayers on Sol-gel processed hafnium oxide as dielectric layers [3112].

1-(2,3,4-Trihydroxyphenyl)-1-octadecanone
(4-Octadecanoylpyrogallol)

[103449-14-5] $C_{24}H_{40}O_4$ mol. wt. 392.58



Syntheses
-Obtained by reaction of stearic acid with pyrogallol,
*in the presence of boron trifluoride for 2–3 h between 65 and 85° (95–98 %) [503];

*in the presence of zinc chloride (Nencki reaction) at 135–140° for 2 h (25 %) [1283].
-Also obtained by reaction of octadecanoyl chloride with pyrogallol in the presence of aluminium chloride in nitrobenzene, first at 5–7° for 2 h, then at r.t. for 2–3 days (40 %) [1726].

-Also refer to: [859, 1317, 2247, 2326].

m.p. 93–94° [2247], 93° [503], 91–93° [1283], 80–81° [859].
N.B.: One of the reported melting point is obviously wrong.
^{1}H NMR [1726].

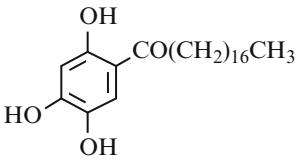
USE: Colour photog. contg. antistaining agent from, [2326].

4-Nitrophenylhydrazone $C_{30}H_{45}N_3O_5$ mol. wt. 527.70

m.p. 154–155° [859].

1-(2,4,5-Trihydroxyphenyl)-1-octadecanone

[57863-94-2] $C_{24}H_{40}O_4$ mol. wt. 392.58



Syntheses
-Preparation by Friedel-Crafts-type catalysts or Fries rearrangements of 1,2,4-trioctadecanoyloxybenzene with aluminium chloride in nitrobenzene [291, 292].
-Also obtained by reaction of stearonitril with phloroglucin (Hoesch reaction) [1608].

-Also refer to: [1708, 1728].

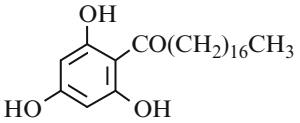
light-yellow [291];
m.p. 126–127° [1608], 118–119° [291, 292].

USE: Antioxidant [1708]; Antioxidant for fats and oils [291]; Antioxidant for fats, oils and paraffin waxes [292]; Heat stabilizers, for bicycloheptene polymers [1728]; Linear polyesters stabilization [1930].

BIOLOGICAL ACTIVITY: Toxicity [1708].

1-(2,4,6-Trihydroxyphenyl)-1-octadecanone

$C_{24}H_{40}O_4$ mol. wt. 392.58



Syntheses
-Obtained by reaction of stearic nitrile with phloroglucinol (Hoesch reaction) [1608].
-Also obtained by reaction of stearic acid with phloroglucinol in the presence of boron trifluoride for 2–3 h between 65 and 85° (95–98 %) [503].

m.p. 126–127° [1608], 126° [503].

Monohydrate $C_{24}H_{40}O_4$, H_2O mol. wt. 410.59

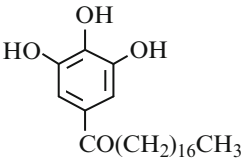
m.p. 118–120° [1608].

Trimethyl ether $C_{27}H_{46}O_4$ mol. wt. 434.66

m.p. 67° [16].

1-(3,4,5-Trihydroxyphenyl)-1-octadecanone

[180894-15-9] $C_{24}H_{40}O_4$ mol. wt. 392.58

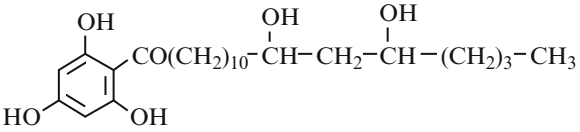


Synthesis
-Refer to: [1639].

USE: Additive; silver halide colour photog. material [1639].

1-(2,4,6-Trihydroxyphenyl)-12,14-dihydroxyoctadecanone
(Byssomeruliol A and B)

[75656-31-4] $C_{24}H_{40}O_6$ mol. wt. 424.59
[83212-66-2]
[83213-39-2]



Syntheses
-Refer to: [1930, 1931].

^{1}H NMR [1930, 1931], ^{13}C NMR [1930, 1931], IR [1930, 1931], UV [1930, 1931], MS [1930, 1931].

Isolation from natural sources
- From fruit bodies and mycelia of *Byssomerulius corium* [1930, 1931].

2,4,6-Trimethyl ether $C_{27}H_{46}O_6$ mol. wt. 466.66

-Refer to: [1930].

^{1}H NMR [1930], UV [1930], MS [1930].

Pentamethyl ether [75679-83-3] [83212-56-0] $C_{29}H_{50}O_6$ mol. wt. 494.71

-Refer to: [1931].

MS [1931].

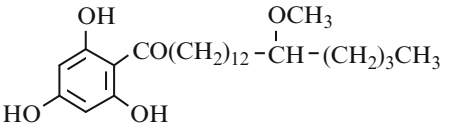
2,4,6-Triacetate $C_{30}H_{46}O_9$ mol. wt. 550.69

-Refer to: [1930].

^{1}H NMR [1930], ^{13}C NMR [1930], UV [1930], MS [1930].

1-(2,4,6-Trihydroxyphenyl)-14-methoxy-1-octadecanone

$C_{25}H_{42}O_5$ mol. wt. 422.61



Synthesis
-Refer to: [1931].

Trimethyl ether

$C_{28}H_{48}O_5$ mol. wt. 464.69

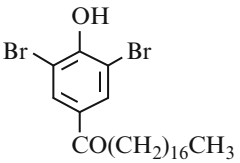
-Refer to: [1931].

MS [1326].

1.2 Substituted Hydroxyketones

1-(3,5-Dibromo-4-hydroxyphenyl)-1-octadecanone

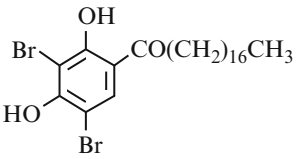
$C_{24}H_{38}Br_2O_2$ mol. wt. 518.37



Synthesis
-Obtained by reaction of bromine with 4-hydroxystearophenone in acetic acid (83 %) [501].
m.p. 80° [501].

1-(3,5-Dibromo-2,4-dihydroxyphenyl)-1-octadecanone
(2,6-Dibromo-4-stearylresorcinol)

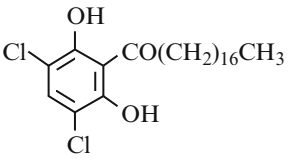
$C_{24}H_{38}Br_2O_3$ mol. wt. 534.37



Synthesis
-Obtained by reaction of bromine with 4-stearylresorcinol in acetic acid at 37–38° for few min [507].
colourless leaflets [507]; m.p. 105° [507].

1-(3,5-Dichloro-2,6-dihydroxyphenyl)-1-octadecanone

[921758-93-2] $C_{24}H_{38}Cl_2O_3$ mol. wt. 445.46

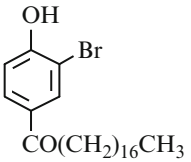


Synthesis
-Refer to: [2320].

USE: Black and white photothermog. material and image forming method using fluorescent intensifying screen [2320].

1-(3-Bromo-4-hydroxyphenyl)-1-octadecanone

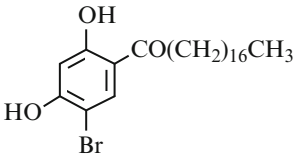
$C_{24}H_{39}BrO_2$ mol. wt. 439.47



Synthesis
-Obtained by reaction of bromine with 4-hydroxy-stearophenone in acetic acid (82 %) [501].
m.p. 96° [501].

1-(5-Bromo-2,4-dihydroxyphenyl)-1-octadecanone

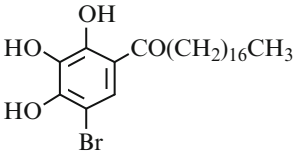
$C_{24}H_{39}BrO_3$ mol. wt. 455.48



Synthesis
-Refer to: [859].
needles [859];
m.p. 98–99° [859].

1-(5-Bromo-2,3,4-trihydroxyphenyl)-1-octadecanone

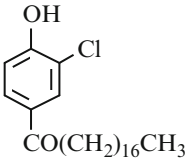
$C_{24}H_{39}BrO_4$ mol. wt. 471.48



Synthesis
-Refer to: [859].
needles [859]; m.p. 86–87° [859].

1-(3-Chloro-4-hydroxyphenyl)-1-octadecanone

$C_{24}H_{39}ClO_2$ mol. wt. 395.03



Synthesis
-Refer to: [3467].

Methyl ether

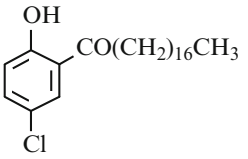
$C_{25}H_{41}ClO_2$ mol. wt. 409.05

-Obtained by reaction of stearoyl chloride with o-chloroanisole in the presence of aluminium chloride in petroleum ether at 0° for 1 h (10 %) [3467].

colourless needles [3467]; m.p. 56–57° [3467].

1-(5-Chloro-2-hydroxyphenyl)-1-octadecanone

$C_{24}H_{39}ClO_2$ mol. wt. 395.03

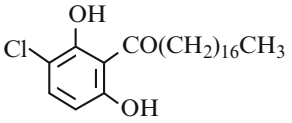


Synthesis
-Refer to: [451].
Oxime, nickel complexes

USE: stabilizers, for propene polymers [451].

1-(3-Chloro-2,6-dihydroxyphenyl)-1-octadecanone

[921758-92-1] $C_{24}H_{39}ClO_3$ mol. wt. 411.02

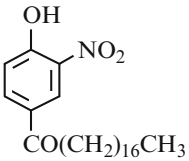


Synthesis
-Refer to: [2320].

USE: Black and white photothermog. material and image forming method using fluorescent intensifying screen [2320].

1-(4-Hydroxy-3-nitrophenyl)-1-octadecanone

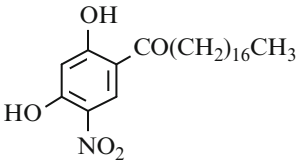
[70079-29-7] $C_{24}H_{39}NO_4$ mol. wt. 405.58



Synthesis
-Obtained by treatment of 4-octadecanoylphenol with concentrated nitric acid in concentrated sulfuric acid at 0° for 1 h 15 min [1222].
m.p. 87.5–88.5° [1222].

1-(2,4-Dihydroxy-5-nitrophenyl)-1-octadecanone

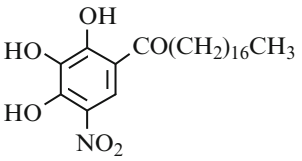
$C_{24}H_{39}NO_5$ mol. wt. 421.58



Synthesis
-Refer to: [859].
pale yellow prisms [859];
m.p. 97–98° [859].

1-(2,3,4-Trihydroxy-5-nitrophenyl)-1-octadecanone

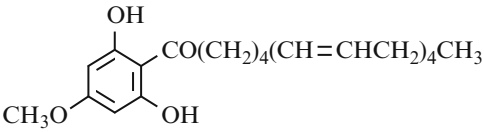
$C_{24}H_{39}NO_6$ mol. wt. 437.58



Synthesis
-Refer to: [859].
m.p. 95–96° [859].

1-(2,6-Dihydroxy-4-methoxyphenyl)-6,9,12,15-tetraen-1-octadecanone

[77464-71-2] $C_{25}H_{34}O_4$ mol. wt. 398.54

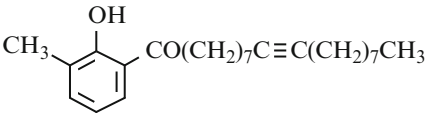


Isolation from natural sources
-From the Brown Alga *Cystophora torulosa* [1165].
pale yellow syrup [1165].

^{1}H NMR [1165], ^{13}C NMR [1165], IR [1165], UV [1165], MS [1165].

1-(2-Hydroxy-3-methylphenyl)-9-octadecyn-1-one
2′-Hydroxy 3′-methyl phenyl heptadecyn-9, one-1

[23803-78-3] $C_{25}H_{38}O_2$ mol. wt. 370.58



Synthesis
-Obtained by Fries rearrangement of o-cresyl stearolate with aluminium chloride at 115–120° for 2 h (23.4 %) [200].

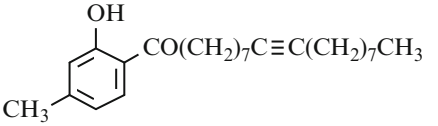
b.p.$_{.6}$ 242° [200].

2,4-Dinitrophenylhydrazone [23803-79-4] $C_{31}H_{42}N_4O_5$ mol. wt. 550.70

m.p. 205° [200].

1-(2-Hydroxy-4-methylphenyl)-9-octadecyn-1-one
2′-Hydroxy 4′-methyl phenyl heptadecyn-9, one-1

[23803-80-7] $C_{25}H_{38}O_2$ mol. wt. 370.58



Synthesis
-Obtained by Fries rearrangement of m-cresyl stearolate with aluminium chloride at 115–120° for 2 h (40.5 %) [200].

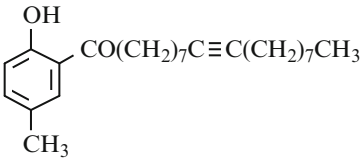
b.p.$_{.3}$ 210° [200].

2,4-Dinitrophenylhydrazone [23803-81-8] $C_{31}H_{42}N_4O_5$ mol. wt. 550.70

m.p. 295° [200].

1-(2-Hydroxy-5-methylphenyl)-9-octadecyn-1-one
2′-Hydroxy 5′-methyl phenyl heptadecyn-9, one-1

[23803-82-9] $C_{25}H_{38}O_2$ mol. wt. 370.58



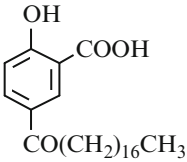
Synthesis
-Obtained by Fries rearrangement of p-cresyl stearolate with aluminium chloride at 115–120° for 2 h (41 %) [200].
b.p.$_3$ 220° [200].

2,4-Dinitrophenylhydrazone [23803-83-0] $C_{31}H_{42}N_4O_5$ mol. wt. 550.70

m.p. 208° [200].

5-(1-Octadecanoyl)-2-hydroxybenzoic acid

[95269-86-6] $C_{25}H_{40}O_4$ mol. wt. 404.59



Syntheses
-Obtained by reaction of stearoyl chloride with salicylic acid in the presence of aluminium chloride in nitrobenzene,
*at r.t. for 12 h, then for 2 h on a water-bad [2784];
*at 25° overnight (70 %) [1029].

-Also refer to: [2170].

m.p. 128–129° [1029], 117–119° [2784];
^{1}H NMR [1029], IR [1029].

Methyl ether $C_{26}H_{42}O_4$ mol. wt. 418.62

-Refer to: [2170]; m.p. 194–196° [2170].

Methyl ether and methyl ester $C_{27}H_{44}O_4$ mol. wt. 432.64

-Refer to: [2170]; m.p. 73–74° [2170].

Na salt [95269-91-3] $C_{25}H_{39}O_4Na$ mol. wt. 426.57

-Obtained by treatment of the keto-acid above mentioned with 2.5 % aqueous sodium hydroxide [2784].
-Also refer to: [2170].

m.p. 240° (d) [2784].

mono-K salt $C_{25}H_{39}O_4K$ mol. wt. 442.68

-Refer to: [2170]; m.p. 224–230° [2170].

N-methylmorpholine salt [95269-97-9] $C_{30}H_{51}NO_5$ mol. wt. 505.74

-Refer to: [2170]; m.p. 98° [2170].

Tris(2-hydroxyethyl)amine salt [95269-96-8] $C_{31}H_{55}NO_7$ mol. wt. 553.78

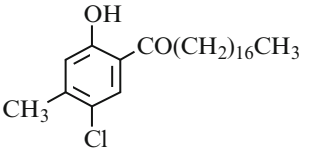
-Refer to: [2170]; m.p. 84° [2170].

Lysine salt [95302-59-3] $C_{31}H_{54}N_2O_6$ mol. wt. 550.78

-Refer to: [2170].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-octadecanone

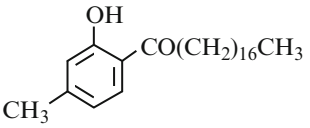
$C_{25}H_{41}ClO_2$ mol. wt. 409.05



Synthesis
-Obtained by reaction of stearic acid with 4-chloro-3-methylphenol in the presence of boron trifluoride for 2–3 h between 65 and 85° (90 %) [503].
m.p. 88° [503].

1-(2-Hydroxy-4-methylphenyl)-1-octadecanone

[909191-71-5] $C_{25}H_{42}O_2$ mol. wt. 374.61



Syntheses
-Obtained by reaction of octadecanoic acid with m-cresol in the presence of graphite and methanesulfonic acid mixture at 120° for 2.5 h (85 %) [2834].
-Also refer to: [451, 1111].

^{1}H NMR [2834], ^{13}C NMR [2834], IR [2834].

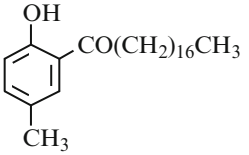
USE: For nickel(2+) or cobalt(2+) extraction in kerosene. Extraction behaviour of nickel and cobalt has been carried out with LIX 84 and compared with the extractant newly synthesized [1111].

Oxime, nickel complexes

USE: stabilizers, for propene polymers [451].

1-(2-Hydroxy-5-methylphenyl)-1-octadecanone

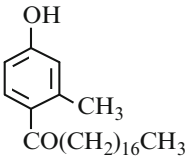
[859992-51-1] $C_{25}H_{42}O_2$ mol. wt. 374.61



Synthesis
-Obtained by reaction of stearic acid with p-cresol [3430] in the presence of boron trifluoride for 2–3 h between 65 and 85° (90–95 %) [503].
m.p. 69° [503].

1-(4-Hydroxy-2-methylphenyl)-1-octadecanone

$C_{25}H_{42}O_2$ mol. wt. 374.61



Synthesis
-Refer to: [2503].

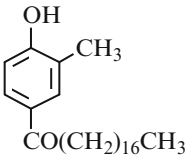
Phenyl ether [791615-82-2]
$C_{31}H_{46}O_2$ mol. wt. 450.71

-Obtained by adding a mixture of m-phenoxytoluene and octadecanoyl chloride to a suspension of aluminium chloride in methylene chloride at 0°, then the mixture was stirred for 1.5–2 h at 3–5° (22 %) [2503].

b.p.$_3$ 280–282° [2503]; m.p. 49–50° [2503];
^{1}H NMR [2503], IR [2503], MS [2503].

1-(4-Hydroxy-3-methylphenyl)-1-octadecanone

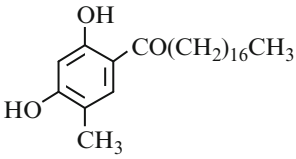
[114398-92-4] $C_{25}H_{42}O_2$ mol. wt. 374.61



Synthesis
-Obtained by reaction of stearic acid with o-cresol in the presence of boron trifluoride [142].
m.p. 72–73° [142].

1-(2,4-Dihydroxy-5-methylphenyl)-1-octadecanone

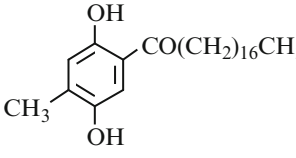
[95185-60-7] $C_{25}H_{42}O_3$ mol. wt. 390.61



Synthesis
-Refer to: [2704].

1-(2,5-Dihydroxy-4-methylphenyl)-1-octadecanone

[101649-67-6] $C_{25}H_{42}O_3$ mol. wt. 390.61

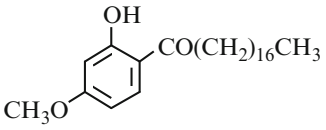


Synthesis
-Refer to: [1477].

USE: Fog inhibitor, for diffusion-transfer heat-developable photothermog. materials contg. silver halide and benzotriazole deriv. silver salt and reductive developer [1477].

1-(2-Hydroxy-4-methoxyphenyl)-1-octadecanone

[95869-36-6] $C_{25}H_{42}O_3$ mol. wt. 390.61



Syntheses

-Obtained by reaction of dimethyl sulfate with 2,4-dihydroxystearophenone in carbon tetrachloride in the presence of 40 % sodium hydroxide at 70–75° [249].

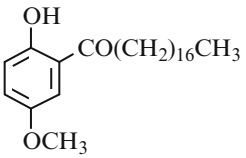
-Also prepared by reaction of stearoyl chloride with 1,3-dimethoxybenzene in the presence of aluminium chloride in chlorobenzene at 10°, and the temperature kept below 20° for 30 min [249].

m.p. 72–73° [249].

USE: Protect mineral and vegetable oils from oxidative degradation, by acting as an ultra-violet absorber [249].

1-(2-Hydroxy-5-methoxyphenyl)-1-octadecanone

[35175-56-5] $C_{25}H_{42}O_3$ mol. wt. 390.61



Syntheses

-Obtained by reaction of octadecanoic acid with p-methoxyphenol in the presence of boron trifluoride,

*in tetrachloroethane for 4 h. The reaction mixture was allowed to stand overnight at r.t. and was then heated on a steam bath for about 3 h (46 %) [142];

*without solvent for 5 h at 95–100° (20 %) [3184, 3185].

-Also obtained by reaction of stearoyl chloride with 1,4-dimethoxybenzene in the presence of aluminium chloride [2226].

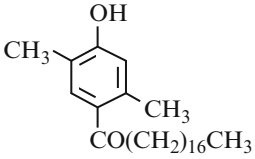
-Also obtained by reaction of octadecanoyl chloride with hydroquinone dimethyl ether in the presence of aluminium chloride [156] in carbon disulfide [159].

-Also obtained by acylating hydroquinone dimethyl ether with stearic acid (72 %) [3186].

b.p.$_{10}$ 187–191° [156];
light yellow crystals [3184, 3185]; m.p. 63–64° [156, 159], 62–63° [3184, 3185], 59.5–61.5° [142];
^{1}H NMR [3184, 3185], IR [3184, 3185].

1-(4-Hydroxy-2,5-dimethylphenyl)-1-octadecanone

[95185-69-6] $C_{26}H_{44}O_2$ mol. wt. 388.63

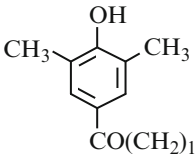


Synthesis

-Refer to: [2704].

1-(4-hydroxy-3,5-dimethylphenyl)-1-octadecanone

[137832-99-6] $C_{26}H_{44}O_2$ mol. wt. 388.63



Syntheses

-Obtained by reaction of octadecanoyl chloride with 2,6-dimethylphenol according to the method described previously [2871], (10 %) [119].

-Also obtained by reaction of octadecanoyl chloride with 2,6-dimethylphenol in the presence of aluminium chloride [1832].

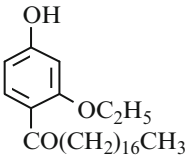
-Also obtained by reaction of octadecanoic acid with 2,6-dimethylphenol in the presence of boron trifluoride [1832].

-Also refer to: [1733].

m.p. 62–62.5° [119]; ^{1}H NMR [119], IR [119].

1-(2-Ethoxy-4-hydroxyphenyl)-1-octadecanone

[76750-11-3] $C_{26}H_{44}O_3$ mol. wt. 404.63



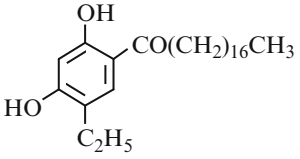
Synthesis

-Refer to: [2790].

USE: Polyamide fibers modified with, transparency of, [2790].

1-5-Ethyl-2,4-dihydroxyphenyl)-1-octadecanone

$C_{26}H_{44}O_3$ mol. wt. 404.63



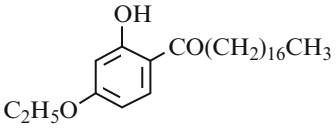
Synthesis

-Refer to: [497].

m.p. 89–90° [497].

1-(4-Ethoxy-2-hydroxyphenyl)-1-octadecanone

[22198-51-2] $C_{26}H_{44}O_3$ mol. wt. 404.63



Syntheses

-Obtained by reaction of stearoyl chloride with resorcinol diethyl ether in the presence of aluminium chloride,

*at 80° for 2 h (66 %) [3469].

*first at 10–15°, then at 80–90° [1195].

-Also obtained by reaction of octadecanoyl chloride with m-diethoxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was

stirred for 1 h at 10°, and then for 6 h at 20–25°. The temperature was then raised to 80° and stirring was continued at that temperature for 5 h (66 %) [1194], (60–73 %) [3470].
-Also obtained by reaction of ethyl bromide with 2,4-dihydroxyoctadecanophenone in the presence of ethanolic potassium hydroxide (90–95 %) [2273].
-Also refer to: [2791].

m.p. 75–75.5° [3469, 3470], 70–70.3° [1194, 1195], 69–70° [2273];
UV [1194, 1195, 3469, 3470].

USE: UV absorber [1194]; Light-stabilizer of polymeric materials [1194]; Detn. of, by potentiometric titration in methylpyrrolidinone [1763]; Nylon 6 monofilaments contg. transparency of, morphol. in relation to, [2791].

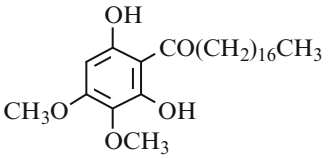
Oxime [33488-77-6] $C_{26}H_{45}NO_3$ mol. wt. 419.65

-Refer to: [1569, 1834].

USE: Extn. by copper, model for, [1569, 1834].

1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-octadecanone

[134082-00-1] $C_{26}H_{44}O_5$ mol. wt. 436.63

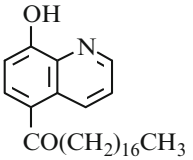


Synthesis
-Preparation by treatment of 1-[6-hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-hexadecanone with potassium carbonate in refluxing methanol for 1–3 h (76 %) [1353].

m.p. 86–87° [1353]; ^{1}H NMR [1353].

1-(8-Hydroxy-5-quinolinyl)-1-octadecanone

[110593-81-2] $C_{27}H_{41}NO_2$ mol. wt. 411.63



Syntheses
-Preparation by Fries rearrangement of 8-hydroxyquinolinyl stearate using aluminium chloride as catalyst [992].
-Also obtained by reaction of octadecanoyl chloride with 8-hydroxyquinoline in the presence of aluminium chloride in nitrobenzene at 80–85° for 15–16 h (50 %) [1725].

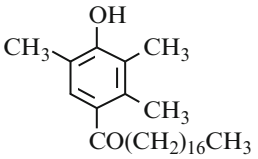
-Also refer to: [993].

m.p. 83.2–85° [1725]; ^{1}H NMR [1725], IR [1725].

USE: Ion-flotation collector [1725]; Ion-flotation with, of gallium [1725].

1-(4-Hydroxy-2,3,5-trimethylphenyl)-1-octadecanone

[137832-97-4] $C_{27}H_{46}O_2$ mol. wt. 402.65

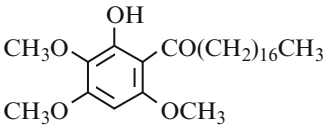


Synthesis

-Obtained by Friedel-Crafts acylation of 2,3,6-trimethylphenol with octadecanoyl chloride in the presence of aluminium chloride in methylene chloride (13 %) [1733].

1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-octadecanone

[134081-69-9] $C_{27}H_{46}O_5$ mol. wt. 450.66



Syntheses

-Obtained by partial selective demethylation of crude 2,3,4,6-tetramethoxyoctadecanophenone with aluminium chloride in acetonitrile at 50° for 1–2 h (87 %) [1353].

-Also refer to: [1351].

m.p. 72.5–74.5° [1353]; ^{1}H NMR [1353].

p-Toluenesulfonic ester [134081-84-8] $C_{34}H_{52}O_7S$ mol. wt. 604.85

-Obtained by reaction of p-toluenesulfonyl chloride with 2-hydroxy-3,4,6-trimethoxy-octadecanophenone in the presence of potassium carbonate in refluxing acetone for 6 to 14 h (92 %) [1353].

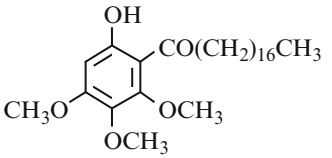
m.p. 67.5–68.5° [1353]; ^{1}H NMR [1353].

Methyl ether $C_{28}H_{48}O_5$ mol. wt. 464.69

-Obtained by reaction of octadecanoyl chloride with 1,2,3,5-tetramethoxybenzene in the presence of aluminium chloride in ethyl ether at 0° for 30 min [1353].

1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-octadecanone

[134081-76-8] $C_{27}H_{46}O_5$ mol. wt. 450.66



Syntheses

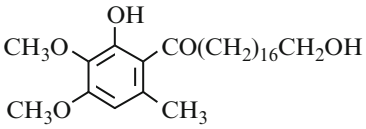
-Obtained by hydrogenation of (6-phenylmethoxy)-2,3,4-trimethoxyoctadecanophenone over 10 % palladium on charcoal in ethyl acetate/methanol (1:1) until the uptake of hydrogen ceased (92 %) [1353].

-Also refer to: [1351].

m.p. 64.5–66° [1353]; ^{1}H NMR [1353].

18-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-octadecanone

[77712-02-8] $C_{27}H_{46}O_5$ mol. wt. 450.66



Synthesis
-Obtained by treatment of its 18-acetyl ester with sodium hydroxide in methanol for 2 h at r.t. (78 %) [1147].

colourless needles [1147]; m.p. 101° [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

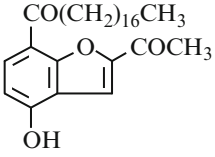
18-Acetyl ester [104988-70-7] $C_{29}H_{48}O_6$ mol. wt. 492.97

-Obtained by Friedel-Crafts reaction of 18-acetoxyoctadecanoyl chloride with 3,4,5-tri-methoxytoluene in 1,2-dichloroethane in the presence of aluminium chloride (2.1 mol) at 20° for 72 h [1147].

colourless oil [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

1-(2-Acetyl-4-hydroxy-7-benzofuranyl)-1-octadecanone

$C_{28}H_{42}O_4$ mol. wt. 442.64



Synthesis
-Refer to: [682].

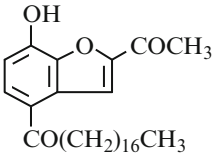
Methyl ether [59445-63-5]
$C_{29}H_{44}O_4$ mol. wt. 456.54

-Obtained by reaction of octadecanoyl chloride with 2-acetyl-4-methoxy-benzofuran with aluminium chloride (2.4 mol) in methylene chloride at r.t. for 24 h (91 %) [682].

m.p. 94° [682].

1-(2-Acetyl-7-hydroxy-4-benzofuranyl)-1-octadecanone

$C_{28}H_{42}O_4$ mol. wt. 442.64



Synthesis
-Refer to: [682].

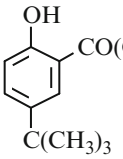
Methyl ether [59445-74-8]
$C_{29}H_{44}O_4$ mol. wt. 456.54

-Obtained by reaction of octadecanoyl chloride with 2-acetyl-7-methoxy-benzofuran with aluminium chloride (2.4 mol) in methylene chloride at r.t. for 24 h (89 %) [682].

m.p. 96° [682].

1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-octadecanone

$C_{28}H_{48}O_2$ mol. wt. 416.69



Synthesis
-Refer to: [976].

Oxime [51830-11-6]
$C_{28}H_{49}NO_2$ mol. wt. 431.70

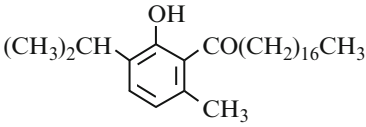
USE: Palladium complex, singlet oxygen quenching by, [976].

Oxime, palladium complex [41894-23-9]

USE: Energy transfer to ligand-field states of, in aromatic hydrocarbon triplet state quenching [92].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-octadecanone

$C_{28}H_{48}O_2$ mol. wt. 416.69

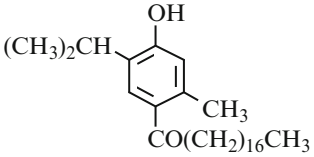


Synthesis
-Obtained by reaction of octadecanoic acid with thymol in the presence of aluminium chloride on heating at reflux for 12 h (80 %) [2960].

b.p.$_{13}$ 128–130° [2960]; m.p. 46° [2960].

1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-octadecanone

$C_{28}H_{48}O_2$ mol. wt. 416.69



Synthesis
-Refer to: [2660].

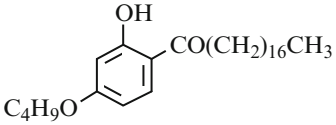
Methyl ether (**XIX**)
$C_{29}H_{50}O_2$ mol. wt. 430.71

-Obtained by reaction of stearoyl chloride with thymol methyl ether in the presence of aluminium chloride in carbon disulfide (30 %) [2660].

b.p.$_{24}$ 318° [2660], m.p. 59.5° [2660].

1-[4-(Butyloxy)-2-hydroxyphenyl]-1-octadecanone

[22198-50-1] $C_{28}H_{48}O_3$ mol. wt. 432.69



Syntheses
-Obtained by reaction of stearoyl chloride with resorcinol dibutyl ether in the presence of aluminium chloride,
*at 80° for 2 h (73 %) [3469];
*first at 10–15°, then at 80–90° [1195].

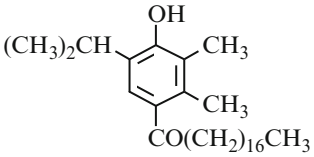
-Also obtained by reaction of octadecanoyl chloride with m-dibutoxybenzene in the presence of aluminium chloride in dichloroethane at 0°. Then, the mixture was stirred for 1 h at 10°, and then for 6 h at 20–25°. The temperature was then raised to 80° and stirring was continued at that temperature for 5 h (73.5 %) [1194], (60–73 %) [3470].

m.p. 52.5–53° [1194, 1195, 3469, 3470];
UV [1194, 1195, 3469, 3470].

USE: UV absorber [1194]; Light-stabilizer of polymeric materials [1194].

1-(4-Hydroxy-2,3-dimethyl-5-(1-methylethyl)phenyl)-1-octadecanone

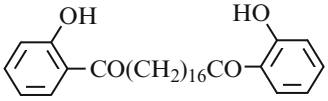
[137833-02-4] $C_{29}H_{50}O_2$ mol. wt. 430.71



Synthesis
-Refer to: [1733].

1,18-Bis-(2-hydroxyphenyl)-1,18-octadecanedione

[115916-09-1] $C_{30}H_{42}O_4$ mol. wt. 466.66



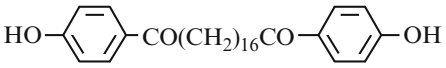
Synthesis
-Refer to: [1188].
m.p. 112–112.5° [1188].

Di-2,4-dinitrophenylhydrazone [117272-01-2] $C_{42}H_{50}N_8O_{10}$ mol. wt. 826.91

m.p. 150° [1188].

1,18-Bis-(4-hydroxyphenyl)-1,18-octadecanedione

[115915-64-5] $C_{30}H_{42}O_4$ mol. wt. 466.66



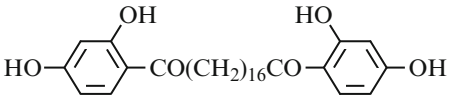
Synthesis
-Refer to: [1188].
m.p. 103.5° [1188].

Di-2,4-dinitrophenylhydrazone [117271-96-2] $C_{42}H_{50}N_8O_{10}$ mol. wt. 826.91

m.p. 170° [1188].

1,18-Bis(2,4-dihydroxyphenyl)-1,18-octadecanedione

[103170-10-1] $C_{30}H_{42}O_6$ mol. wt. 498.66



Synthesis
-Obtained by reaction of 1,18-octadecanedioic acid with resorcinol in the presence of zinc chloride at 140° for 5 h [445].

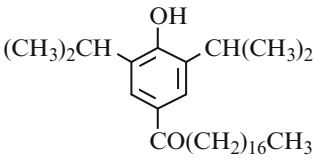
m.p. 139–140° [445].

Tetraacetate $C_{38}H_{50}O_{10}$ mol. wt. 666.81

m.p. 90° [445].

1-(4-Hydroxy-3,5-bis(1-methylethyl)phenyl)-1-octadecanone

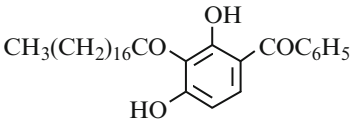
[137833-00-2] $C_{30}H_{52}O_2$ mol. wt. 444.74



Synthesis
-Refer to: [1733].

1-(3-Benzoyl-2,6-dihydroxyphenyl)-1-octadecanone

$C_{31}H_{44}O_4$ mol. wt. 480.69

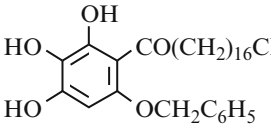


Synthesis
-Refer to: [133].

USE: Stabilization of vinyl halide resins and polyolefins against photodegradation [133].

1-[2,3,4-Trihydroxy-6-(phenylmethoxy)phenyl]-1-octadecanone

$C_{31}H_{46}O_5$ mol. wt. 498.70



Synthesis
-Refer to: [1353].

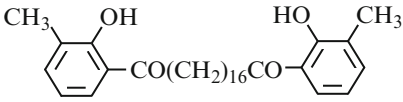
Trimethyl ether

$C_{34}H_{52}O_5$ mol. wt. 540.78

-Refer to: [1353].

1,18-Bis-(2-hydroxy-3-methylphenyl)-1,18-octadecanedione

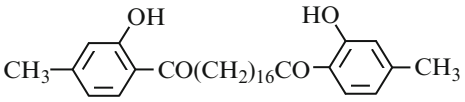
[119039-49-5] $C_{32}H_{46}O_4$ mol. wt. 494.72



Synthesis
-Refer to: [1188].
m.p. 106° [1188].

1,18-Bis-(2-hydroxy-4-methylphenyl)-1,18-octadecanedione

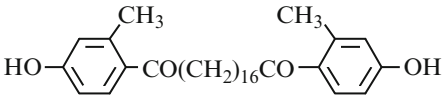
[119039-38-2] $C_{32}H_{46}O_4$ mol. wt. 494.72



Synthesis
-Refer to: [1188].
m.p. 124° [1188].

1,18-Bis-(4-hydroxy-2-methylphenyl)-1,18-octadecanedione

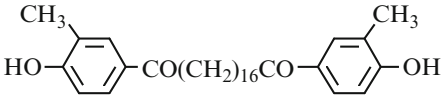
[119039-37-1] $C_{32}H_{46}O_4$ mol. wt. 494.72



Synthesis
-Refer to: [1188].
m.p. 112.5° [1188].

1,18-Bis-(4-hydroxy-3-methylphenyl)-1,18-octadecanedione

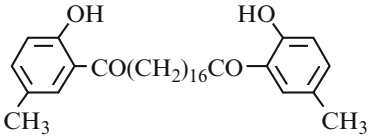
[119039-35-9] $C_{32}H_{46}O_4$ mol. wt. 494.72



Synthesis
-Refer to: [1188].
m.p. 95° [1188].

1,18-Bis-(2-hydroxy-5-methylphenyl)-1,18-octadecanedione

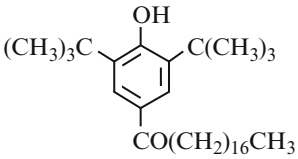
[119039-36-0] $C_{32}H_{46}O_4$ mol. wt. 494.72



Synthesis
-Refer to: [1188].
m.p. 127° [1188].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-octadecanone

[28459-33-8] $C_{32}H_{56}O_2$ mol. wt. 472.80



Syntheses

-Preparation by reaction of octadecanoyl chloride with 2,6-di-tert-butylphenol in the presence of aluminium chloride in 1,1,2-trichloroethane at −10 to −20° [951].

-Also refer to: [1733].

m.p. 62–63° [951].

USE: Stabilize plastics, oils, and fats against heat, light, and oxidation [951].

K salt $C_{32}H_{55}O_2K$ mol. wt. 510.89

-Refer to: [951].

Acetate [30392-07-5] $C_{34}H_{58}O_3$ mol. wt. 514.83

-Refer to: [228].

b.p.$_{11}$ 305–308° [228].

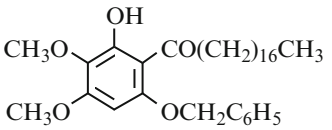
Methyl ether [30492-53-6] $C_{33}H_{58}O_2$ mol. wt. 486.82

-Refer to: [228].

b.p.$_{11}$ 300–305° [228].

1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-octadecanone

[134082-08-9] $C_{33}H_{50}O_5$ mol. wt. 526.76



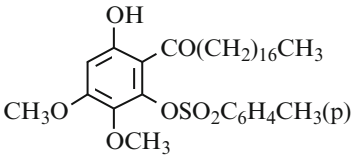
Synthesis

-Obtained by elimination of one phenylmethyl group in 2-position by treatment of 1-(2,6-dibenzyloxy-3,4-dimethoxyphenyl)-1-octadecanone with concentrated hydrochloric acid and acetic acid at r.t. for 2–3 h (85 %) [1353].

m.p. 83–84° [1353]; ^{1}H NMR [1353].

1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-octadecanone

[134081-92-8] $C_{33}H_{50}O_7S$ mol. wt. 590.82

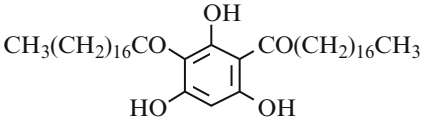


Synthesis
-Obtained by treatment of 1-(2-tosyloxy-3,4,6-trimethoxyphenyl)-1-octadecanone with 25 % aluminium bromide in acetonitrile at r.t. for 2–3 h (72 %) [1353].

m.p. 58–60° [1353]; ^{1}H NMR [1353].

1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-octadecanone

[1103524-18-0] $C_{42}H_{74}O_5$ mol. wt. 659.05

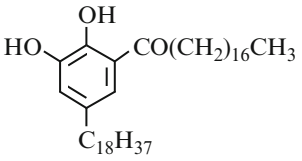


Synthesis
-Obtained by reaction of octadecanoic acid with phloroglucinol in the presence of boron trifluoride etherate at 100° for 2 h (50–75 %) [338].

BIOLOGICAL ACTIVITY: As a new class of GPR40 (FFAR1) agonists [338].

1-(2,3-Dihydroxy-5-octadecylphenyl)-1-octadecanone

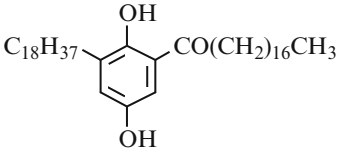
[74061-22-6] $C_{42}H_{76}O_3$ mol. wt. 629.06



Syntheses
-Refer to: [1605, 2761].
m.p. 59–60° [1604, 1605];
^{1}H NMR [1604, 1605],
IR [1604, 1605].

1-(2,5-Dihydroxy-3-octadecylphenyl)-1-octadecanone

[72306-96-8] $C_{42}H_{76}O_3$ mol. wt. 629.06

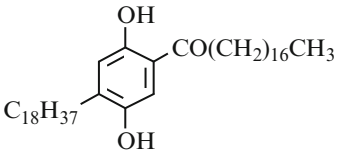


Syntheses
-Obtained by reaction of stearic acid with 2-octadecyl-4-methoxyphenol (m.p. 76°) in the presence of boron trifluoride for 7 h at 150–160°, then at 20° for 15 h (2 %) [3184, 3185].

greyish crystals [3184, 3185]; m.p. 85–86° [3184, 3185];
^{1}H NMR [3184, 3185], IR [3184, 3185].

1-(2,5-Dihydroxy-4-octadecylphenyl)-1-octadecanone

[72306-97-9] $C_{42}H_{76}O_3$ mol. wt. 629.06



Syntheses

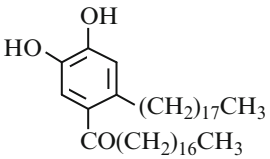
-Obtained by reaction of stearic acid with 2-octadecyl-4-methoxyphenol (m.p. 76°) in the presence of boron trifluoride for 7 h at 150–160°, then at 20° for 15 h (19 %) [3184].

-Also refer to: [309, 3185 (19 %)].

colourless crystals [3184, 3185];
m.p. 101° [309], 100–102° [3184, 3185];
^{1}H NMR [3184, 3185], IR [3184, 3185].

1-(4,5-Dihydroxy-2-octadecylphenyl)-1-octadecanone

$C_{42}H_{76}O_3$ mol. wt. 629.06



Synthesis

-Refer to: [3112].

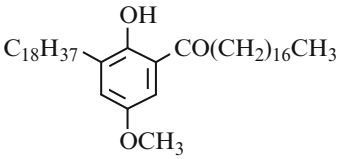
Dimethyl ether [1111287-73-0]
$C_{44}H_{80}O_3$ mol. wt. 657.10

-Refer to: [3112].

USE: Formation of self-assembled monolayers on Sol-gel processed hafnium oxide as dielectric layers [3112].

1-(2-Hydroxy-5-methoxy-3-octadecylphenyl)-1-octadecanone

[72306-95-7] $C_{43}H_{78}O_3$ mol. wt. 643.09



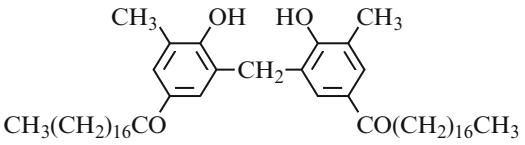
Syntheses

-Obtained by reaction of stearic acid with 2-octadecyl-4-methoxyphenol (m.p. 76°) in the presence of boron trifluoride for 7 h at 150–160° (37 %) [3185], then at 20° for 15 h (26 %) [3184].

light-yellow crystals [3184, 3185]; m.p. 74–75° [3184, 3185];
^{1}H NMR [3184, 3185], IR [3184, 3185].

1,1′-[Methylenebis(2-hydroxy-3-methyl-5,1-phenylene)]bis-1-octadecanone

$C_{51}H_{84}O_4$ mol. wt. 761.23



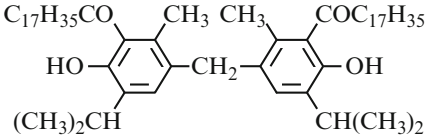
Syntheses
-Obtained by reaction of octadecanoyl chloride with bis (2-hydroxy-3-methylphenyl) methane according to the method described

previously [2871], (65 %) [119].

m.p. 87.4–90° [119]; ^{1}H NMR [119], IR [119].

1,1′-[Methylenebis[4-hydroxy-5-(1-methylethyl)-2-methyl-3,1-phenylene]]bis-1-octadecanone

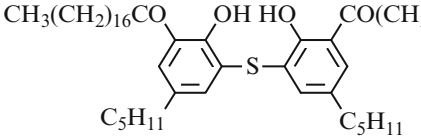
$C_{57}H_{96}O_4$ mol. 845.39



Synthesis
-Refer to: [2961].
m.p. 175–187° [2961].

1,1′-[Thiobis(2-hydroxy-5-pentyl-3,1-phenylene)]bis-1-octadecanone
3′,3‴-Thiobis[2′-hydroxy-5′-pentyl-octadecanophenone

$C_{58}H_{98}O_4S$ mol. wt. 891.48



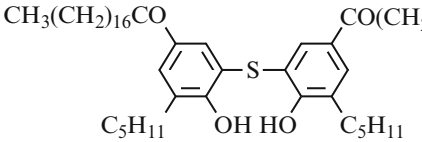
Syntheses
-Refer to: [825, 826].

USE: Polycarboxylic acid esters of oxypropylated, [825];

Polycarboxylic acid esters of oxypropylated, in breaking petroleum emulsions [826].

1,1′-[Thiobis(6-hydroxy-5-pentyl-3,1-phenylene)]bis-1-octadecanone
3′,3‴-Thiobis[6′-hydroxy-5′-pentyl-octadecanophenone

$C_{58}H_{98}O_4S$ mol. wt. 891.48



Syntheses
-Refer to: [825, 826].

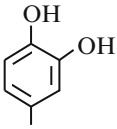
USE: Polycarboxylic acid esters of oxypropylated, [825];

Polycarboxylic acid esters of oxypropylated, in breaking petroleum emulsions [826].

2 Aromatic Hydroxyketones Derived from Various Halogenooctadecanoic Acids

9,10,12,13,15,16-Hexabromo-1-(3,4-dihydroxyphenyl)-1-octadecanone

[100559-75-9] $C_{24}H_{34}Br_6O_3$ mol. wt. 849.96



$CO(CH_2)_7CHBrCHBrCH_2CHBrCHBrCH_2CHBrCHBrCH_2CH_3$

Synthesis
-Refer to: [3093].

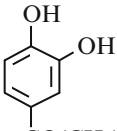
Dimethyl ether [100559-74-8] $C_{26}H_{38}Br_6O_3$ mol. wt. 878.01

-Obtained by reaction of 9,10,12,13,15,16 hexabromooctanoyl chloride with veratrole in the presence of aluminium chloride in tetrachloroethylene at 120° (15.8 %) [3097].
-Also refer to: [3093].

USE: Useful as intermediate for urushiol [3097].

9,10,12,13-Tetrabromo-1-(3,4-dihydroxyphenyl)-1-octadecanone

[100559-78-2] $C_{24}H_{36}Br_4O_3$ mol. wt. 692.16



$CO(CH_2)_7CHBrCHBrCH_2CHBrCHBrC_5H_{11}$

Synthesis
-Obtained by treatment of its dimethyl ether below with boron tribromide in methylene chloride at −60° (68.7 %) [3095].

Dimethyl ether [100559-77-1] $C_{26}H_{40}Br_4O_3$ mol. wt. 720.22

-Obtained by reaction of 9,10,12,13-tetrabromooctadecanoyl chloride with veratrole in the presence of aluminium chloride in refluxing carbon disulfide (42.6 %) [3095, 3096].

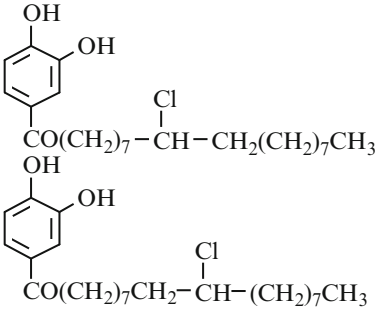
9-Chloro-1-(3,4-dihydroxyphenyl)-1-octadecanone

[97911-40-5] $C_{24}H_{39}ClO_3$ mol. wt. 411.02

and

10-Chloro-1-(3,4-dihydroxyphenyl)-1-octadecanone

[97911-41-6] $C_{24}H_{39}ClO_3$ mol. wt. 411.02



Synthesis

-Obtained by Fries rearrangement of pyrocatechol oleate in the presence of aluminium chloride. There is fixation of one molecule hydrogen chloride on the double bond during the reaction (36 %) [1505].

colourless waxy solid [1505];

m.p. 85–87° [1505];

^{1}H NMR [1505], IR [1505], UV [1505].

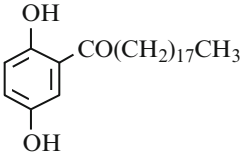
Chapter 17
Nonadecanones

1 Aromatic Hydroxyketones Derived from Nonadecanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2,5-Dihydroxyphenyl)-1-nonadecanone

$C_{25}H_{42}O_3$ mol. wt. 390.61



Synthesis
-Refer to: [1820].
Dimethyl ether [103099-04-3]
$C_{27}H_{46}O_3$ mol. wt. 418.66

-Obtained by condensation of nonadecanoyl chloride with hydroquinone dimethyl ether [1820].

colourless prisms [1820]; m.p. 55–56° [1820]; IR [1820].

2,4-Dinitrophenylhydrazone of the methyl ether

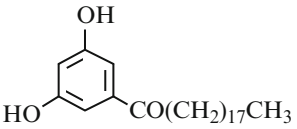
[103325-22-0] $C_{33}H_{50}N_4O_6$ mol. wt. 598.78

red prisms [1820]; m.p. 81–82° [1820].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_17

1-(3,5-Dihydroxyphenyl)-1-nonadecanone

$C_{25}H_{42}O_3$ mol. wt. 390.61



Syntheses
-Refer to: [2876, 2877, 2948].

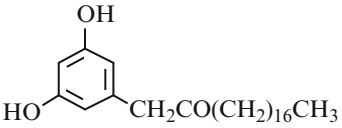
Dimethyl ether [22168-75-8] $C_{27}H_{46}O_3$ mol. wt. 418.66

-Obtained by reaction of octadecylmagnesium bromide with 3,5-dimethoxybenzamide in ether (56%) [2876, 2948].
-Refer to: [2877].

m.p. 69–71° [2948], 67–71° [2876].

1-(3,5-Dihydroxyphenyl)-2-nonadecanone

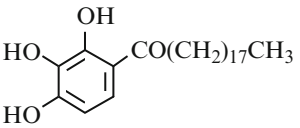
[142611-25-4] $C_{25}H_{42}O_3$ mol. wt. 390.61



Isolation from natural sources
-From etiolated rice seedlings [3003].

1-(2,3,4-Trihydroxyphenyl)-1-nonadecanone

[114808-66-1] $C_{25}H_{42}O_4$ mol. wt. 406.61

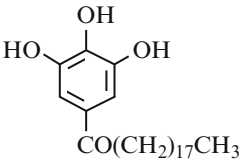


Syntheses
-Refer to: [2714–2716].

USE: Thermal recording material contg. [2716]; For IR-absorbing image [2715]; Thermal recording materials contg. higher fatty acid metal double salts and, for improved image contrast and resistance to oils and optical readability [2714].

1-(3,4,5-Trihydroxyphenyl)-1-nonadecanone

[87667-31-0] $C_{25}H_{42}O_4$ mol. wt. 406.61



Syntheses
-Refer to: [1327, 2229].

USE: Hydrophilic colloid layer contg., as photog. additive [2229]; Colour mixing effect prevention by, in photog. films [1327].

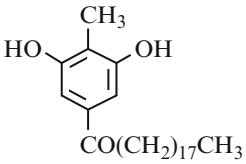
Trimethyl ether $C_{28}H_{48}O_4$ mol. wt. 448.69

m.p. 78° [1326].

1.2 Substituted Hydroxyketones

1-(3,5-Dihydroxy-4-methylphenyl)-1-nonadecanone

$C_{26}H_{44}O_3$ mol. wt. 404.63

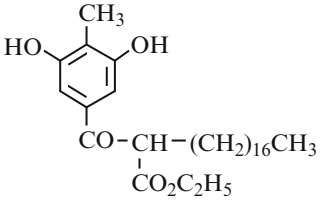


Synthesis
-Refer to: [1326].
Dimethyl ether
$C_{28}H_{48}O_3$ mol. wt. 432.69

-Refer to: [1326]; m.p. 82° [1326].

2-(3,5-Dihydroxy-4-methylbenzoyl)nonadecanoic acid ethyl ester

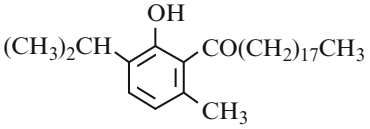
$C_{29}H_{48}O_5$ mol. wt. 476.70



Synthesis
-Refer to: [1326].
Dimethyl ether
$C_{31}H_{52}O_5$ mol. wt. 504.75
m.p. 70.5° [1326].

1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-nonadecanone

$C_{29}H_{50}O_2$ mol. wt. 430.71

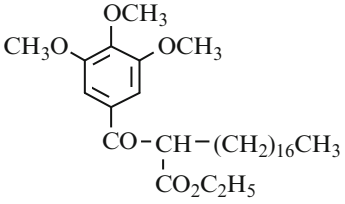


Synthesis
-Obtained by reaction of nonadecanoic acid with thymol in the presence of aluminium chloride on heating at reflux for 12 h (72%) [2960].

b.p.$_{16}$ 131–133° [2960]; m.p. 44.5° [2960].

2-(3,4,5-Trimethoxybenzoyl)nonadecanoic acid ethyl ester

$C_{31}H_{52}O_6$ mol. wt. 520.75

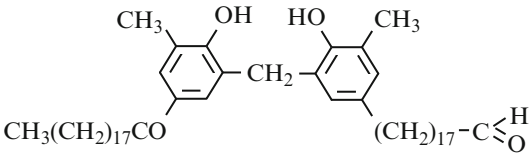


Synthesis
-Refer to: [1326].
m.p. 66.3° [1326].

1-[4-Hydroxy-3-[[2-hydroxy-3-methyl-5-(1-oxooctadecyl)phenyl]methyl]-5-methylphenyl]-1-nonadecanone (Chemical Abstracts)

18-[4-Hydroxy-3-(2-hydroxy-3-methyl-5-nonadecanoylbenzyl)-5-methylphenyl]-octadecanal (IUPAC)

[169553-39-3] $C_{52}H_{86}O_4$ mol. wt. 775.24



Synthesis
-Refer to: [120].

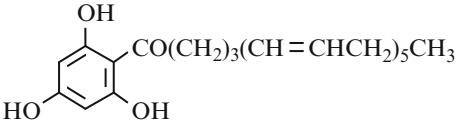
Chapter 18
Eicosanones

1 Aromatic Hydroxyketones Derived from Eicosanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2,4,6-Trihydroxyphenyl)-5,8,11,14,17-eicosapentaen-1-one (all *Z*)

[79553-90-5] $C_{26}H_{34}O_4$ mol. wt. 410.55

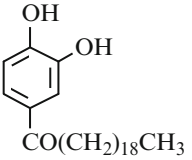


Isolation from natural sources
-From *Zonaria tournefortii* (Lamour) Mont. (Dictyotaceae) [102].

pale yellow oil [102];
^{1}H NMR [102, 103], ^{13}C NMR [102, 103, 1103], IR [102, 1103], UV [102, 1103], MS [102, 1103]; TLC [102].

1-(3,4-Dihydroxyphenyl)-1-eicosanone

[151029-60-6] $C_{26}H_{44}O_3$ mol. wt. 404.63



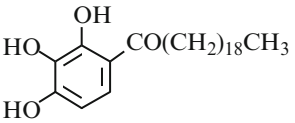
Isolation from natural sources
-From *Plectranthus sylvestris* [1551].

BIOLOGICAL ACTIVITY: Refer to: [1551].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_18

1-(2,3,4-Trihydroxyphenyl)-1-eicosanone

[96070-21-2] $C_{26}H_{44}O_4$ mol. wt. 420.63



Syntheses

-Obtained by reaction of arachidic acid with pyrogallol in the presence of boron trifluoride and hydrogen fluoride in xylene on a water-bath at 70° (90 %) [505].

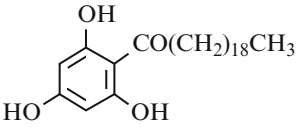
-Also refer to: [500].

b.p.$_{14}$ 308–310° [500]; m.p. 101° [500], 99° [505].

BIOLOGICAL ACTIVITY: Potential activity against lethal radiations [505].

1-(2,4,6-Trihydroxyphenyl)-1-eicosanone

[79553-91-6] $C_{26}H_{44}O_4$ mol. wt. 420.63



Synthesis

-Obtained by mild catalytic hydrogenation of 1-(2,4,6-trihydroxyphenyl)-1-eicosanone, 5,8,11,14,17-pentaene [102].

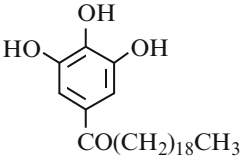
Isolation from natural sources

-From the brown alga *Zonaria tournefortii* [102].

m.p. 136° [102]; ^{1}H NMR [102], IR [102], UV [102], MS [102, 581].

1-(3,4,5-Trihydroxyphenyl)-1-eicosanone

$C_{26}H_{44}O_4$ mol. wt. 420.63



Synthesis

-Refer to: [1326].

Trimethyl ether

$C_{29}H_{50}O_4$ mol. wt. 462.71

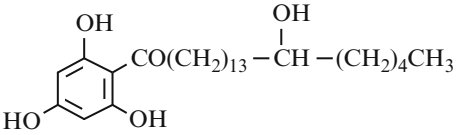
-Refer to: [1326].

m.p. 82° [1326].

1-(2,4,6-Trihydroxyphenyl)-15-hydroxy-1-eicosanone

2-Eicosanoylphloroglucinol decahydro derivative

$C_{26}H_{44}O_5$ mol. wt. 436.63

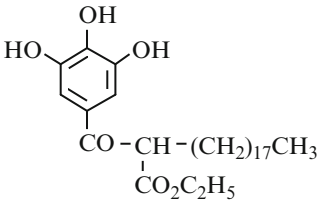


Synthesis

-Refer to: [103].

2-(3,4,5-Trihydroxybenzoyl)eicosanoic acid ethyl ester

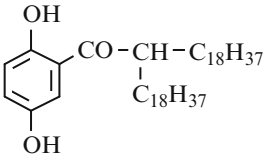
$C_{29}H_{48}O_6$ mol. wt. 492.70



Synthesis
-Refer to: [1326].
Trimethyl ether
$C_{32}H_{54}O_6$ mol. wt. 534.78
m.p. 66.5° [1326].

1-(2,5-Dihydroxyphenyl)-2-octadecyl-1-eicosanone

$C_{44}H_{80}O_3$ mol. wt. 657.10

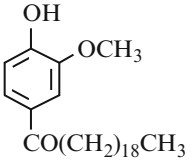


Synthesis
-Refer to: [2225].
Dimethyl ether [125697-50-9]
$C_{46}H_{84}O_3$ mol. wt. 685.17
-Refer to: [2225].

1.2 Substituted Hydroxyketones

1-(4-Hydroxy-3-methoxyphenyl)-1-eicosanone

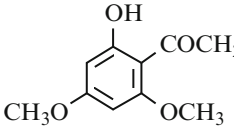
$C_{27}H_{46}O_3$ mol. wt. 418.65



Synthesis
-Refer to: [2369].
m.p. 70.5–71.5° [2369].

1-(2-Hydroxy-4,6-dimethoxyphenyl)-1,3-eicosanedione
ω-n-Octadecanoyl-2-hydroxy-4,6-dimethoxyacetophenone

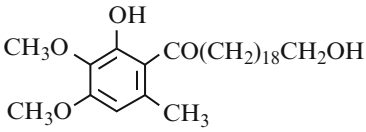
$C_{28}H_{46}O_5$ mol. wt. 462.67



Synthesis
-Refer to: [3167].
m.p. 94–96° [3167].

20-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-eicosanone

[104966-98-5] $C_{29}H_{50}O_5$ mol. wt. 478.71



Synthesis
-Obtained by treatment of its 20-acetyl ester with sodium hydroxide in methanol for 2 h at r.t. (64 %) [1147].

colourless needles [1147]; m.p. 105° [1147];
^{1}H NMR [1147], IR [1147], MS [1147].

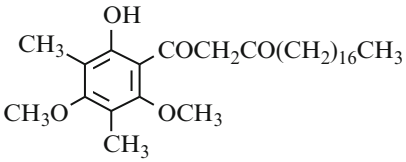
20-Acetyl ester [104966-94-1] $C_{31}H_{52}O_6$ mol. wt. 520.75

-Obtained by Friedel-Crafts reaction of 20-acetoxyeicosanoyl chloride with 3,4,5-trimethoxy-toluene in 1,2-dichloroethane in the presence of aluminium chloride (2.1 mol) at 20° for 72 h [1147].

colourless oil [1147];
IR [1147], ^{1}H NMR [1147], MS [1147].

1-(2-Hydroxy-4,6-dimethoxy-3,5-dimethylphenyl)-1,3-eicosanedione

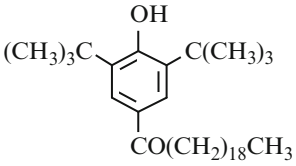
$C_{30}H_{50}O_5$ mol. wt. 490.72



Synthesis
-Refer to: [3167].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-eicosanone

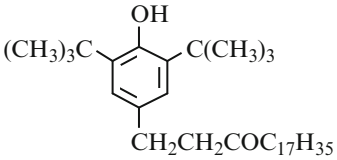
[28441-04-5] $C_{34}H_{60}O_2$ mol. wt. 500.85



Synthesis
-Refer to: [951].
m.p. 74–76° [951].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-eicosanone

[54685-34-6] $C_{34}H_{60}O_2$ mol. wt. 500.85



Synthesis
-Refer to: [2758].

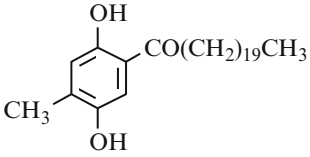
USE: Reaction of, with sodium cyanide and ammonium carbonate in preparation of hydantoins [2758].

Chapter 19
Heneicosanones

1 Aromatic Hydroxyketones Derived from Heneicosanoic Acids

1-(2,5-Dihydroxy-4-methylphenyl)-1-heneicosanone

[13736-51-1] $C_{28}H_{48}O_3$ mol. wt. 432.69



Synthesis
-Obtained by hydrolysis of 5-heneicosanoate with a mixture (1:1) concentrated hydrochloric acid/ethanol for 8 h (13.5 %) [3416].
yellow needles [3416];

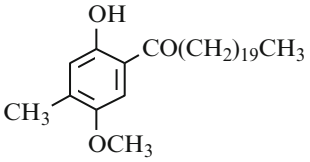
m.p. 95–97° [3416]; IR [3416].

5-Heneicosanoyl ether [13736-50-0] $C_{49}H_{88}O_4$ mol. wt. 741.24

m.p. 45–48° [3416]; IR [3416].

1-(2-Hydroxy-5-methoxy-4-methylphenyl)-1-heneicosanone

[13736-49-7] $C_{29}H_{50}O_3$ mol. wt. 446.71



Synthesis
-Obtained by Friedel-Crafts condensation of heneicosanoyl chloride with 2,5-dimethoxytoluene in the presence of aluminium chloride in refluxing carbon disulfide for 20 h (63.2 %) [3416].

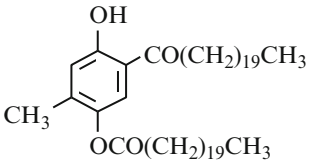
pale yellow plates [3416]; m.p. 82–83° [3416]; IR [3416].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_19

1-(5-Heneicosanoyloxy-2-hydroxy-4-methylphenyl)-1-heneicosanone

2,5-Dihydroxy-4-methylheneicosanophenone 5-heneicosanoate

[13736-50-0] $C_{49}H_{88}O_4$ mol. wt. 741.24



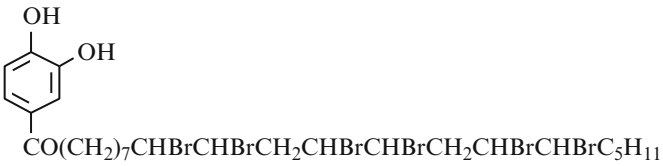
Synthesis
-Obtained by Friedel-Crafts condensation of heneicosanoyl chloride with 2,5-dimethoxytoluene in the presence of aluminium chloride in refluxing carbon disulfide for 20 h (9.2 %) [3416].

yellow needles [3416]; m.p. 45–48° [3416]; IR [3416].

2 Aromatic Hydroxyketones Derived from Bromoheneicosanoic Acid

9,10,12,13,15,16-Hexabromo-1-(3,4-dihydroxyphenyl)-1-heneicosanone

[100559-80-6] $C_{27}H_{40}Br_6O_3$ mol. wt. 892.04



Synthesis
-Refer to: [3094].

Dimethyl ether [100568-25-0] $C_{29}H_{44}Br_6O_3$ mol. wt. 920.09

-Refer to: [3097].

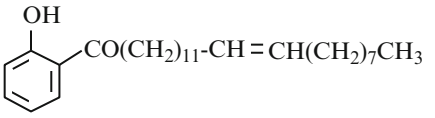
Chapter 20
Docosanones

1 Aromatic Hydroxyketones Derived from Docosanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(2-Hydroxyphenyl)-13-docosen-1-one
2′-Hydroxy phenyl heneicosen-13, one-1 [200]

$C_{28}H_{46}O_2$ mol. wt. 414.67



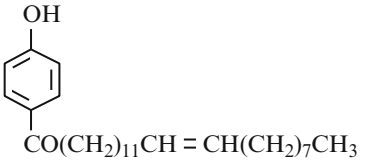
Synthesis
-Obtained by Fries rearrangement of phenyl erucate with aluminium chloride at 115–120° for 2 h (27 %) [200].

2,4-Dinitrophenylhydrazone $C_{34}H_{50}N_4O_5$ mol. wt. 594.79

m.p. 140° [200].

1-(4-Hydroxyphenyl)-13-docosen-1-one
4′-Hydroxy phenyl heneicosen-13, one-1 [200]

$C_{28}H_{46}O_2$ mol. wt. 414.67



Synthesis
-Obtained by Fries rearrangement of phenyl erucate with aluminium chloride at 115–120° for 2 h (7 %) [200].
b.p.$_{10}$ 260° [200].

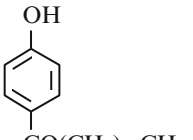
R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_20

2,4-Dinitrophenylhydrazone $C_{34}H_{50}N_4O_5$ mol. wt. 594.79

m.p. 167° [200].

1-(4-Hydroxyphenyl)-1-docosanone

[47660-65-1] $C_{28}H_{48}O_2$ mol. wt. 416.69



Synthesis
-Obtained by reaction of behenic acid with phenol in the presence of boron trifluoride for 2–3 h between 65 and 85° (75 %) [503].
m.p. 96–97° [503].

iso-Nicotinylhydrazone [103396-94-7] $C_{34}H_{53}N_3O_2$ mol. wt. 535.81

m.p. 131° [520, 521].

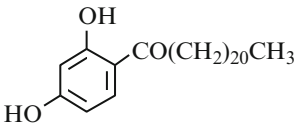
USE: In chemotherapy of leprosy [520, 521].

Polymer with formaldehyde [27029-47-6]

USE: Point depressant for fuel oil [1344].

1-(2,4-Dihydroxyphenyl)-1-docosanone
(4-Behenylresorcinol)

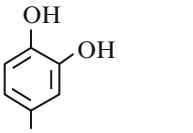
[856360-21-9] $C_{28}H_{48}O_3$ mol. wt. 432.69



Synthesis
-Obtained by reaction of behenic acid with resorcinol in the presence of zinc chloride at 150–160° for 4 h [507].
colourless needles [507]; m.p. 103° [507].

1-(3,4-Dihydroxyphenyl)-1-docosanone
(4-Behenylcatechol)

$C_{28}H_{48}O_3$ mol. wt. 432.69

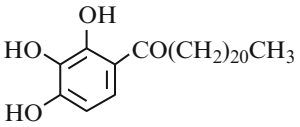


Syntheses
-Obtained by reaction of behenic acid with pyrocatechol,
*in the presence of zinc chloride (Nencki reaction) (10 %) [507];
*in the presence of boron trifluoride at 80° (75 %) [507].
colourless prisms [507]; m.p. 103° [507].

BIOLOGICAL ACTIVITY: Protection against whole-body irradiation [1810]; Protection against X-rays [1811].

1-(2,3,4-Trihydroxyphenyl)-1-docosanone
(4-Behenylpyrogallol)

[103279-18-1] $C_{28}H_{48}O_4$ mol. wt. 448.69



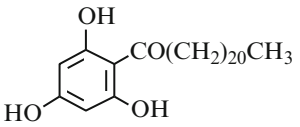
Syntheses
-Obtained by reaction of behenic acid with pyrogallol in the presence of zinc chloride at 150–160° for 4 h (70 %) [507].
-Also refer to: [1810, 1811, 2778].

colourless needles [507]; $b.p._{0.2}$ 250° [507]; m.p. 100–101° [507].

BIOLOGICAL ACTIVITY: Protection against whole-body irradiation [1810]; Protection against X-rays [1811]; Radiation damage prevention by, [2778].

1-(2,4,6-Trihydroxyphenyl)-1-docosanone

$C_{28}H_{48}O_4$ mol. wt. 448.69

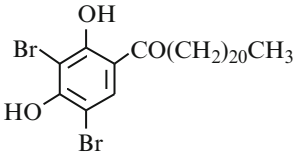


Synthesis
-Refer to: [581].
HRMS [581], ESI [581].

1.2 Substituted Hydroxyketones

1-(3,5-Dibromo-2,4-dihydroxyphenyl)-1-docosanone
(2,6-Dibromo-4-behenylresorcinol)

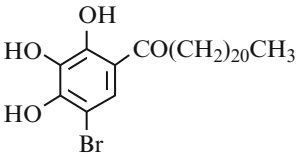
$C_{28}H_{46}Br_2O_3$ mol. wt. 590.48



Synthesis
-Obtained by reaction of bromine with 4-behenylresorcinol in acetic acid at 37–38° for few min (92 %) [507].
colourless needles [507]; m.p. 110° [507].

1-(5-Bromo-2,3,4-trihydroxyphenyl)-1-docosanone
(6-Bromo-4-behenylpyrogallol)

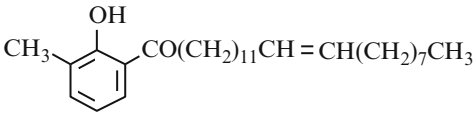
$C_{28}H_{47}BrO_4$ mol. wt. 527.58



Synthesis
-Obtained by reaction of bromine with 4-behenylpyrogallol in acetic acid at r.t. (85 %) [507].
colourless needles [507]; m.p. 99° [507].

1-(2-Hydroxy-3-methylphenyl)-13-docosen-1-one
2′-Hydroxy 3′-methyl phenyl heneicosen-13, one-1 [200]

$C_{29}H_{48}O_2$ mol. wt. 428.70



Synthesis
-Obtained by Fries rearrangement of o-cresyl erucate with aluminium chloride at 115–120° for 2 h (19 %) [200].

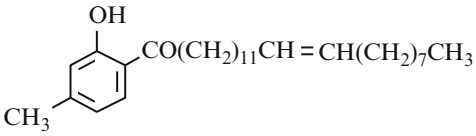
b.p.$_3$ 225° [200].

2,4-Dinitrophenylhydrazone $C_{35}H_{52}N_4O_5$ mol. wt. 608.82

m.p. 139° [200].

1-(2-Hydroxy-4-methylphenyl)-13-docosen-1-one
2′-Hydroxy 4′-methyl phenyl heneicosen-13, one-1 [200]

$C_{29}H_{48}O_2$ mol. wt. 428.70



Synthesis
-Obtained by Fries rearrangement of m-cresyl erucate with aluminium chloride at 115–120° for 2 h (33 %) [200].

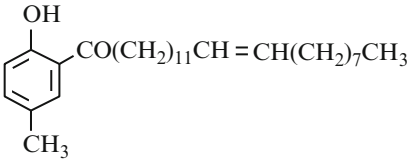
b.p.$_4$ 230° [200].

2,4-Dinitrophenylhydrazone $C_{35}H_{52}N_4O_5$ mol. wt. 608.82

m.p. 130° [200].

1-(2-Hydroxy-5-methylphenyl)-13-docosen-1-one
2′-Hydroxy 5′-methyl phenyl heneicosen-13, one-1 [200]

$C_{29}H_{48}O_2$ mol. wt. 428.70



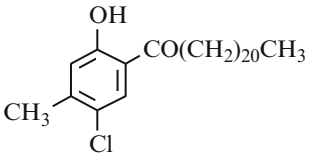
Synthesis
-Obtained by Fries rearrangement of p-cresyl erucate with aluminium chloride at 115–120° for 2 h (39 %) [200].
b.p.$_4$ 243° [200].

2,4-Dinitrophenylhydrazone $C_{35}H_{52}N_4O_5$ mol. wt. 608.82

m.p. 110° [200].

1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-docosanone

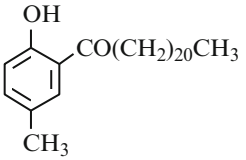
$C_{29}H_{49}ClO_2$ mol. wt. 465.16



Synthesis
-Obtained by reaction of behenic acid with 4-chloro-3-methylphenol in the presence of boron trifluoride for 2–3 h between 65 and 85° (90 %) [503].
m.p. 92–93° [503].

1-(2-Hydroxy-5-methylphenyl)-1-docosanone

$C_{29}H_{50}O_2$ mol. wt. 430.71



Synthesis
-Obtained by reaction of behenic acid with p-cresol in the presence of boron trifluoride for 2–3 h between 65 and 85° (90–95 %) [503].
m.p. 80–81° [503].

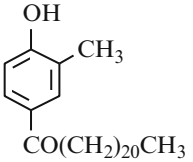
Methyl ether [103398-74-9] $C_{30}H_{52}O_2$ mol. wt. 444.74

-Obtained by refluxing a mixture of 2-hydroxy-5-methylbehenophenone and methyl iodide in the presence of potassium hydroxide for 2 h [518].

silky needles [370]; m.p. 76° [518].

1-(4-Hydroxy-3-methylphenyl)-1-docosanone

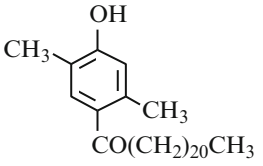
[95185-70-9] $C_{29}H_{50}O_2$ mol. wt. 430.71



Synthesis
-Refer to: [2704].

1-(4-Hydroxy-2,5-dimethylphenyl)-1-docosanone

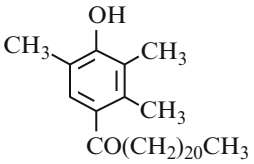
[95185-61-8] $C_{30}H_{52}O_2$ mol. wt. 444.74



Synthesis
-Refer to: [2704].

1-(4-Hydroxy-2,3,5-trimethylphenyl)-1-docosanone

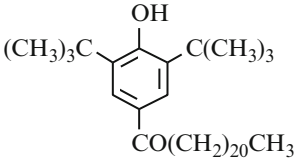
[137833-01-3] $C_{31}H_{54}O_2$ mol. wt. 458.77



Synthesis
-Refer to: [1733].

1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-docosanone

[28441-05-6] $C_{36}H_{64}O_2$ mol. wt. 528.90

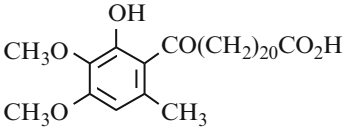


Synthesis
-Preparation by reaction of docosanoyl chloride with 2,6-di-tert-butylphenol in the presence of aluminium chloride in 1,1,2-trichloroethane at −10 to −20° [951].
m.p. 66–69° [951].

2 Aromatic Hydroxyketones Derived from 22-Oxodocosanoic Acid

22-(2-Hydroxy-3,4-dimethoxy-6-methylphenyl)-22-oxo-1-docosanoic acid
21-(2-Hydroxy-3,4-dimethoxy-6-methylbenzoyl)heneicosanoic acid

[79330-93-1] $C_{31}H_{52}O_6$ mol. wt. 520.75



Synthesis
-Obtained by reaction of ethyl chloroformyl-eicosanoate with 3,4,5-trimethoxytoluene in the presence of aluminium chloride in nitrobenzene first at 0°, then at r.t. [2325].

m.p. 103–105° [2325]; IR [2325].

Methyl ether [84978-10-9] $C_{32}H_{54}O_6$ mol. wt. 534.78

-Obtained by reaction of ethyl chloroformyl-eicosanoate with 3,4,5-trimethoxytoluene in the presence of aluminium chloride in nitrobenzene first at 0°, then at r.t. [2325].

m.p. 88–90° [2325]; IR [2325].

Methyl ester [77711-94-5] $C_{32}H_{54}O_6$ mol. wt. 534.78

Methyl 21-(2-hydroxy-3,4-dimethoxy-6-methylbenzoyl)heneicosanoate

-Obtained by esterification of the title acid [2325].

m.p. 75–76° [2325]; ^{1}H NMR [1432], IR [2325].

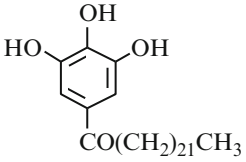
Chapter 21
Tricosanones

1 Aromatic Hydroxyketones Derived from Tricosanoic Acid

1.1 Unsubstituted Hydroxyketones

1-(3,4,5-Trihydroxyphenyl)-1-tricosanone

[155084-01-8] $C_{29}H_{50}O_4$ mol. wt. 462.71



Syntheses
-Refer to: [2082–2085, 2981] (Japanese patents).

USE: Blotting-resistant thermographic recording sheet containing [2083]; Thermographic recording sheet for high sensitive and plasticizer-resistant images [2084]; Thermal recording material containing electron donor from, [2082].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_21

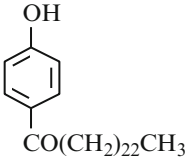
Chapter 22
Tetracosanones

1 Aromatic Hydroxyketones Derived from Tetracosanoic Acids

1.1 Unsubstituted Hydroxyketones

1-(4-Hydroxyphenyl)-1-tetracosanone

$C_{30}H_{52}O_2$ mol. wt. 444.74

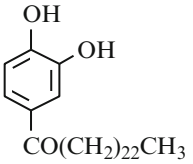


Synthesis
-Refer to: [1344]
Polymer with formaldehyde [27029-46-5]

USE: Pour point depressant for fuel oil [1344].

1-(3,4-Dihydroxyphenyl)-1-tetracosanone

[191284-02-3] $C_{30}H_{52}O_3$ mol. wt. 460.74



Synthesis
-Refer to: [2215].

USE: Thermal printing material for images with good solvent resistance [2215].

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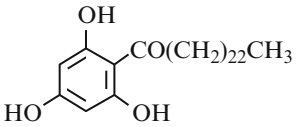
1-(2,4,6-Trihydroxyphenyl)-1-tetracosanone

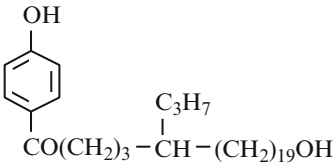
$C_{30}H_{52}O_4$ mol. wt. 476.74



Synthesis
-Refer to: [581].
HRMS [581]; ESI [581].

4-(24-Hydroxy-1-oxo-5-n-propyltetracosanyl)phenol

$C_{33}H_{58}O_3$ mol. wt. 502.82



Synthesis
-Refer to: [2092].

Isolation from natural sources
-From the shoots of *Leucas aspera* Spreng [2092].

m.p. 80–81° [2092];
^{1}H NMR [2092], ^{13}C NMR [2092], IR [2092], UV [2092], MS [2092];
$(\alpha)_D^{35} = -10.4°$ (ethanol) [2092].

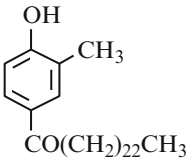
Diacetate $C_{37}H_{62}O_5$ mol. wt 586.90

m.p. 68–70° [2092]; IR [2092], MS [2092].

1.2 Substituted Hydroxyketones

1-(4-Hydroxy-3-methylphenyl)-1-tetracosanone

[95102-15-1] $C_{31}H_{54}O_2$ mol. wt. 458.77



Syntheses
-Refer to: [1595, 2704].

USE: Colour developer, for thermal recording materials [1595].

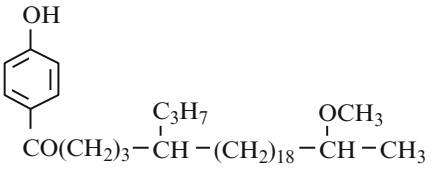
Chapter 23
Pentacosanones

1 Aromatic Hydroxyketones Derived from Pentacosanoic Acid

1.1 Unsubstituted Hydroxyketones

1-(4-Hydroxyphenyl)-5-propyl-24-methoxy-1-pentacosanone
4-(24-Methoxy-24-methyl-1-oxo-5-n-propyltetracosanyl)phenol

$C_{35}H_{62}O_3$ mol. wt. 530.88



Synthesis
-Refer to: [1545].

Isolation from natural sources
-From *Mimosa pudica* Linn [1545].

m.p. 112–113° [1545];
^{1}H NMR [1545], ^{13}C NMR [1545], IR [1545], UV [1545], MS [1545];
$(\alpha)_D^{25} = -6.9°$ (ethanol) [1545].

Acetate $C_{37}H_{64}O_4$ mol. wt. 572.91

m.p. 88–90° [1545]; IR [1545], MS [1545].

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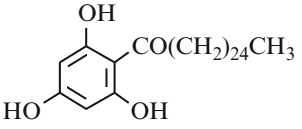
Chapter 24
Hexacosanones

1 Aromatic Hydroxyketones Derived from Hexacosanoic Acid

1.1 Unsubstituted Hydroxyketone

1-(2,4,6-Trihydroxyphenyl)-1-hexacosanone

$C_{32}H_{56}O_4$ mol. wt. 504.79



Synthesis
-Refer to: [581].
HRMS [581]; ESI [581].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_24

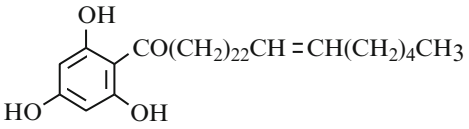
Chapter 25
Triacontanones

1 Aromatic Hydroxyketones Derived from Triacontanoic Acid

1.1 Unsubstituted Hydroxyketone

1-(2,4,6-Trihydroxyphenyl)-1-[24-triacontenone
2,4,6-Trihydroxyphenyl-(24*Z*)-triacontene-1-one
(Tenulphenone C)

$C_{36}H_{62}O_4$ mol. wt. 558.89



Synthesis
-Refer to: [1513].

Isolation from natural sources
-From the cortexes of *Polygala tenuifolia* [1513].

m.p. 197–200° [1513];
^{1}H NMR [1513], ^{13}C NMR [1513], IR [1513].

R. Martin, J.-P. Buisson, *Aromatic Hydroxyketones: Preparation & Physical Properties*, DOI 10.1007/978-3-319-14185-5_25

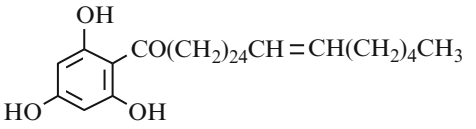
Chapter 26
Dotriacontanones

1 Aromatic Hydroxyketones Derived from Dotriacontanoic Acid

1.1 Unsubstituted Hydroxyketone

1-(2,4,6-Trihydroxyphenyl)-1-[24-dotriacontenone
2,4,6-Trihydroxyphenyl-(24*Z*)-dotriacontene-1-one
(Tenulphenone D)

$C_{38}H_{66}O_4$ mol. wt. 586.94



Synthesis
-Refer to: [1513].

Isolation from natural sources.
-From the cortexes of *Polygala tenuifolia* [1513].

m.p. 197–200° [1513];
^{1}H NMR [1513], ^{13}C NMR [1513], IR [1513].

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Common Abbreviations

Å	Angström units
b.p.	Boiling point (for example, $b.p._{0.1}$ 100° means boils at 100° if the pressure is 0.1 mmHg)
^{13}C	Nuclear Magnetic Resonance relative to carbon 13
(d)	Decomposition
20°	20 degrees Celsius
d	Density (for example, d_{20} specific gravity at 20 °C referred to water et 4 °C)
equiv.	Equivalent
(E)	Geometric stereodescriptor used for compounds having achiral elements resulting from double bonds where the groups of highest priority are on the opposite side of the vertical reference plane
^{19}F	Nuclear Magnetic Resonance relative to fluorine 19
GC	Gaz chromatography
GC-MS	Gaz chromatography-mass spectroscopy
GLC	Gaz-liquid chromatography
h	Hour
^{1}H NMR	Nuclear Magnetic Resonance relative to proton
HPLC	High Pressure Liquid Chromatography
IR	Infrared spectra
iso-	Aliphatic hydrocarbon having two methyl groups on the terminal carbon atom of the chain (for example, $(CH_3)_2CH\text{-}CH_2\text{-}CH_2\text{-}$)
LD_{50}	Median lethal dose, the quantity of a chemical that is estimated to be fatal to 50 % of the organisms tested
m-	Meta-
M	Molar (concentration)
min	Minute
Mol	Molecule
mol. wt.	Molecular weight

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m.p.	Melting point
MS	Mass spectra
n-	Normal (as n-butyl)
N	Normal (equivalents per liter, as applied to concentration)
N.B.	Nota Bene
n_D^{25}	Index of refraction (for 25° and sodium light)
nm	Nanometre
o-	Ortho-
p-	Para-
Pd/C	Palladium on charcoal
pK_a	Log of the reciprocal of the dissociation constant
r.t.	Room temperature
Sadtler	Sadtler Research Laboratories, Philadelphia (USA)
sec-	Secondary-
SM	Starting Material
tert-	Tertiary-
TLC	Thin Layer Chromatography
UV	Ultraviolet spectra
vol.	Volume
(Z)	Opposite of (E)

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Molecular Formula Index

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$C_{12}H_{16}O_3$

$C_{13}H_{18}O_3$

Chemical Abstracts Registry Numbers

[114-42-1]	3,5-Dihydroxy-4,4-dimethyl-2-(1-oxobutyl)-6-[[2,4,6-trihydroxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,5-cyclohexadien-1-one, 341
[319-30-2]	1-(5-Fluoro-2-hydroxyphenyl)-1-pentanone, 484
[319-31-3]	1-(5-Fluoro-2-hydroxyphenyl)-1-hexanone, 627
[329-44-2]	1-(3-Bromo-5-fluoro-4-hydroxyphenyl)-1-hexanone, 620
[347-65-9]	1-(3-Fluoro-4-methoxyphenyl)-1-butanone, 33
[350-16-3]	1-(3-Fluoro-4-hydroxy-5-iodophenyl)-1-hexanone, 623
[350-26-5]	1-(3-Fluoro-4-hydroxyphenyl)-1-pentanone, 483
[392-02-9]	1-(5-Fluoro-2-hydroxyphenyl)-1-decanone, 880
[402-81-3]	1-(3-Bromo-5-fluoro-4-hydroxyphenyl)-1-decanone, 877
[402-82-4]	1-(3-Fluoro-4-hydroxy-5-iodophenyl)-1-decanone, 878
[403-08-7]	1-(3-Fluoro-4-hydroxyphenyl)-1-decanone, 880
[437-72-9]	1-(2,6-Dihydroxy-4-methoxyphenyl)-1-butanone, 58
[449-31-0]	1-(3-Fluoro-4-hydroxyphenyl)-1-pentanone (isoNicotinylhydrazone), 483
[450-16-8]	7-Methoxy-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 203
[455-53-8]	1-(3-Bromo-5-fluoro-4-hydroxyphenyl)-1-pentanone, 478
[455-77-6]	1-(3-Fluoro-4-methoxyphenyl)-1-decanone, 880
[478-48-8]	1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-1-butanone, 73
[478-67-1]	5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 237
[479-96-9]	1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-1-butanone, 72
[480-27-3]	1-(2,4,6-Trimethoxyphenyl)-1,3-butanedione, 327
[519-40-4]	1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-1-butanone, 72
[521-38-0]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 236
[575-67-7]	1-(5-Fluoro-2-hydroxyphenyl)-1-butanone, 33
[584-28-1]	2-[[2,6-Dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-3,5-dihydroxy-4,4-dimethyl-6-(1-oxobutyl)-2,5-cyclohexadien-1-one, 342
[584-28-1]	3′-[(5-Butyryl-2,4-dihydroxy-3,3-dimethyl-6-oxo-1,4-cyclohexadien-1-yl)methyl]-2′,4′-dihydroxy-6′-methoxy-5′-methyl-1-butanone, 342

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[586-03-8]	1-(3-Bromo-5-fluoro-4-hydroxyphenyl)-1-butanone, 20
[586-18-5]	1-(3-Fluoro-4-hydroxyphenyl)-1-butanone, 32
[586-20-9]	1-(3-Fluoro-4-methoxyphenyl)-1-pentanone, 484
[749-41-7]	1-(3,4-Dimethoxyphenyl)-4-(4-ethoxy-3-methoxyphenyl)-2,3-dimethyl-1,4-butanedione, 371
[784-64-5]	1-(5-Fluoro-2-hydroxyphenyl)-1-octanone, 788
[860-34-4]	1-(5-Fluoro-2-hydroxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 627
[881-43-6]	2-Bromo-1-(4-methoxyphenyl)-1-butanone, 270
[949-06-4]	5-Chloro-1-(4-methoxyphenyl)-1-pentanone, 568
[986-89-0]	1,4-Bis(4-ethoxy-3-methoxyphenyl)-2,3-dimethyl-1,4-butanedione, 371
[1009-11-6]	1-(4-Hydroxyphenyl)-1-butanone, 4
[1084-74-8]	4-(2,5-Dimethoxyphenyl)-4-oxo-1-butanoic acid, 406
[1086-77-7]	Methyl 4-(2,5-dimethoxyphenyl)-4-oxo-1-butanoate, 406
[1130-98-9]	1-(2-Chloro-4-hydroxyphenyl)-1-butanone, 28
[1133-33-1]	1-(2,6-Dichloro-4-hydroxyphenyl)-1-butanone, 24
[1133-34-2]	1-(2,4-Dichloro-6-hydroxyphenyl)-1-butanone, 23
[1133-58-0]	1-(2-Chloro-3-methoxyphenyl)-1-butanone, 28
[1134-09-4]	1-(3-Bromo-2-chloro-4-hydroxyphenyl)-1-butanone, 20
[1148-02-3]	4-(4-Chlorobutyryl)-3-methylphenoxyacetic acid, 287
[1154-71-8]	2-[2,3-Dichloro-4-(4-methylvaleryl)phenoxy]acetic acid, 548
[1154-72-9]	1-(2,3,4-Trihydroxyphenyl)-1-decanone, 875
[1158-20-9]	1-(3,4-Dihydroxyphenyl)-1-dodecanone, 948
[1177-44-2]	1-(3,4-Dihydroxyphenyl)-1-octadecanone, 1067
[1200-95-9]	1-(2-Hydroxy-6-methylphenyl)-1-butanone, 50
[1201-04-3]	1-(2-Chloro-3-hydroxyphenyl)-1-butanone, 28
[1203-88-9]	1-(5-Hydroxy-2,4-dimethylphenyl)-1-butanone, 69
[1210-21-5]	1-(2,3-Dichloro-4-hydroxyphenyl)-4-methyl-1-pentanone, 546
[1210-91-9]	1-(4-Hydroxy-2-methyl-3-nitrophenyl)-1-butanone, 46
[1211-07-0]	1-[2-(Acetylamino)-4-hydroxyphenyl]-1-butanone, 64
[1248-88-0]	1,5-Bis(3,4-dimethoxyphenyl)-1,5-pentanedione, 521
[1421-63-2]	1-(2,4,5-Trihydroxyphenyl)-1-butanone, 16
[1441-41-4]	1-(2,6-Dichloro-3-hydroxyphenyl)-1-butanone, 24
[1480-47-3]	1-(5-Fluoro-2-hydroxyphenyl)-1-dodecanone, 955
[1506-72-5]	1-(2,3-Dichloro-4-hydroxyphenyl)-3-methyl-1-butanone, 185
[1506-73-6]	1-(2-Chloro-4-hydroxyphenyl)-3,3-dimethyl-1-butanone, 252
[1509-06-4]	1-(2,4,6-Trihydroxy-3-methylphenyl)-1-butanone, 59
[1509-10-0]	1-[3-(3-Butyryl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl-2,6-dihydroxy-4-methoxyphenyl]-1-butanone, 339
[1539-14-6]	1-(2,3-Dichloro-4-hydroxyphenyl)-2-ethyl-1-butanone, 171
[1639-85-6]	1-(2-Hydroxy-4,6-dimethylphenyl)-1-butanone, 67
[1644-57-1]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-hexanone, 621
[1644-98-0]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-pentanone (2,4-Dinitrophenylhydrazone), 478
[1671-76-7]	1-(4-Methoxyphenyl)-1-pentanone, 466

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[1702-68-7]	4-(2,4,5-Trimethoxyphenyl)-2-methyl-4-oxo-1-butanoic acid, 417
[1702-69-8]	Methyl 4-(2,4,5-trimethoxyphenyl)-2-methyl-4-oxo-1-butanoate, 417
[1702-70-1]	4-(2,4,5-Trimethoxyphenyl)-3-methyl-4-oxo-1-butanoic acid, 418
[1760-65-2]	4-Cyclohexyl-1-(4-hydroxyphenyl)-1-butanone, 256
[1813-21-4]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-pentanone, 478
[1813-22-5]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-pentanone, 479
[1814-29-5]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-heptanone, (2,4-Dinitrophenylhydrazone), 732
[1841-68-5]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 620
[1847-68-3]	Methyl 5-(4-methoxyphenyl)-5-oxo-1-pentanoate, 579
[1854-63-3]	1-(2,3-Dimethoxyphenyl)-1-octanone (2,4-Dinitrophenylhydrazone), 778
[1854-64-4]	1-(2,3-Dimethoxyphenyl)-1-octanone, 778
[1854-68-8]	1-(2,3-Dimethoxyphenyl)-1-heptanone (2,4-Dinitrophenylhydrazone), 725
[1854-69-9]	1-(2,3-Dimethoxyphenyl)-1-heptanone, 725
[1854-72-4]	1-(2,3-Dimethoxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 606
[1854-73-5]	1-(2,3-Dimethoxyphenyl)-1-hexanone, 606
[1867-82-9]	1-[3-[[2,4-Dihydroxy-6-methoxy-5-methyl-3-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxy-5-methylphenyl]-1-butanone, 340
[1957-52-4]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 621
[1957-56-8]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-butanone, 20
[1960-58-3]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-hexanone, 620
[1995-70-6]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 20
[1995-74-0]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 22
[2010-80-2]	Methyl 4-(2,4,5-trimethoxyphenyl)-3-methyl-4-oxo-1-butanoate, 418
[2015-80-7]	1-(2,5-Dihydroxy-4-methoxyphenyl)-1-butanone, 58
[2017-96-1]	1-[(2,5-Diphenylmethoxy)-4-methoxyphenyl]-1-butanone, 58
[2020-73-7]	1-(2,4,5-Trimethoxyphenyl)-1-butanone, 17
[2035-55-4]	1-(5-Hydroxy-2,3-diphenyl-6-benzofuranyl)-1,3-butanedione, 333
[2108-54-5]	1-(4-Methoxyphenyl)-1,4-pentanedione, 460
[2193-04-6]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-pentanone (2,4-Dinitrophenylhydrazone), 479
[2194-77-6]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-octanone (2,4-Dinitrophenylhydrazone), 785
[2250-71-7]	1-[5-Fluoro-3-(4-fluorobenzoyl)-2-hydroxyphenyl]-1-butanone, 386
[2262-19-3]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-octanone, 784
[2262-21-7]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-octanone, 785
[2289-11-4]	5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*;8*H*-pyrano [2,3-f]chromen-2-one, 243
[2289-30-7]	9,10-Dihydro-8,8-dimethyl-5-hydroxy-6-(3-methyl-1-oxobutyl)-4-phenyl-8*H*-pyrano-[2,3-*f*]chromen-2-one, 247
[2317-60-4]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-heptanone (2,4-Dinitrophenylhydrazone), 731

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[2341-98-2]	1-(5-Fluoro-2-hydroxyphenyl)-1-dodecanone (2,4-Dinitrophenylhydrazone), 956
[2342-47-4]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-heptanone, 731
[2342-49-6]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-heptanone, 732
[2350-46-1]	1-(2,3-Dichloro-4-hydroxyphenyl)-1-butanone, 23
[2414-79-1]	1-(3-Bromo-5-fluoro-2-hydroxyphenyl)-1-octanone (2,4-Dinitrophenylhydrazone), 785
[2437-61-8]	1-(2,3,4-Trihydroxyphenyl)-1-butanone, 15
[2437-62-9]	1-(2,4,6-Trihydroxyphenyl)-1-butanone, 18
[2525-01-1]	1-(3,4-Dihydroxyphenyl)-1-pentanone, 472
[2525-08-8]	1-(3,4-Dihydroxyphenyl)-1-heptanone, 727
[2525-88-4]	1,10-Bis(4-methoxyphenyl)-1,10-decanedione, 901
[2525-89-5]	1,9-Bis(4-methoxyphenyl)-1,9-nonanedione, 850
[2533-59-7]	1,10-Bis(4-hydroxyphenyl)-1,10-decanedione, 900
[2533-60-0]	1,9-Bis(4-hydroxyphenyl)-1,9-nonanedione (Di-2,4-dinitrophenyl-hydrazone), 850
[2533-61-1]	1,9-Bis(4-acetyloxyphenyl)-1,9-nonanedione, 850
[2533-62-2]	1,9-Bis(4-hydroxyphenyl)-1,9-nonanedione, 850
[2546-82-9]	1-(5-Fluoro-2-hydroxyphenyl)-1-decanone (2,4-Dinitrophenylhydrazone), 880
[2585-70-8]	1-(3-Chloro-5-fluoro-2-hydroxyphenyl)-1-butanone, 22
[2589-71-1]	1-(4-Hydroxyphenyl)-1-pentanone, 465
[2589-72-2]	1-(4-Hydroxyphenyl)-1-hexanone, 601
[2589-73-3]	1-(4-Hydroxyphenyl)-1-octanone, 774
[2589-74-4]	1-(4-Hydroxyphenyl)-1-dodecanone, 941
[2589-75-5]	1-(4-Hydroxyphenyl)-1-tetradecanone, 1004
[2589-76-6]	1-(4-Hydroxyphenyl)-1-hexadecanone, 1032
[2589-77-7]	1-(4-Hydroxyphenyl)-1-octadecanone, 1063
[2589-83-5]	1-(2-Hydroxyphenyl)-1-dodecanone, 939
[2589-84-6]	1-(2-Hydroxyphenyl)-1-hexadecanone, 1031
[2589-85-7]	1-(2-Hydroxyphenyl)-1-octadecanone, 1062
[2619-46-7]	1,10-Bis(4-acetyloxyphenyl)-1,10-decanedione, 901
[2630-99-1]	1,10-Bis(4-hydroxyphenyl)-1,10-decanedione (Di-2,4-dinitrophenyl-hydrazone), 900
[2728-92-9]	1-(5-Fluoro-2-hydroxyphenyl)-1-octanone (2,4-Dinitrophenylhydrazone), 788
[2754-54-3]	1-(3,4-Dihydroxyphenyl)-1-decanone, 874
[2887-61-8]	1-(2-Hydroxyphenyl)-1-butanone, 1
[2904-87-2]	1-(3,5-Dibromo-4-hydroxyphenyl)-1-butanone, 22
[2954-68-9]	Ethyl 4-(4-methoxy-3-methylphenyl)-4-oxo-1-butanoate, 436
[2999-10-2]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-3-methyl-1-butanone, 303
[2999-11-3]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-decanone, 914
[2999-12-4]	1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-nonanone, 863
[2999-14-6]	4-Methyl-1-(2,4,6-trihydroxyphenyl)-1-pentanone, 546
[2999-16-8]	1,1′-(5-Bromo-2,4,6-trihydroxy-1,3-phenylene)bis-1-butanone, 297

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[2999-17-9]	1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-4-methyl-1-pentanone, 552
[2999-18-0]	1-(2,4,6-Trihydroxyphenyl)-1-pentanone, 476
[2999-21-5]	1,1′-(4,6-Dihydroxy-1,3-phenylene)bis-1-butanone, 298
[2999-22-6]	1,1′-(2,4-Dihydroxy-1,3-phenylene)bis-1-butanone, 298
[2999-37-3]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-butanone, 75
[3088-14-0]	1,10-Bis(2,4-dihydroxyphenyl)-1,10-decanedione, 901
[3098-40-6]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-butanone, 298
[3118-32-9]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-pentanone, 512
[3118-33-0]	1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-pentanone, 526
[3118-34-1]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-hexanone, 681
[3118-36-3]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-heptanone, 759
[3118-37-4]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-4-methyl-1-pentanone, 551
[3118-38-5]	1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-hexanone, 684
[3118-39-6]	1,1-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-heptanone, 762
[3118-42-1]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-nonanone, 862
[3118-45-4]	1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-octanone, 824
[3118-46-5]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-octanone, 821
[3136-48-9]	1,1′-(5-Bromo-2,4,6-trihydroxy-1,3-phenylene)bis-1-pentanone, 510
[3144-54-5]	1-(2,4-Dihydroxyphenyl)-1-hexanone, 606
[3153-44-4]	4-(4-Methoxyphenyl)-4-oxo-1-butanoic acid, 400
[3226-15-1]	1-(2-Hydroxyphenyl)-1-hexanone, 598
[3226-16-2]	1-(5-Chloro-2-hydroxyphenyl)-1-hexanone, 625
[3226-17-3]	1-(3-Chloro-2-hydroxyphenyl)-1-hexanone, 624
[3226-18-4]	1-(3,5-Dichloro-2-hydroxyphenyl)-1-hexanone, 621
[3226-27-5]	1-(2-Hydroxyphenyl)-1-octanone, 772
[3226-35-5]	1-(3-Chloro-4-hydroxyphenyl)-1-hexanone, 624
[3307-03-7]	1-(4,5-Dimethoxy-2-methylphenyl)-1-butanone, 72
[3307-04-8]	1-(4,5-Dimethoxy-2-methylphenyl)-1-hexanone, 642
[3307-23-1]	1-(4,5-Dimethoxy-2-methylphenyl)-1-hexanone (Phenylhydrazone), 642
[3329-02-0]	1-(3,4,5-Trihydroxyphenyl)-1-butanone, 19
[3567-96-2]	3-Methyl-1-(2,4,6-trimethoxy-3,5-dimethylphenyl)-1-butanone, 200
[3728-78-7]	Methyl 4-(3-ethyl-4-methoxyphenyl)-4-oxo-1-butanoate, 443
[3728-79-8]	4-(3-Ethyl-4-methoxyphenyl)-4-oxo-1-butanoic acid, 442
[3773-25-9]	3,5-Dihydroxy-4,4-dimethyl-2-(1-oxopropyl)-6-[[2,4,6-trihydroxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,5-cyclohexadien-1-one, 337
[3781-76-8]	1-(5-Ethyl-2-methoxyphenyl)-1-butanone, 66
[3787-68-6]	1-(4,5-Dimethoxy-2-methylphenyl)-1-hexanone (Semicarbazone), 642
[4009-78-3]	1-(3,4-Dihydroxyphenyl)-1-hexanone, 609
[4023-80-7]	1-(4-Methoxyphenyl)-1,3-butanedione, 311
[4069-47-0]	1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-1-butanone, 84
[4069-49-2]	1,1′-[Methylenebis(2,4,6-trihydroxy-5-methyl-3,1-phenylene)]bis-1-butanone, 338
[4070-68-2]	1-(2-Chloro-4-methoxyphenyl)-1-butanone, 29
[4070-69-3]	1-(4-Chloro-2-methoxyphenyl)-1-butanone, 30

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[4091-11-6]	2-Bromo-1-(2,3-dichloro-4-hydroxyphenyl)-2-ethyl-1-butanone, 293
[4101-16-0]	1-(3,4-Dimethoxyphenyl)-4-methyl-1-pentanone, 544
[4115-00-8]	1-(2,3-Dichloro-4-hydroxyphenyl)-2-methylene-1-butanone, 131
[4115-02-0]	1-(2 Chloro-4-hydroxyphenyl)-2-methylene-1-butanone, 132
[4133-95-3]	1-(4-Chloro-2-hydroxyphenyl)-1-butanone, 30
[4139-74-6]	4-Hydroxy-3-(1-oxobutyl)-2*H*-1-benzopyran-2-one, 78
[4139-75-7]	4-Hydroxy-3-(3-methyl 1-oxobutyl)-2*H*-1-benzopyran-2-one, 202
[4160-51-4]	1-(4-Methoxyphenyl)-1-butanone, 6
[4196-61-6]	1-(6-Hydroxy-2,3-dimethyl-5-benzofuranyl)-1,3-butanedione, 329
[4280-49-3]	1,6-Bis(4-methoxyphenyl)-1,6-hexanedione, 673
[4280-50-6]	1,8-Bis(4-methoxyphenyl)-1,8-octanedione, 811
[4280-52-8]	1,12-Bis(4-methoxyphenyl)-1,12-dodecanedione, 977
[4349-54-6]	1-(7-Hydroxy-2,3-dimethyl-6-benzofuranyl)-1,3-butanedione, 329
[4374-24-7]	1-(3-Fluoro-4-methoxyphenyl)-3-methyl-1-butanone, 186
[4374-92-9]	1-[2,4,6-Trihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone, 152
[4374-93-0]	3-Methyl-1-[2,4,6-trihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-1-butanone, 231
[4378-55-6]	5-(3,4-Dimethoxyphenyl)-5-oxo-1-pentanoic acid, 582
[4390-92-5]	1-(2,4-Dihydroxyphenyl)-1-butanone, 9
[4390-93-6]	1-(2,6-Dihydroxy-4-methylphenyl)-1-butanone, 54
[4440-92-0]	1,4-Bis(3,4-dimethoxyphenyl)-2,3-dimethyl-1,4-butanedione, 367
[4592-82-9]	5-(4-Hydroxy-3-methylphenyl)-5-oxo-1-pentanoic acid, 592
[4592-83-0]	1,5-Bis(4-hydroxy-3-methylphenyl)-1,5-pentanedione, 532
[4592-84-1]	1,5-Bis(4-hydroxy-2-methylphenyl)-1,5-pentanedione (Dioxime), 532
[4605-98-5]	Ethyl 4-(4-methoxy-3-methylphenyl)-4-oxo-1-butanoate (Semicarbazone), 437
[4609-06-7]	5-(5-Chloro-2-hydroxy-4-methylphenyl)-5-oxo-1-pentanoic acid, 590
[4609-08-9]	1,5-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,5-pentanedione, 530
[4609-09-0]	1,5-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,5-pentanedione (Dioxime), 530
[4609-10-3]	5-(4-Methoxyphenyl)-5-oxo-1-pentanoic acid, 579
[4609-11-4]	1,5-Bis(4-methoxyphenyl)-1,5-pentanedione, 518
[4626-83-9]	5-(4-Methoxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 579
[4642-26-6]	1,5-Bis(4-hydroxy-3-methylphenyl)-1,5-pentanedione (Dioxime), 533
[4642-27-7]	5-(2-Hydroxy-3-methylphenyl)-5-oxo-1-pentanoic acid, 590
[4642-28-8]	5-(2-Hydroxy-3-methylphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 591
[4642-30-2]	5-(4-Methoxy-3-methylphenyl)-5-oxo-1-pentanoic acid, 592
[4642-31-3]	1,5-Bis(4-methoxy-3-methylphenyl)-1,5-pentanedione, 533
[4642-32-4]	5-(4-Hydroxy-2-methylphenyl)-5-oxo-1-pentanoic acid, 592
[4642-33-5]	5-(4-Hydroxy-2-methylphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 592
[4642-34-6]	1,5-Bis(4-hydroxy-2-methylphenyl)-1,5-pentanedione, 532
[4642-35-7]	5-(2-Hydroxy-4-methylphenyl)-5-oxo-1-pentanoic acid, 591

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[4642-36-8]	5-(2-Hydroxy-4-methylphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 591
[4642-37-9]	5-(4-Methoxy-2-methylphenyl)-5-oxo-1-pentanoic acid, 592
[4642-38-0]	1,5-Bis(4-methoxy-2-methylphenyl)-1,5-pentanedione, 532
[4642-40-4]	1,5-Bis(2-hydroxy-4-methoxyphenyl)-1,5-pentanedione, 534
[4642-41-5]	5-(2-Hydroxy-4-methoxyphenyl)-5-oxo-1-pentanoic acid, 593
[4642-42-6]	5-(2-Hydroxy-4-methoxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 594
[4642-43-7]	5-(2,4-Dihydroxyphenyl)-5-oxo-1-pentanoic acid, 580
[4642-44-8]	5-(2,4-Dihydroxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 581
[4648-94-6]	5-(4-Hydroxyphenyl)-5-oxo-1-pentanoic acid, 578
[4648-95-7]	5-(4-Hydroxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 579
[4648-96-8]	5-(4-Acetyloxyphenyl)-5-oxo-1-pentanoic acid, 579
[4648-97-9]	5-(2-Hydroxyphenyl)-5-oxo-1-pentanoic acid, 577
[4648-98-0]	5-(2-Hydroxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 578
[4649-01-8]	5-(2-Hydroxy-5-methylphenyl)-5-oxo-1-pentanoic acid, 591
[4649-02-9]	5-(2-Hydroxy-5-methylphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 592
[4649-03-0]	1,5-Bis(2-hydroxy-5-methylphenyl)-1,5-pentanedione, 531
[4649-04-1]	1,5-Bis(2-hydroxy-5-methylphenyl)-1,5-pentanedione (Dioxime), 532
[4650-71-9]	1,4-Bis(3,4-dimethoxyphenyl)-1,4-butanedione, 363
[4654-07-3]	5-(2,4-Dimethoxyphenyl)-5-oxo-1-pentanoic acid, 581
[4680-89-1]	5-(4-Hydroxy-3-methylphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 592
[4693-16-7]	1-(2,5-Dihydroxyphenyl)-1-butanone, 11
[4693-17-8]	1-(2,5-Dihydroxyphenyl)-1-pentanone, 471
[4693-18-9]	1-(2,5-Dihydroxyphenyl)-1-hexanone, 608
[4693-19-0]	1-(2,5-Dihydroxyphenyl)-1-octanone, 780
[4693-29-2]	1-(2,5-Dihydroxyphenyl)-1-octadecanone, 1066
[4693-30-5]	1-(2,5-Dihydroxyphenyl)-1-dodecanone, 946
[4714-77-6]	1,5-Bis(2-hydroxy-4-methoxyphenyl)-1,5-pentanedione (Dioxime), 534
[4798-10-1]	1-(3-Chloro-4-hydroxy-2-methylphenyl)-2-ethyl-1-butanone, 172
[4798-12-3]	1-(3-Chloro-4-hydroxyphenyl)-2-propyl-1-pentanone, 560
[4804-56-2]	1-(2-Chloro-4-hydroxyphenyl)-2-ethyl-1-butanone, 171
[4807-43-6]	1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-decanone, 915
[4808-89-3]	1-(4-Methoxyphenyl)-1,3,5-hexanetrione, 595
[4848-01-5]	Methyl 4-(2-amino-4,5-dimethoxyphenyl)-4-oxo-1-butanoate, 429
[4878-81-3]	4-(4-Methoxy-7-benzo[*b*]thiophene)-4-oxo-1-butanoic acid, 441
[4890-45-3]	4-(2,4,6-Trihydroxyphenyl)-4-oxo-1-butanoic acid, 413
[4945-79-3]	1,5-Bis(2-hydroxyphenyl)-1,5-pentanedione, 517
[4963-67-1]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-pentanone (Piperazine salt), 513
[5022-20-8]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one (Racemic), 153

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[5022-22-0]	5,7-Dihydroxy-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 143
[5022-23-1]	5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 143
[5085-54-1]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 120
[5085-55-2]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one, 158
[5224-54-4]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 245
[5259-08-5]	1-(3,5-Dimethoxyphenyl)-1-tridecanone, 998
[5310-91-8]	1-(4-Hydroxy-2-methylphenyl)-3-methyl-2-(1-methylethyl)-1-butanone, 209
[5333-29-9]	1-(3,5-Dimethoxyphenyl)-1-pentanone, 474
[5333-34-6]	4-(3,4-Dimethoxyphenyl)-4-oxo-1-butanoic acid, 408
[5340-05-6]	1-(2-Methoxy-5-methylphenyl)-1-butanone, 50
[5377-72-0]	1,1′-[Methylenebis(2,6-dihydroxy-4-methoxy-5-methyl-3,1-phenylene)] bis-1-butanone, 342
[5394-88-7]	1-(4-Methoxy-3-methylphenyl)-1-pentanone, 494
[5408-44-6]	1-(3,5-Dibromo-4-hydroxyphenyl)-1-pentanone, 478
[5447-74-5]	Methyl 4-(4-methoxyphenyl)-4-oxo-1-butanoate, 401
[5485-73-4]	6-(4-Hydroxyphenyl)-6-oxo-1-hexanoic acid (2,4-Dinitrophenylhydrazone), 710
[5485-77-8]	6-(4-Methoxy-3-methylphenyl)-6-oxo-1-hexanoic acid, 717
[5537-75-7]	6-(4-Hydroxyphenyl)-6-oxo-1-hexanoic acid, 710
[5537-76-8]	6-(4-Methoxyphenyl)-6-oxo-1-hexanoic acid, 711
[5538-07-8]	6-(4-Hydroxy-3-methylphenyl)-6-oxo-1-hexanoic acid, 716
[5538-08-9]	1,6-Bis(4-hydroxy-3-methylphenyl)-1,6-hexanedione (Dioxime), 686
[5538-09-0]	6-(4-Methoxy-3-methylphenyl)-6-oxo-1-hexanoic acid (2,4-Dinitrophenylhydrazone), 717
[5538-10-3]	1,6-Bis(4-methoxy-3-methylphenyl)-1,6-hexanedione, 686
[5538-11-4]	6-(4-Hydroxy-2-methylphenyl)-6-oxo-1-hexanoic acid, 716
[5538-12-5]	6-(4-Hydroxy-2-methylphenyl)-6-oxo-1-hexanoic acid (2,4-Dinitrophenylhydrazone), 716
[5538-13-6]	1,6-Bis(4-hydroxy-2-methylphenyl)-1,6-hexanedione (Dioxime), 686
[5538-14-7]	6-(4-Methoxy-2-methylphenyl)-6-oxo-1-hexanoic acid, 716
[5538-16-9]	1,6-Bis(4-methoxy-2-methylphenyl)-1,6-hexanedione (Oxime), 686
[5550-52-7]	6-(4-Hydroxy-3-methylphenyl)-6-oxo-1-hexanoic acid (2,4-Dinitrophenylhydrazone), 716
[5550-53-8]	1,6-Bis(4-methoxy-3-methylphenyl)-1,6-hexanedione (Dioxime), 686
[5550-54-9]	1,6-Bis(4-hydroxy-2-methylphenyl)-1,6-hexanedione, 685
[5550-55-0]	6-(4-Methoxy-2-methylphenyl)-6-oxo-1-hexanoic acid (2,4-Dinitrophenylhydrazone), 716
[5550-56-1]	1,6-Bis(4-methoxy-2-methylphenyl)-1,6-hexanedione, 686
[5590-61-4]	1-(2-Chloro-4-hydroxyphenyl)-2-ethyl-3-methyl-1-butanone, 196
[5665-89-4]	1-(2,4,6-Trihydroxyphenyl)-1-hexanone, 612

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[5673-08-5]	1-(2,6-Dimethoxyphenyl)-1-hexanone, 609
[5717-16-8]	4-(4-Methoxyphenyl)-2-methyl-4-oxo-1-butanoic acid, 415
[5862-05-5]	1-(4-Hydroxy-2,3-dimethylphenyl)-1-butanone, 68
[5862-11-3]	1-(2,6-Dichloro-3-methoxyphenyl)-1-butanone, 24
[5862-26-0]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-pentanone (Tri-Na salt), 513
[6016-44-0]	1,6-Bis(4-hydroxy-3-methylphenyl)-1,6-hexanedione, 686
[6048-89-1]	1-(2,4,6-Trihydroxyphenyl)-1-decanone, 875
[6268-56-0]	1,6-Bis(3,4-dimethylenedioxyphenyl)-1,6-hexanedione, 676
[6324-54-5]	7-Hydroxy-4-methyl-8-(1-oxopentyl)-2*H*-1-benzopyran-2-one, 506
[6345-66-0]	1-(3,4,5-Trihydroxyphenyl)-1-hexanone, 614
[6397-82-6]	1-(4-Methoxyphenyl)-1-hexanone, 603
[6565-75-9]	1-(2,4-Dimethoxyphenyl)-1-octanone, 779
[6575-51-5]	4-(4,5-Dimethoxy-2-methylphenyl)-4-oxo-1-butanoic acid, 438
[6703-00-0]	1-(2,4-Dimethoxyphenyl)-1-butanone, 10
[6790-21-2]	1-(2,4,6-Trihydroxyphenyl)-1-dodecanone, 951
[6916-62-7]	5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 160
[7058-70-0]	5,7-dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 160
[7150-55-2]	4-Chloro-1-(4-hydroxyphenyl)-1-butanone, 279
[7282-05-5]	1-(2-Hydroxy-4,6-dimethylphenyl)-1-dodecanone, 964
[7337-50-0]	1-(2,5-Dihydroxyphenyl)-1-decanone, 873
[7356-03-8]	4-(2-Hydroxy-3,5-dimethylphenyl)-4-oxo-1-butanoic acid, 443
[7573-11-7]	1-(2,3-Dihydroxyphenyl)-1-decanone, 872
[7640-25-7]	1,9-Bis(2,4-dihydroxyphenyl)-1,9-nonanedione, 851
[7658-30-2]	1,7-Bis(2,4-dihydroxyphenyl)-1,7-heptanedione, 754
[10121-26-3]	1-(2,6-Dihydroxyphenyl)-1-butanone, 12
[10262-13-2]	1-(4-Methoxyphenyl)-1,2-butanedione (Dioxime), 307
[10201-46-4]	1-(4-Methoxyphenyl)-1,2-butanedione, 307
[10351-89-0]	1,4-Bis(2-hydroxy-3,4-dimethoxylphenyl)-1,4-butanedione, 371
[10351-90-3]	1,6-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,6-hexanedione, 691
[10351-91-4]	1,7-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,7-heptanedione, 763
[10351-92-5]	1,8-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,8-octanedione, 825
[10351-93-6]	1,10-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,10-decanedione, 913
[10365-10-3]	1,10-Bis(2,5-dimethoxyphenyl)-1,10-decanedione, 902
[10365-21-6]	1,4-Bis(2,5-dimethoxyphenyl)-1,4-butanedione, 362
[10365-22-7]	1,5-Bis(2,5-dimethoxyphenyl)-1,5-pentanedione, 520
[10365-23-8]	1,6-Bis(2,5-dimethoxyphenyl)-1,6-hexanedione, 675
[10365-24-9]	1,7-Bis(2,5-dimethoxyphenyl)-1,7-heptanedione, 755
[10365-25-0]	1,9-Bis(2,5-dimethoxyphenyl)-1,9-nonanedione, 851
[10365-28-3]	1,6-Bis(2-hydroxy-5-methoxyphenyl)-1,6-hexanedione, 687
[10365-29-4]	1,7-Bis(2-hydroxy-5-methoxyphenyl)-1,7-heptanedione, 761
[10365-30-7]	1,9-Bis(2-hydroxy-5-methoxyphenyl)-1,9-nonanedione, 861
[10365-31-8]	1,10-Bis(2-hydroxy-5-methoxyphenyl)-1,10-decanedione, 910
[10365-32-9]	1,5-Bis(2-acetyloxy-5-methoxyphenyl)-1,5-pentanedione, 534

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[10365-33-0]	1,6-Bis(2-acetyloxy-5-methoxyphenyl)-1,6-hexanedione, 687
[10365-34-1]	1,7-Bis(2-acetyloxy-5-methoxyphenyl)-1,7-heptanedione, 761
[10365-35-2]	1,8-Bis(2-acetyloxy-5-methoxyphenyl)-1,8-octanedione, 820
[10365-36-3]	1,9-Bis(2-acetyloxy-5-methoxyphenyl)-1,9-nonanedione, 861
[10365-37-4]	1,10-Bis(2-acetyloxy-5-methoxyphenyl)-1,10-decanedione, 910
[10365-53-4]	1,5-Bis(3-hydroxyphenyl)-1,5-pentanedione, 517
[10365-54-5]	1,7-Bis(3-hydroxyphenyl)-1,7-heptanedione, 754
[10365-55-6]	1,10-Bis(3-hydroxyphenyl)-1,10-decanedione, 900
[10365-60-3]	1,7-Bis(4-methoxyphenyl)-1,7-heptanedione, 754
[10365-65-8]	1,5-Bis(2-hydroxy-3-methylphenyl)-1,5-pentanedione, 531
[10365-66-9]	1,7-Bis(2-hydroxy-3-methylphenyl)-1,7-heptanedione, 760
[10365-74-9]	1,5-Bis(2-hydroxy-5-methoxyphenyl)-1,5-pentanedione, 534
[10373-31-6]	1,6-Bis(2,3,4-trimethoxyphenyl)-1,6-hexanedione, 677
[10373-32-7]	1,8-Bis(2,3,4-trimethoxyphenyl)-1,8-octanedione, 813
[10373-33-8]	1,10-Bis(2,3,4-trimethoxyphenyl)-1,10-decanedione, 904
[10388-38-2]	1,4-Bis(2,3,4-trimethoxyphenyl)-1,4-butanedione, 363
[10388-39-3]	1,4-Bis(2,3,4-trimethoxyphenyl)-1,4-butanedione (2,4-Dinitrophenylhydrazone), 364
[10400-43-8]	1,10-Bis(2-hydroxy-4-methylphenyl)-1,10-decanedione, 907
[10400-49-4]	1,5-Bis(2-methoxy-5-methylphenyl)-1,5-pentanedione, 532
[10400-50-7]	1,7-Bis(2-methoxy-5-methylphenyl)-1,7-heptanedione, 761
[10400-51-8]	1,10-Bis(2-methoxy-5-methylphenyl)-1,10-decanedione, 908
[10400-56-3]	1,10-Bis-(5-chloro-2-methoxyphenyl)-1,10-decanedione, 899
[10401-04-4]	1,7-Bis(2-hydroxyphenyl)-1,7-heptanedione, 753
[10401-05-5]	1,10-Bis(2-hydroxyphenyl)-1,10-decanedione, 900
[10475-16-8]	1,5-Bis(2,3,4-trimethoxyphenyl)-1,5-pentanedione, 522
[10475-17-9]	1,7-Bis(2,3,4-trimethoxyphenyl)-1,7-heptanedione, 756
[10475-18-0]	1,9-Bis(2,3,4-trimethoxyphenyl)-1,9-nonanedione, 852
[10483-67-7]	1,5-Bis(2-hydroxy-3,4-dimethoxylphenyl)-1,5-pentanedione, 536
[10483-68-8]	1,9-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,9-nonanedione, 862
[10483-69-9]	1,10-Bis(2-hydroxy-3-methylphenyl)-1,10-decanedione, 907
[10491-14-2]	1,8-Bis(2,5-dimethoxyphenyl)-1,8-octanedione, 820
[10491-15-3]	1,8-Bis(2-hydroxy-5-methoxyphenyl)-1,8-octanedione, 820
[10571-10-5]	1,5-Bis(2-hydroxy-4-methylphenyl)-1,5-pentanedione, 531
[10586-43-3]	1-(3,5-Dimethoxyphenyl)-2-methyl-1-heptanone, 730
[13149-43-4]	11-Bromo-1-(4-hydroxy-3-methoxyphenyl)-1-undecanone, 936
[13149-44-5]	11-Bromo-1-(4-allyloxy-3-methoxyphenyl)-1-undecanone, 936
[13149-48-9]	17-Bromo-1-(4-hydroxy-3-methoxyphenyl)-1-heptadecanone, 1060
[13149-49-0]	17-Bromo-1-(4-allyloxy-3-methoxyphenyl)-1-heptadecanone, 1060
[13178-17-1]	1,10-Bis(2,3,4-trihydroxyphenyl)-1,10-decanedione, 903
[13178-43-3]	1,10-Bis(4-hydroxy-3-methylphenyl)-1,10-decanedione, 909
[13210-98-5]	1-(4-Acetyloxyphenyl)-1-butanone, 5
[13221-24-4]	1,7-Bis(2-hydroxy-4-methylphenyl)-1,7-heptanedione, 760
[13282-23-0]	1,4-Bis(2-hydroxy-5-methylphenyl)-1,4-butanedione, 366
[13282-24-1]	1,6-Bis(2-hydroxy-5-methylphenyl)-1,6-hexanedione, 685

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[14814-73-4]	1-(5-Benzoyl-2,4-dihydroxyphenyl)-1-dodecanone, 981
[15041-68-6]	1,1′-(5-Benzoyl-2,4-dihydroxy-1,3-phenylene)bis-1-dodecanone, 992
[15116-03-7]	1-(2,3-Dimethoxyphenyl)-3-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 177
[15116-04-8]	1-(2,3-Dimethoxyphenyl)-2-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 127
[15116-05-9]	1-(2,3-Dimethoxyphenyl)-1-pentanone (2,4-Dinitrophenylhydrazone), 470
[15116-06-0]	1-(2-Hydroxy-3-methoxyphenyl)-3-methyl-1-butanone, 192
[15116-07-1]	1-(2-Hydroxy-3-methoxyphenyl)-2-methyl-1-butanone, 134
[15116-08-2]	1-(2-Hydroxy-3-methoxyphenyl)-1-pentanone, 496
[15116-13-9]	1-(2,4-Dihydroxyphenyl)-1-pentanone, 470
[15116-14-0]	1-(2,4-Dihydroxyphenyl)-3-methyl-1-butanone, 177
[15116-15-1]	1-(2,4-Dihydroxyphenyl)-2-methyl-1-butanone, 127
[15118-48-6]	4-(4-Methoxyphenyl)-2,2-dimethyl-4-oxo-1-butanoic acid, 418
[15118-67-9]	Ethyl 4-(4-methoxyphenyl)-4-oxo-1-butanoate, 401
[15118-68-0]	Ethyl 4-(4-methoxyphenyl)-2-methyl-4-oxo-1-butanoate, 415
[15118-69-1]	Methyl 4-(4-methoxyphenyl)-2,2-dimethyl-4-oxo-1-butanoate, 419
[15121-98-9]	1-(2,3-Dimethoxyphenyl)-3-methyl-1-butanone, 177
[15121-99-0]	1-(2,3-Dimethoxyphenyl)-2-methyl-1-butanone, 127
[15122-00-6]	1-(2,3-Dimethoxyphenyl)-1-pentanone, 470
[15191-69-2]	1-(2-Methoxyphenyl)-4,4,4-trifluoro-1,3-butanedione, 308
[15251-74-8]	1-(2,3,4-Trihydroxyphenyl)-1-dodecanone, 950
[15572-01-7]	4-(4-Chloro-2-hydroxyphenyl)-4-oxo-1-butanoic acid, 423
[15572-02-8]	4-(4-Chloro-2-methoxyphenyl)-4-oxo-1-butanoic acid, 423
[15572-03-9]	4-(2-Chloro-4-methoxyphenyl)-4-oxo-1-butanoic acid, 422
[15572-05-1]	Methyl 4-(5-chloro-2-methoxyphenyl)-4-oxo-1-butanoate, 424
[15572-06-2]	4-(3-Chloro-2-hydroxyphenyl)-4-oxo-1-butanoic acid, 422
[15982-64-6]	1,4-Bis(4-methoxyphenyl)-1,4-butanedione, 360
[16093-14-4]	5-(5-Bromo-2,4-dihydroxyphenyl)-5-oxo-1-pentanoic acid, 586
[16093-15-5]	1,5-Bis(2,4,6-trihydroxyphenyl)-1,5-pentanedione (Di-2,4-Dinitrophenylhydrazone), 522
[16093-16-6]	5-(2,3,4-Trimethoxyphenyl)-5-oxo-1-pentanoic acid, 582
[16093-17-7]	5-(2,3,4-Trimethoxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 583
[16093-18-8]	5-(5-Chloro-2,4-dihydroxyphenyl)-5-oxo-1-pentanoic acid, 588
[16093-19-9]	5-(5-Chloro-2,4-dihydroxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 588
[16093-22-4]	1,5-Bis(2,4-dihydroxyphenyl)-1,5-pentanedione, 520
[16093-23-5]	1,5-Bis(2,4-dihydroxyphenyl)-1,5-pentanedione (Dioxime), 520
[16093-26-8]	1,5-Bis(5-chloro-2,4-dihydroxypheny)l-1,5-pentanedione, 516
[16093-27-9]	1,5-Bis(5-chloro-2,4-dihydroxypheny)l-1,5-pentanedione (Dioxime), 516
[16093-28-0]	1,5-Bis(5-chloro-2,4-dimethoxypheny)l-1,5-pentanedione, 516
[16093-29-1]	1,5-Bis(5-chloro-2,4-dimethoxypheny)l-1,5-pentanedione (Dioxime), 516
[16093-30-4]	5-(5-Chloro-2,4-dimethoxyphenyl)-5-oxo-1-pentanoic acid, 588

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[16093-31-5]	5-(5-Chloro-2,4-dimethoxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 588
[16093-32-6]	1,5-Bis(5-bromo-2,4-dihydroxyphenyl)-1,5-pentanedione, 515
[16093-33-7]	1,5-Bis(5-bromo-2,4-dihydroxyphenyl)-1,5-pentanedione (Di-2,4-Dinitrophenylhydrazone), 515
[16093-34-8]	1,5-Bis(5-bromo-2,4-dimethoxyphenyl)-1,5-pentanedione, 516
[16093-35-9]	1,5-Bis(5-bromo-2,4-dimethoxyphenyl)-1,5-pentanedione (Dioxime), 516
[16093-36-0]	5-(5-Bromo-2,4-dimethoxyphenyl)-5-oxo-1-pentanoic acid, 586
[16093-37-1]	5-(5-Bromo-2,4-dimethoxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 586
[16093-39-3]	5-(2,4-Dihydroxy-6-methylphenyl)-5-oxo-1-pentanoic acid, 593
[16093-40-6]	5-(2,4-Dihydroxy-6-methylphenyl)-5-oxo-1-pentanoic acid (Oxime), 593
[16093-41-7]	5-(2,4-Dimethoxy-6-methylphenyl)-5-oxo-1-pentanoic acid, 593
[16093-42-8]	5-(2,4-Dimethoxy-6-methylphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 593
[16093-43-9]	5-(5-Chloro-2,4-dihydroxy-6-methylphenyl)-5-oxo-1-pentanoic acid, 590
[16093-44-0]	5-(5-Chloro-2,4-dihydroxy-6-methylphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 590
[16093-45-1]	5-(5-Bromo-2,4-dihydroxy-6-methylphenyl)-5-oxo-1-pentanoic acid, 589
[16093-46-2]	5-(5-Bromo-2,4-dihydroxy-6-methylphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 590
[16093-47-3]	5-(5-Bromo-2,4-dimethoxy-6-methylphenyl)-5-oxo-1-pentanoic acid, 590
[16093-48-4]	1,5-Bis(2,4,6-trihydroxyphenyl)-1,5-pentanedione, 522
[16093-49-5]	1,5-Bis(5-chloro-2,4-dimethoxy-6-methylpheny)l-1,5-pentanedione (Di-2,4-Dinitrophenylhydrazone), 530
[16093-59-7]	5-(5-Bromo-2,4-dihydroxyphenyl)-5-oxo-1-pentanoic acid (2,4-Dinitrophenylhydrazone), 586
[16117-33-2]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-(1-methylpropyl)-2*H*-1-benzopyran-2-one, 156
[16148-67-7]	1,5-Bis(2-hydroxy-3,4-dimethoxylphenyl)-1,5-pentanedione (Dioxime), 536
[16148-68-8]	1,5-Bis(5-chloro-2,4-dimethoxy-6-methylpheny)l-1,5-pentanedione, 530
[16148-93-9]	1,5-Bis(3,4-dimethoxyphenyl)-1,5-pentanedione (Di-2,4-Dinitrophenylhydrazone), 521
[16197-54-9]	1,4-Bis(5-chloro-2-hydroxyphenyl)-1,4-butanedione, 356
[16197-55-0]	1,4-Bis(5-chloro-2-hydroxyphenyl)-1,4-butanedione (Di-2,4-dinitrophenylhydrazone), 356
[16197-56-1]	1,4-Bis(2-hydroxy-5-methylphenyl)-1,4-butanedione (Di-2,4-dinitrophenylhydrazone), 366
[16197-57-2]	1,4-Bis(2-hydroxy-5-methylphenyl)-1,4-butanedione (Dioxime), 366
[16197-58-3]	1,4-Bis(5-bromo-2-hydroxyphenyl)-1,4-butanedione, 356
[16197-59-4]	1,4-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,4-butanedione, 365
[16197-60-7]	1,4-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,4-butanedione (Di-2,4-dinitrophenylhydrazone), 365
[16197-61-8]	1,4-Bis(3-chloro-6-hydroxy-2,4-dimethylphenyl)-1,4-butanedione, 369
[16197-62-9]	1,4-Bis(3-chloro-6-hydroxy-2,4-dimethylphenyl)-1,4-butanedione (Di-2,4-dinitrophenylhydrazone), 369
[16197-64-1]	1,4-Bis(5-chloro-2-hydroxyphenyl)-1,4-butanedione (Dioxime), 356

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[16286-63-8]	1,4-Bis(5-bromo-2-hydroxyphenyl)-1,4-butanedione (Di-2,4-dinitrophenylhydrazone), 356
[16290-14-5]	1,4-Bis(2,4-dihydroxyphenyl)-1,4-butanedione, 361
[16290-15-6]	1,4-Bis(2,4-diacetyloxyphenyl)-1,4-butanedione, 361
[16290-17-8]	1,4-Bis(2,4-dihydroxyphenyl)-1,4-butanedione (Di-phenylhydrazone), 361
[16290-18-9]	1,4-Bis(2-hydroxy-4-methoxyphenyl)-1,4-butanedione, 368
[16290-20-3]	1,4-Bis(2,4-dimethoxyphenyl)-1,4-butanedione, 362
[16636-62-7]	1-(2-Hydroxyphenyl)-1,3-butanedione, 309
[16636-64-9]	1-(2-Hydroxy-5-methylphenyl)-1,3-butanedione, 317
[16648-70-7]	1-[4-Hydroxy-3-(1-methylpropyl)phenyl]-1-butanone, 92
[16850-80-9]	1-(2-Hydroxyphenyl)-1,4-pentanedione, 460
[16850-82-1]	1-(2-Hydroxyphenyl)-4-phenyl-1,3-butanedione, 354
[16850-97-8]	7-Methoxy-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (2,4-Dinitrophenylhydrazone), 203
[17055-14-0]	2-Bromo-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-butanone, 274
[17055-15-1]	2-Bromo-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-pentanone, 577
[17055-16-2]	2-Bromo-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-methyl-1-butanone, 295
[17103-73-0]	4-(3,5-Dimethoxyphenyl)-3-methyl-4-oxo-1-butanoic acid, 417
[17386-89-9]	1-(3,4-Dihydroxyphenyl)-1-butanone, 13
[17744-45-5]	1-(4-Hydroxyphenyl)-1-decanone (2,4-Dinitrophenylhydrazone), 870
[17744-53-5]	1-(2-Hydroxyphenyl)-1-pentanone (2,4-Dinitrophenylhydrazone), 462
[17744-54-6]	1-(2-Hydroxyphenyl)-1-octanone (2,4-Dinitrophenylhydrazone), 773
[17765-30-9]	1-(4-Hydroxyphenyl)-1-octanone (2,4-Dinitrophenylhydrazone), 775
[17766-59-5]	4-Chloro-1-(3,4,5-trimethoxyphenyl)-1-butanone, 283
[18110-28-6]	1-[2-(2,3-Epoxypropyloxy)phenyl]-1-decanone, 869
[18110-29-7]	1-[2-(2,3-Epoxypropyloxy)phenyl]-1-dodecanone, 940
[18110-30-0]	1-[4-(2,3-Epoxypropyloxy)phenyl]-1-dodecanone, 944
[18110-31-1]	1-[2-(2,3-Epoxypropyloxy)phenyl]-1-tetradecanone, 1004
[18110-32-2]	1-[4-(2,3-Epoxypropyloxy)phenyl]-1-tetradecanone, 1005
[18211-87-5]	1-[4-(2,3-Epoxypropyloxy)phenyl]-1-decanone, 872
[18211-88-6]	1-(4-Hydroxyphenyl)-1-hexadecanone (2,3-Epoxypropoxy ether), 1034
[18405-71-5]	1-(2-Hydroxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 599
[18430-91-6]	1-(2-Hydroxyphenyl)-1-pentanone, 462
[18483-64-2]	5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 245
[18787-32-1]	1-(2,5-Dihydroxyphenyl)-4-methyl-1-pentanone, 544
[18787-33-2]	1-(2,5-Dihydroxyphenyl)-1-heptanone, 726
[19019-21-7]	1-(2-Hydroxyphenyl)-3-methyl-1-butanone, 173
[19343-46-5]	1,6-Bis(2,4,6-trihydroxyphenyl)-1,6-hexanedione, 677
[19343-47-6]	1,6-Bis(2,4-dihydroxyphenyl)-1,6-hexanedione, 674
[19347-50-3]	1-(4-Ethoxy-2-hydroxyphenyl)-1-hexanone, 652
[19347-51-4]	1-(4-Butoxy-2-hydroxyphenyl)-1-hexanone, 666
[19347-52-5]	1-(4-Ethoxy-2-hydroxyphenyl)-1-hexadecanone, 1044
[19347-74-1]	6-Chloro-1-(3,4-dimethoxyphenyl)-1-hexanone, 701

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[19513-15-6]	1-[4-(2-Chloroallyloxy)-2-hydroxyphenyl]-1-tridecanone (Compound with nickel chloride, hexahydrate), 1000
[19809-98-4]	1-[5-Chloro-2-hydroxy-(4-undecanoyloxy)phenyl]-1-undecanone, 930
[19809-99-5]	1-(5-Chloro-2,4-dihydroxyphenyl)-1-undecanone, 929
[19810-00-5]	1-(5-Chloro-2,4-dihydroxyphenyl)-1-undecanone (2,4-Dinitrophenylhydrazone), 929
[19810-03-8]	1-[2-Hydroxy-(4-undecanoyloxy)phenyl]-1-undecanone, 926
[19810-04-9]	1-(2,4-Dihydroxyphenyl)-1-undecanone, 925
[19810-05-0]	1-(2,4-Dihydroxyphenyl)-1-undecanone (Di-3,5-dinitrobenzoate), 926
[20031-96-3]	4-Hydroxy-3-valeroylbenzoic acid, 489
[20035-78-3]	Methyl 4-hydroxy-3-valeroylbenzoate, 489
[20038-59-9]	1-(2,4-Dihydroxyphenyl)-5-phenyl-1-pentanone, 525
[20359-54-0]	1-(2-Methoxyphenyl)-1-pentanone, 463
[20359-55-1]	1-(3-Methoxyphenyl)-1-pentanone, 464
[20483-30-1]	Methyl 4-(2-methoxy-5-methylphenyl)-4-oxo-1-butanoate, 434
[20683-49-2]	1-(3,5-Dibromo-4-hydroxyphenyl)-1-hexanone, 620
[20683-50-5]	1-(3,5-Dibromo-4-hydroxyphenyl)-1-heptanone, 732
[20683-51-6]	1-(3,5-Dibromo-4-hydroxyphenyl)-1-octanone, 785
[20683-53-8]	1-(3,5-Dibromo-4-hydroxyphenyl)-1-decanone, 878
[20800-12-8]	1-[4-(N-Morpholinoethoxy)-2-hydroxyphenyl]-1-butanone (Hydrochloride), 109
[20800-24-2]	1-(2-Hydroxy-4-methoxyphenyl)-1-butanone, 54
[20803-52-5]	1-(4-Hydroxyphenyl)-1-dodecanone (Oxime), 942
[20803-53-6]	1-(2-Hydroxyphenyl)-1-dodecanone (Semicarbazone), 940
[20803-54-7]	1-(4-Hydroxyphenyl)-1-dodecanone (Semicarbazone), 942
[20803-93-4]	1-(2-Hydroxyphenyl)-1-dodecanone (Oxime), 940
[20825-28-9]	1-(4-Ethoxy-2-hydroxyphenyl)-1-decanone, 888
[20837-35-8]	1,5-Bis(4-hydroxyphenyl)-1,5-pentanedione, 518
[20837-37-0]	1,6-Bis(4-hydroxyphenyl)-1,6-hexanedione, 673
[20837-38-1]	1,7-Bis(4-hydroxyphenyl)-1,7-heptanedione, 754
[20869-99-2]	1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-3-methyl-1-butanone, 213
[20870-01-3]	1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-3-methyl-1-butanone, 213
[20924-70-3]	4-Hydroxy-3-(1-oxodecyl)-2*H*-1-benzopyran-2-one, 889
[20924-71-4]	4-Hydroxy-3-(1-oxotetradecyl)-2*H*-1-benzopyran-2-one, 1016
[21092-65-9]	1-[2-(N-Morpholinoethoxy)-4-methoxyphenyl]-1-butanone (Hydrochloride), 108
[21093-22-1]	1-(2,4-Dihydroxyphenyl)-1-octadecanone, 1065
[21182-57-0]	1-(2-Hydroxy-5-methoxyphenyl)-1-octanone, 796
[21182-58-1]	1-(2-Hydroxy-5-octanoyloxyphenyl)-1-octanone, 821
[21182-60-5]	1-(2-Hydroxy-5-methoxy-4-methylphenyl)-1-octanone, 802
[21182-61-6]	1-(2,5-Dihydroxy-4-methylphenyl)-1-octanone, 795
[21182-64-9]	1-(2,5-Dihydroxy-4-methylphenyl)-1-hexadecanone, 1042
[21182-66-1]	1-(2-Hydroxy-5-methoxy-4-octylphenyl)-1-octanone, 825

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[21185-39-7]	1-(2,4-Dihydroxy-6-methoxyphenyl)-1-butanone, 57
[21390-01-2]	1,14-Bis(3,5-dimethoxyphenyl)-1,14-tetradecanedione, 1020
[21390-11-4]	1,14-Bis(3,5-dimethoxy-4-methylphenyl)-1,14-tetradecanedione, 1021
[21550-01-6]	1-(4-Methoxyphenyl)-4-methyl-1-pentanone, 542
[21550-06-1]	1-(3-Methoxyphenyl)-1-butanone, 3
[21550-10-7]	1-(2-Acetyloxyphenyl)-1-butanone, 2
[21667-43-6]	1-(2-Hydroxyphenyl)-1-butanone (Oxime), 2
[21772-21-4]	1,16-Bis(2,5-dimethoxyphenyl)-1,16-hexadecanedione, 1050
[21772-22-5]	1,16-Bis(2-hydroxy-5-methoxyphenyl)-1,16-hexadecanedione, 1051
[21999-97-3]	1-(3-Acetyloxyphenyl)-1-butanone, 3
[22168-75-8]	1-(3,5-Dimethoxyphenyl)-1-nonadecanone, 1094
[22198-47-6]	1-(4-Ethoxy-2-hydroxyphenyl)-1-octanone, 801
[22198-48-7]	1-[4-(Heptyloxy)-2-hydroxyphenyl]-1-butanone, 112
[22198-49-8]	1-[4-(Nonyloxy)-2-hydroxyphenyl]-1-butanone, 117
[22198-50-1]	1-[4-(Butyloxy)-2-hydroxyphenyl]-1-octadecanone, 1082
[22198-51-2]	1-(4-Ethoxy-2-hydroxyphenyl)-1-octadecanone, 1078
[22362-59-0]	1-(2-Hydroxyphenyl)-1-heptanone, 719
[22362-60-3]	1-(2-Hydroxyphenyl)-1-nonanone, 835
[22362-68-1]	1-(3,5-Dibromo-2-hydroxyphenyl)-1-butanone, 21
[22362-69-2]	1-(3,5-Dibromo-2-hydroxyphenyl)-1-pentanone, 478
[22421-07-4]	11-Bromo-1-(3,4-dihydroxyphenyl)-1-undecanone, 935
[22421-08-5]	1-(3,4-Dihydroxyphenyl)-11-acetyloxy-1-undecanone, 928
[22526-26-7]	1-(2-Hydroxyphenyl)-4-methyl-1-pentanone, 541
[22526-27-8]	1-(2-Methoxyphenyl)-4-methyl-1-pentanone, 541
[22620-38-8]	4-Chloro-1-(4-phenoxyphenyl)-1-butanone, 281
[22748-59-0]	3-Methyl-1-[2,4,6-trihydroxy-3,5-bis(3-methylbutyl)phenyl]-1-butanone, 234
[22811-84-3]	7-(4-Hydroxy-2-methylphenyl)-7-oxo-1-heptanoic acid, 769
[22811-89-8]	8-(4-Hydroxyphenyl)-8-oxo-1-octanoic acid, 830
[22811-90-1]	1,8-Bis(4-hydroxyphenyl)-1,8-octanedione, 811
[22811-95-6]	1,8-Bis(4-methoxyphenyl)-1,8-octanedione (Di-2,4-dinitrophenyl-hydrazone), 812
[22811-96-7]	8-(4-Hydroxy-3-methylphenyl)-8-oxo-1-octanoic acid, 833
[22811-98-9]	1,8-Bis(4-hydroxy-3-methylphenyl)-1,8-octanedione, 819
[22812-00-6]	8-(4-Hydroxy-2-methylphenyl)-8-oxo-1-octanoic acid, 832
[22812-02-8]	1,8-Bis(4-hydroxy-2-methylphenyl)-1,8-octanedione, 819
[22812-06-2]	8-(2-Hydroxy-5-chlorophenyl)-8-oxo-1-octanoic acid, 832
[22812-09-5]	8-(2-Hydroxy-4-methylphenyl)-8-oxo-1-octanoic acid, 832
[22859-96-7]	1,7-Bis(4-hydroxy-3-methylphenyl)-1,7-heptanedione, 760
[22860-00-0]	1,7-Bis(4-hydroxy-2-methylphenyl)-1,7-heptanedione, 760
[22919-59-1]	1-(2,4-Dihydroxyphenyl)-1-butanone (Oxime), 9
[22994-79-2]	7-(5-Chloro-2-hydroxyphenyl)-7-oxo-1-heptanoic acid, 768
[23187-42-0]	1-(4-Ethoxy-2-hydroxyphenyl)-1-butanone, 70
[23293-67-6]	12-(4-Hydroxyphenyl)-12-oxo-1-dodecanoic acid, 994
[23298-90-0]	3-Butyryl-4-acetyloxybenzoic acid, 43

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[23474-83-1]	2-Bromo-1-(3,4-dimethoxyphenyl)-1-butanone, 271
[23666-67-3]	1-(4-Hydroxy-3,5-dimethylphenyl)-1-dodecanone, 965
[23803-76-1]	1-(2-Hydroxyphenyl)-9-octadecyn-1-one (2,4-Dinitrophenylhydrazone), 1061
[23803-77-2]	1-(4-Hydroxyphenyl)-9-octadecyn-1-one (2,4-Dinitrophenylhydrazone), 1062
[23803-78-3]	1-(2-Hydroxy-3-methylphenyl)-9-octadecyn-1-one, 1073
[23803-79-4]	1-(2-Hydroxy-3-methylphenyl)-9-octadecyn-1-one (2,4-Dinitrophenylhydrazone), 1073
[23803-80-7]	1-(2-Hydroxy-4-methylphenyl)-9-octadecyn-1-one, 1073
[23803-81-8]	1-(2-Hydroxy-4-methylphenyl)-9-octadecyn-1-one (2,4-Dinitrophenylhydrazone), 1073
[23803-82-9]	1-(2-Hydroxy-5-methylphenyl)-9-octadecyn-1-one, 1074
[23803-83-0]	1-(2-Hydroxy-5-methylphenyl)-9-octadecyn-1-one (2,4-Dinitrophenylhydrazone), 1074
[23842-91-3]	1-(4-Hydroxyphenyl)-9-octadecyn-1-one, 1061
[23951-55-5]	4′-[4-Hydroxy-3,5-(diiodo)diphenyl]ether-4-(1-dodecanone), 976
[24070-03-9]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-pentanone (Mg salt), 513
[24085-13-0]	Methyl 5-(2-bromo-1-oxobutyl)-2-hydroxybenzoate, 271
[24294-76-6]	1-(4-Butoxy-2-hydroxyphenyl)-1-octanone, 808
[24313-92-6]	1-(4-Butoxy-2-hydroxyphenyl)-1-hexadecanone, 1049
[24313-95-9]	1-(2,4-Dihydroxyphenyl)-1-decanone, 872
[24313-96-0]	1-[4-(Butyloxy)-2-hydroxyphenyl]-1-decanone, 896
[24323-47-5]	1-(2-Hydroxy-5-methylphenyl)-1-butanone, 49
[24336-93-4]	1,9-Bis(4-methoxyphenyl)-1,9-nonanedione (Di-2,4-dinitrophenyl-hydrazone), 850
[24336-94-5]	1,9-Bis(4-hydroxy-3-methylphenyl)-1,9-nonanedione, 860
[24336-96-7]	1,9-Bis(4-methoxy-3-methylphenyl)-1,9-nonanedione, 860
[24336-97-8]	1,9-Bis(4-hydroxy-2-methylphenyl)-1,9-nonanedione, 859
[24339-80-8]	10-(4-Methoxyphenyl)-10-oxo-1-decanoic acid (2,4-Dinitrophenylhydrazone), 919
[24339-81-9]	1,10-Bis(4-methoxyphenyl)-1,10-decanedione (Di-2,4-dinitrophenyl-hydrazone), 901
[24339-82-0]	1,9-Bis(4-hydroxy-2-methylphenyl)-1,9-nonanedione (Di-2,4-dinitrophenyl-hydrazone), 859
[24339-87-5]	9-(5-Chloro-2-hydroxyphenyl)-9-oxo-1-nonanoic acid (2,4-Dinitrophenylhydrazone), 865
[24339-88-6]	10-(4-Hydroxy-3-methylphenyl)-10-oxo-1-decanoic acid (2,4-Dinitrophenylhydrazone), 921
[24339-89-7]	10-(4-Hydroxy-3-methylphenyl)-10-oxo-1-decanoic acid, 921
[24339-93-3]	10-(4-Methoxyphenyl)-10-oxo-1-decanoic acid, 918
[24339-95-5]	10-(4-Hydroxyphenyl)-10-oxo-1-decanoic acid, 918
[24339-96-6]	10-(4-Hydroxyphenyl)-10-oxo-1-decanoic acid (2,4-Dinitrophenylhydrazone), 918
[24339-99-9]	1,10-Bis(4-methoxy-3-methylphenyl)-1,10-decanedione, 909
[24340-00-9]	1,10-Bis(4-hydroxy-2-methylphenyl)-1,10-decanedione, 908

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[24340-01-0]	1,10-Bis(4-hydroxy-2-methylphenyl)-1,10-decanedione (Di-2,4-dinitrophenylhydrazone), 908
[24340-02-1]	1,10-Bis(4-methoxy-2-methylphenyl)-1,10-decanedione, 908
[24340-03-2]	1,10-Bis(4-methoxy-2-methylphenyl)-1,10-decanedione (Di-2,4-dinitrophenylhydrazone), 908
[24340-04-3]	10-(5-Chloro-2-hydroxyphenyl)-10-oxo-1-decanoic acid, 920
[24340-05-4]	10-(5-Chloro-2-hydroxyphenyl)-10-oxo-1-decanoic acid (2,4-Dinitrophenylhydrazone), 920
[24340-07-6]	1,10-Bis(2-hydroxy-5-methylphenyl)-1,10-decanedione (Di-2,4-dinitrophenylhydrazone), 908
[24381-67-7]	9-(5-Chloro-2-hydroxyphenyl)-9-oxo-1-nonanoic acid, 865
[24490-27-5]	1-(2-Chloro-6-hydroxy-4-methylphenyl)-1-hexanone, 635
[24490-29-7]	1-(2-Chloro-6-hydroxy-4-methylphenyl)-1-hexadecanone, 1041
[25065-15-0]	3-Butyryl-4-hydroxybenzoic acid, 43
[25305-58-2]	Ethyl 5-(4-methoxyphenyl)-5-oxo-1-pentanoate, 580
[25632-60-4]	1-(2,4-Dihydroxyphenyl)-1-dodecanone, 945
[25715-26-8]	1,9-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,9-nonanedione, 858
[25715-27-9]	1,9-Bis(5-chloro-2-hydroxy-4-methylphenyl)-1,9-nonanedione (Di-2,4-dinitrophenylhydrazone), 859
[25715-28-0]	1,10-Bis(3-chloro-6-hydroxy-2-methylphenyl)-1,10-decanedione, 906
[25779-68-4]	1,10-Bis(3-chloro-6-hydroxy-2-methylphenyl)-1,10-decanedione (Di-2,4-dinitrophenylhydrazone), 906
[25804-38-0]	4-Cyclohexyl-1-(4-hydroxy-3-methylphenyl)-1-butanone, 258
[25804-39-1]	4-Cyclohexyl-1-(4-hydroxy-3-methylphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 258
[25804-40-4]	4-Cyclohexyl-1-(2-hydroxy-5-methylphenyl)-1-butanone, 258
[25804-41-5]	4-Cyclohexyl-1-(2-hydroxy-5-methylphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 258
[25804-66-4]	4-Cyclohexyl-1-(2-hydroxyphenyl)-1-butanone, 256
[25804-67-5]	4-Cyclohexyl-1-(2-hydroxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 256
[25804-69-7]	4-Cyclohexyl-1-(4-hydroxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 256
[25915-31-5]	1-[2,4-Dihydroxy-3,5-bis(3-methylbutyl)phenyl]-3-methyl-1-butanone, 234
[26086-74-8]	1,8-Bis(2,4-dihydroxyphenyl)-1,8-octanedione, 812
[26086-77-1]	1,8-Bis(2-hydroxy-4-methoxyphenyl)-1,8-octanedione, 819
[26086-78-2]	1,9-Bis(2-hydroxy-4-methoxyphenyl)-1,9-nonanedione, 861
[26086-80-6]	1,7-Bis(5-chloro-2,4-dihydroxyphenyl)-1,7-heptanedione, 753
[26086-81-7]	1,8-Bis(5-chloro-2,4-dihydroxyphenyl)-1,8-octanedione, 811
[26086-82-8]	1,9-Bis(5-chloro-2,4-dihydroxyphenyl)-1,9-nonanedione, 849
[26086-83-9]	1,7-Bis(5-chloro-2,4-dimethoxyphenyl)-1,7-heptanedione, 753
[26086-84-0]	1,8-Bis(5-chloro-2,4-dimethoxyphenyl)-1,8-octanedione, 811
[26086-85-1]	1,9-Bis(5-chloro-2,4-dimethoxyphenyl)-1,9-nonanedione, 850
[26086-86-2]	1,10-Bis(5-chloro-2,4-dimethoxyphenyl)-1,10-decanedione, 899
[26103-97-9]	3-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone, 182

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[26103-99-1]	1,1′-(3,5,2′,4′,6′-Pentahydroxy[1,1′-biphenyl]-4-yl)-3-methyl-1-butanone, 262
[26104-01-8]	3-Methyl-1-[2,4,6-trihydroxy-3-(3-methylbutyl)phenyl]-1-butanone, 217
[26104-02-9]	1,1′-[2,4,6-Trihydroxy-5-(3-methylbutyl)-1,3-phenylene]bis-3-methyl-1-butanone, 306
[26104-08-5]	3-Methyl-1-[2,4,6-tribenzoyloxy-3,5-bis(3-methylbutyl)phenyl]-1-butanone, 234
[26115-81-1]	1-(3,4-Dihydroxyphenyl)-4-methyl-1-pentanone, 544
[26195-11-9]	1,10-Bis(5-chloro-2,4-dihydroxyphenyl)-1,10-decanedione, 899
[26477-64-5]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 242
[26477-65-6]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 157
[26477-66-7]	4-[1-(Acetyloxy)propyl]-5,7-dimethoxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 158
[26481-09-4]	4-[1-(Acetyloxy)propyl]-5,7-dimethoxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 243
[26639-19-0]	1-(2,5-Dihydroxyphenyl)-1-heptadecanone, 1055
[26945-71-1]	1-[(4-Phenylmethoxy)phenyl]-1-butanone, 6
[26976-83-0]	4-(4-Methoxy-3-nitrophenyl)-4-oxo-1-butanoic acid, 426
[26993-72-6]	5-[[(2-Hydroxy-5-methylphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone, 981
[26993-73-7]	5-[[(5-Chloro-2-hy2,3,4-Trihydroxyphenyl)enyl]-1-dodecanone, 977
[26993-74-8]	5-[[(5-Aminosulfonyl-2-hydroxyphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone, 979
[26993-75-9]	5-[[(2-Carboxyphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone, 980
[27020-17-3]	5-[[(2-Hydroxyphenyl)azo]-2,4-dihydroxyphenyl]-1-dodecanone, 978
[27029-46-5]	1-(4-Hydroxyphenyl)-1-tetracosanone (Polymer with formaldehyde), 1113
[27029-47-6]	1-(4-Hydroxyphenyl)-1-docosanone (Polymer with formaldehyde), 1104
[27117-71-1]	Methyl 4-(4-methoxyphenyl)-2,3-dibromo-4-oxo-1-butanoate (threo), 397
[27117-72-2]	Methyl 4-(4-methoxyphenyl)-2,3-dibromo-4-oxo-1-butanoate (erythro), 397
[27127-44-2]	5,7-Diacetyloxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 246
[27581-18-6]	1-(4-Chloro-2-hydroxyphenyl)-1-pentanone, 482
[27686-81-3]	1,4-Bis(3,4-dimethoxyphenyl)-2,3-dimethyl-1,4-butanedione (racemic), 368
[27763-55-9]	1-(4-Methoxyphenyl)-2-methyl-1-butanone (2*S*), 126
[27883-47-2]	1-(2,4-Dihydroxyphenyl)-1-heptanone, 725
[27883-48-3]	1-(2,4-Dihydroxyphenyl)-1-nonanone, 838
[28319-38-2]	4-[1-(Acetyloxy)propyl]-6-(3,7-dimethyl-2,6-octadienyl)-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 167
[28441-00-1]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-octanone, 822
[28441-02-3]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-dodecanone, 982
[28441-03-4]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-hexadecanone, 1051
[28441-04-5]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-eicosanone, 1100
[28441-05-6]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-docosanone, 1108
[28459-33-8]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-octadecanone, 1086

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[28583-62-2]	1-[4-(Acetylamino)-2-hydroxyphenyl]-1-butanone, 64
[28583-76-8]	1-[5-(Acetylamino)-2-hydroxyphenyl]-1-butanone, 64
[29207-19-0]	Methyl 5-(2-methoxy-4-methylphenyl)-5-oxo-1-pentanoate, 591
[29207-22-5]	Methyl 5-(2-methoxy-4-carbomethoxyphenyl)-5-oxo-1-pentanoate, 594
[29389-23-9]	Methyl 6-(4-methoxyphenyl)-6-oxo-1-hexanoate, 711
[29665-49-4]	1-(4-Methoxy-3,5-dimethylphenyl)-1-tetradecanone, 1015
[29665-52-9]	1-(4-Methoxy-3-methylphenyl)-1-butanone, 52
[29665-55-2]	1-(4-Hydroxy-3-methylphenyl)-1-dodecanone, 960
[29665-56-3]	1-(4-hydroxy-3,5-dimethylphenyl)-1-decanone, 888
[29666-10-2]	1-(2-Hydroxy-4-methylphenyl)-1-dodecanone (Oxime, nickel complex), 958
[29681-99-0]	1-(3-Methoxyphenyl)-1,3-butanedione, 310
[30151-74-7]	1,12-Bis(3,4-dihydroxyphenyl)-1,12-dodecanedione, 977
[30299-35-5]	1-(4-Methoxyphenyl)-4-methyl-1-pentanone (Semicarbazone), 543
[30299-36-6]	1-(4-Ethoxyphenyl)-4-methyl-1-pentanone, 543
[30299-37-7]	1-(4-Ethoxyphenyl)-4-methyl-1-pentanone (Semicarbazone), 543
[30390-12-6]	5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 154
[30392-06-4]	1-[3,5-Bis(1,1-dimethylethyl)-4-acetyloxyphenyl]-1-octanone, 822
[30392-07-5]	1-[3,5-Bis(1,1-dimethylethyl)-4-acetyloxyphenyl]-1-octadecanone, 1086
[30414-64-3]	7-(2,4-Dihydroxyphenyl)-7-oxo-1-heptanoic acid, 767
[30414-65-5]	1-(2,4-Dihydroxy-6-methylphenyl)-1-octanone, 795
[30414-67-6]	1-(2,6-Dihydroxy-4-methylphenyl)-1,7-octanedione, 790
[30414-68-7]	1-(2,6-Dimethoxy-4-methylphenyl)-1,7-octanedione, 790
[30492-53-6]	1-[3,5-Bis(1,1-dimethylethyl)-4-methoxyphenyl]-1-octadecanone, 1086
[30509-74-1]	1,1′-(5-Bromo-2,4,6-trihydroxy-1,3-phenylene)bis-1-pentanone (4-Trichloromethane sulfenate), 511
[30509-76-3]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-pentanone (1,3,5-Tris-trichloromethane sulfenate), 513
[30563-62-3]	8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2′,3′:5,6]benzo[1,2-b]pyran-2-one, 247
[30839-20-4]	1,4-Bis(4-methoxyphenyl)-2,3-bis(phenyl)-1,4-butanedione, 373
[31526-44-0]	5-(4-Methoxyphenyl)-3,3-dimethyl-5-oxo-1-pentanoic acid, 585
[31526-46-2]	Ethyl 5-(4-methoxyphenyl)-3,3-dimethyl-5-oxo-1-pentanoate, 585
[31914-19-9]	4-(2,4,5-Trimethoxyphenyl)-4-oxo-1-butanoic acid, 412
[32085-87-3]	1-(2,6-DImethoxyphenyl)-1,3-butanedione, 321
[32190-32-2]	1,1′-[Methylenebis(2,4-dihydroxy-6-methoxy-3,1-phenylene)]bis-1-butanone, 337
[32246-17-6]	8-(2,4-Dihydroxy-5-bromophenyl)-8-oxo-1-octanoic acid, 831
[32246-62-1]	1,7-Bis(2,4-dimethoxyphenyl)-1,7-heptanedione, 755
[32246-63-2]	1,7-Bis(2,4-dimethoxyphenyl)-1,7-heptanedione (Dioxime), 755
[32246-69-8]	1,7-Bis(3,4-dimethoxyphenyl)-1,7-heptanedione, 755
[32246-72-3]	7-(5-Bromo-2,4-dihydroxyphenyl)-7-oxo-1-heptanoic acid, 767
[32246-77-8]	8-(2,4-Dihydroxyphenyl)-8-oxo-1-octanoic acid, 830
[32246-82-5]	1,8-Bis(2,4-dimethoxyphenyl)-1,8-octanedione, 812
[32246-86-9]	8-(2,4-Dihydroxy-5-chlorophenyl)-8-oxo-1-octanoic acid, 832

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[32246-91-6]	1,8-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,8-octanedione (Dioxime), 825
[32246-93-8]	1,8-Bis(3,4-dimethoxyphenyl)-1,8-octanedione (Di-2,4-dinitrophenyl-hydrazone), 813
[32246-94-9]	8-(3,4-Dimethoxyphenyl)-8-oxo-1-octanoic acid, 831
[32246-95-0]	1,8-Bis(5-bromo-2,4-dihydroxyphenyl)-1,8-octanedione, 811
[32339-34-7]	1,1′-(4′-Methoxy[1,1′-biphenyl]-4-yl)-1-butanone, 261
[32339-35-8]	1,1′-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-butanone, 261
[32340-75-3]	7-(5-Chloro-2,4-dihydroxyphenyl)-7-oxo-1-heptanoic acid, 768
[32340-79-7]	8-(3,4-Dimethoxyphenyl)-8-oxo-1-octanoic acid (2,4-Dinitrophenylhydrazone), 831
[32354-10-2]	1,7-Bis(2,4-dihydroxyphenyl)-1,7-heptanedione (2,4-Dinitrophenylhydrazone), 755
[32435-18-0]	1,8-Bis(3,4-dimethoxyphenyl)-1,8-octanedione, 812
[33245-77-1]	5-Chloro-1-(3,4-dimethoxyphenyl)-1-pentanone, 569
[33245-78-2]	5-Chloro-1-(2,4-dimethoxyphenyl)-1-pentanone, 569
[33446-14-9]	4-(4-Methoxy-3-methylphenyl)-4-oxo-1-butanoic acid, 436
[33488-76-5]	1-(4-Ethoxy-2-hydroxyphenyl)-1-nonanone (Oxime), 845
[33488-77-6]	1-(4-Ethoxy-2-hydroxyphenyl)-1-heptadecanone (Oxime), 1057
[33488-77-6]	1-(4-Ethoxy-2-hydroxyphenyl)-1-octadecanone (Oxime), 1079
[33720-04-6]	2-Bromo-1-(4-methoxyphenyl)-4-methyl-1-pentanone, 574
[33809-55-1]	2-Bromo-1-(4-methoxyphenyl)-1-hexanone, 697
[34052-09-0]	1-(2,3-Dimethoxyphenyl)-1-butanone, 8
[34128-24-0]	1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1,3-butanedione, 332
[34190-36-8]	1-(3-Chloro-4-hydroxyphenyl)-1-pentanone, 482
[34670-10-5]	5-(4-Ethoxyphenyl)-5-oxo-1-pentanoic acid, 580
[34767-67-4]	11-Bromo-1-(3,4-diacetyloxyphenyl)-1-undecanone, 935
[34887-83-7]	1-(4-Hydroxyphenyl)-3-methyl-1-butanone, 175
[34927-48-5]	4-(2-Hydroxy-3,4,6-trimethylphenyl)-2-methyl-4-oxo-1-butanoic acid, 449
[34927-49-6]	4-(2-Hydroxy-3,4,6-trimethylphenyl)-2-methyl-4-oxo-1-butanoic acid, 449
[35031-70-0]	1-(2-Methoxyphenyl)-1-hexanone, 599
[35031-73-3]	1-(4-Ethoxyphenyl)-1-butanone, 8
[35031-74-4]	1-(4-Ethoxyphenyl)-1-hexanone, 605
[35049-65-1]	1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-1-pentanone, 511
[35081-43-3]	2-Bromo-1-[(4-phenylmethoxy)phenyl]-1-butanone, 270
[35081-44-8]	1-(4-Benzyloxyphenyl)-1-pentanone, 466
[35081-50-6]	2-Bromo-1-(4-benzyloxyphenyl)-1-pentanone, 565
[35115-14-1]	1-(2-Hydroxyphenyl)-2-methyl-1,3-butanedione, 314
[35115-15-2]	1-(2-Hydroxyphenyl)-1,3-pentanedione, 459
[35175-56-5]	1-(2-Hydroxy-5-methoxyphenyl)-1-octadecanone, 1077
[35446-28-7]	2-Bromo-1-(4-methoxyphenyl)-3-methyl-1-butanone, 293
[36287-37-3]	1,4-Bis(3,4-dimethoxyphenyl)-2,3-dimethyl-1,4-butanedione (meso-isomer), 368
[36287-37-3]	1,4-Bis(3,4-dimethoxyphenyl)-2,3-dimethyl-1,4-butanedione (meso), 370
[36330-86-6]	4-(4-Phenoxyphenyl)-4-oxo-1-butanoic acid, 402

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[36330-87-7]	4-(4′-Methoxybiphenyl)-4-oxo-1-butanoic acid, 452
[36375-38-9]	1-(2-Hydroxy-3-methylphenyl)-1-butanone, 47
[36412-64-3]	2-Bromo-1-(4-methoxyphenyl)-1-pentanone, 565
[36478-56-5]	5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one, 148
[36481-17-1]	Methyl 5-butyryl-2-hydroxybenzoate, 43
[36677-71-1]	1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-decanone, 915
[36756-42-0]	1-(4,4′-Dihydroxy[1,1′-biphenyl]-3-yl)-1-decanone, 905
[36946-07-3]	1-(2-Hydroxy-5-methylphenyl)-1-octanone, 792
[36946-08-4]	1-(2-Hydroxy-5-methylphenyl)-1-tetradecanone, 1012
[36953-87-4]	4-Hydroxy-3-(1-oxopentyl)-2*H*-1-benzopyran-2-one, 502
[36953-90-9]	4-Hydroxy-3-(1-oxooctyl)-2*H*-1-benzopyran-2-one, 803
[37166-86-2]	1,9-Bis(2,4-dihydroxyphenyl)-1,9-nonanedione (Dioxime), 851
[37166-89-5]	1,9-Bis(2,4-dimethoxyphenyl)-1,9-nonanedione, 851
[37166-91-9]	1,9-Bis(5-chloro-2,4-dihydroxyphenyl)-1,9-nonanedione (Dioxime), 850
[37166-92-0]	9-(5-Chloro-2,4-dihydroxyphenyl)-9-oxo-1-nonanoic acid, 865
[37166-94-2]	1,9-Bis(5-chloro-2,4-dimethoxyphenyl)-1,9-nonanedione (Dioxime), 850
[37166-96-4]	1,9-Bis(2-hydroxy-3,4-dimethoxyphenyl)-1,9-nonanedione (Di-2,4-dinitrophenylhydrazone), 863
[37166-99-7]	1,10-Bis(2,4-dihydroxyphenyl)-1,10-decanedione (Di-2,4-dinitrophenylhydrazone), 902
[37167-01-4]	1,10-Bis(2-hydroxy-4-methoxyphenyl)-1,10-decanedione (Di-2,4-dinitrophenylhydrazone), 910
[37167-02-5]	1,10-Bis(2,4-dimethoxyphenyl)-1,10-decanedione, 902
[37174-76-8]	1,10-Bis(5-chloro-2,4-dimethoxyphenyl)-1,10-decanedione (Di-2,4-dinitrophenylhydrazone), 899
[37174-78-0]	1,10-Bis(5-bromo-2,4-dihydroxyphenyl)-1,10-decanedione, 898
[37174-79-1]	1,10-Bis(5-bromo-2,4-dimethoxyphenyl)-1,10-decanedione, 898
[37174-80-4]	1,10-Bis(5-bromo-2,4-dimethoxyphenyl)-1,10-decanedione (Dioxime), 898
[37401-99-3]	1,10-Bis(5-chloro-2,4-dihydroxyphenyl)-1,10-decanedione (Dioxime), 899
[37402-01-0]	1,10-Bis(5-bromo-2,4-dihydroxyphenyl)-1,10-decanedione (Dioxime), 898
[37402-33-8]	1,9-Bis(2-hydroxy-4-methoxyphenyl)-1,9-nonanedione (Di-2,4-dinitrophenylhydrazone), 861
[37402-34-9]	1,10-Bis(2,4-dimethoxyphenyl)-1,10-decanedione (Di-2,4-dinitrophenylhydrazone), 902
[37622-68-7]	1-(2,4-Dihydroxyphenyl)-1-octanone, 778
[37622-78-9]	1-(3,4-Dihydroxyphenyl)-1-octanone, 781
[37765-93-8]	1-(2-Hydroxyphenyl)-5-phenyl-1-pentanone, 523
[37972-55-7]	5,7-Dihydroxy-8-(3-methylbutyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 248
[37972-56-8]	[5,7-Dihydroxy-6-(3-methylbutyryl)-2-oxo-4-phenyl-2*H*-chromen-8-yl]acetaldehyde, 393
[37975-64-7]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 153
[37975-69-2]	5,7-Dihydroxy-6-(3-methylbutyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 239

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[38051-39-7]	1-[4-(4-Octanoylphenyloxy)phenyl]-1-octanone, 777
[38071-42-0]	1-(2,4-Dibenzyloxy-6-methylphenyl)-1,3,5-hexanetrione, 629
[38071-43-1]	7-(2,4-Dibenzyloxy-6-methylphenyl)-3,5,7-trioxo-1-heptanoic acid, 769
[38071-44-2]	Methyl 7-(2,4-dibenzyloxy-6-methylphenyl)-3,5,7-trioxo-1-heptanoate, 769
[38071-45-3]	Methyl 7-(2,4-dihydroxy-6-methylphenyl)-3,5,7-trioxo-1-heptanoate, 769
[38071-49-7]	Methyl 7-(2,4-dimethoxy-6-methylphenyl)-3,5,7-trioxo-1-heptanoate, 768
[38409-24-4]	7-Methoxy-6-(2,2-dideuterio-3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 202
[38534-63-3]	5,7-Diacetyloxy-4-(1-acetyloxypropyl)-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 238
[38534-70-2]	5,7-Diacetyloxy-4-(1-acetyloxypropyl)-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 155
[38534-76-8]	5,7-Dihydroxy-4-(1-hydroxypropyl)-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 238
[38534-77-9]	5,7-Dihydroxy-4-(1-hydroxypropyl)-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 155
[38534-84-8]	4-[1-(Acetyloxy)propyl]-5,7-diacetyloxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 243
[38537-84-7]	5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 120
[38767-74-7]	6-(3,4-Dimethoxyphenyl)-6-oxo-1-hexanoic acid, 713
[38789-16-1]	5,7-Diacetyloxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 236
[38843-82-2]	1-(2,5-Dimethoxyphenyl)-1-pentanone, 472
[38844-02-9]	1-(2,5-Dimethoxy-4-pentylphenyl)-1-pentanone, 514
[39192-51-3]	1-(3,5-Dimethoxyphenyl)-1-heptanone, 728
[39192-52-4]	1-(3,5-Diacetyloxyphenyl)-1-heptanone, 728
[39192-54-6]	1-(3,5-Dihydroxyphenyl)-1-heptanone, 728
[39496-84-9]	Ethyl 4-(2-hydroxyphenyl)-4-oxo-1-butanoate, 399
[39496-86-1]	4-(3-Amino-4-methoxyphenyl)-4-oxo-1-butanoic acid, 428
[39496-87-2]	4-(3-Chloro-4-methoxyphenyl)-4-oxo-1-butanoic acid, 423
[39560-29-7]	4-(2,4-Diethoxyphenyl)-4-oxo-1-butanoic acid, 404
[39560-34-4]	4-(2-Hydroxyphenyl)-4-oxo-1-butanoic acid, 398
[39575-43-4]	1-(2-Hydroxyphenyl)-3-methyl-1-pentanone, 553
[39575-44-5]	1-(2-Hydroxy-3-methylphenyl)-3-methyl-1-pentanone (+), 558
[39575-45-6]	1-(2-Hydroxy-4-methylphenyl)-3-methyl-1-pentanone (+), 558
[39575-46-7]	1-(2-Hydroxy-5-methylphenyl)-3-methyl-1-pentanone (+), 558
[39575-47-8]	1-(3-Chloro-2-hydroxyphenyl)-3-methyl-1-pentanone (+), 557
[39575-48-9]	1-(4-Chloro-2-hydroxyphenyl)-3-methyl-1-pentanone (+), 557
[39575-49-0]	1-(5-Chloro-2-hydroxyphenyl)-3-methyl-1-pentanone (+), 557
[39652-80-7]	2-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone, 129
[39652-87-4]	1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-2-methyl-1-butanone, 141
[39652-88-5]	1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-2-methyl-1-butanone, 141

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[39652-89-6]	1-[2,4,6-Tribenzoyloxy-3,5-bis(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone, 153
[39757-32-9]	Methyl 4-(2,4-dimethoxyphenyl)-2,4-dioxo-1-butanoate, 397
[39911-73-4]	1-(3,5-Dimethoxyphenyl)-1-butanone, 15
[40000-60-0]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-dodecanone, 967
[40220-94-8]	1-(2,4,6-Triacetyloxyphenyl)-1-dodecanone, 952
[40336-21-8]	1-(3,4,5-Trihydroxyphenyl)-1-dodecanone, 953
[40366-12-9]	1-(2,3,4-Trihydroxyphenyl)-1-hexadecanone, 1038
[40372-78-9]	4-Hexadecanoylsalicylic acid, 1041
[40372-79-0]	1-(2,4-Dihydroxyphenyl)-1-hexadecanone, 1035
[40690-25-3]	1-(2-Hydroxy-4-methylphenyl)-1-dodecanone (Oxime, nickel complex), 958
[40690-30-0]	1-(2-Hydroxy-4-methylphenyl)-1-tridecanone (Oxime, nickel complex), 1000
[40867-42-3]	1-(2-Hydroxy-4-methylphenyl)-1-dodecanone (Oxime), 958
[40877-17-6]	4-Chloro-1-(2-methoxyphenyl)-1-butanone, 279
[40877-19-8]	4-Chloro-1-(4-methoxyphenyl)-1-butanone, 280
[40991-98-8]	1-(2-Hydroxy-4-methylphenyl)-1-butanone, 47
[40991-99-9]	1-(2-Hydroxy-3-methoxy-6-methylphenyl)-1-butanone, 71
[41082-97-7]	1-(4-Hydroxy-5-methoxy-2-methylphenyl)-1-butanone, 72
[41497-32-9]	1-(3,5-Dimethoxyphenyl)-1-hexanone, 611
[41497-33-0]	1-(3,5-Dimethoxyphenyl)-1-undecanone, 927
[41715-70-2]	1-(2,3-Dichloro-4-methoxyphenyl)-1-butanone, 23
[41729-72-0]	1-(2,4-Dihydroxyphenyl)-1-hexadecanone (Na salt), 1035
[41764-07-2]	4-(3,4-Methylenedioxyphenyl)-4-oxo-1-butanoic acid, 410
[41826-92-0]	4-(2,4,5-Triethoxyphenyl)-4-oxo-1-butanoic acid, 412
[41826-96-4]	4-(4,5-Diethoxy-2-methylphenyl)-4-oxo-1-butanoic acid, 438
[41826-97-5]	4-(5-Chloro-2,4-dimethoxyphenyl)-4-oxo-1-butanoic acid, 425
[41826-99-7]	4-(5-Ethoxy-4-methoxy-2-propylphenyl)-4-oxo-1-butanoic acid, 451
[41827-00-3]	4-(4-Methoxy-5-propoxy-2-propylphenyl)-4-oxo-1-butanoic acid, 454
[41827-02-5]	4-(5-Chloro-2,4-diethoxyphenyl)-4-oxo-1-butanoic acid, 425
[41827-04-7]	4-(2,4-Diethoxy-5-ethylphenyl)-4-oxo-1-butanoic acid, 445
[41827-05-8]	4-(4-Chloro-2,5-dimethoxyphenyl)-4-oxo-1-butanoic acid, 424
[41827-06-9]	4-(6-Methoxybenzodioxol-5-yl)-4-oxo-1-butanoic acid, 431
[41827-08-1]	4-(2-Ethoxy-4-methyl-5-methylthiophenyl)-4-oxo-1-butanoic acid, 445
[41827-09-2]	4-(2,4,5-Tributoxyphenyl)-4-oxo-1-butanoic acid, 413
[41827-10-5]	Ethyl 4-(4,5-diethoxy-2-methylphenyl)-4-oxo-1-butanoate, 439
[41827-11-6]	4-(2,5-Diethoxy-4-methylphenyl)-4-oxo-1-butanoic acid, 437
[41827-12-7]	4-(2-Hydroxy-4,5-dimethoxyphenyl)-4-oxo-1-butanoic acid, 447
[41894-23-9]	1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-octadecanone (Oxime, palladium complex), 1082
[41894-24-0]	1-(2-Hydroxy-4-methylphenyl)-1-dodecanone (Oxime, palladium complex), 958
[42290-21-1]	5-Hydroxy-8,8-dimethyl-6-(1-oxobutyl)-4-phenyl-2*H*,8*H*-benzo[1,2-b:5,6-b′]dipyran-2-one, 122
[42782-77-4]	1-(4,7-Dimethoxy-2,3-dimethyl-6-benzofuranyl)-1-decanone, 894

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[42907-96-0]	Methyl 4-(2-hydroxy-4-methoxyphenyl)-4-oxo-1-butanoate, 439
[42916-80-3]	Ethyl 6-(4-methoxyphenyl)-6-oxo-1-hexanoate, 711
[43043-25-0]	1-(2,3,4-Trihydroxyphenyl)-1-pentanone, 475
[43043-26-1]	1-(2,3,4-Trihydroxyphenyl)-1-hexanone, 611
[43043-27-2]	1-[2,3,4-Trihydroxyphenyl]-1-heptanone, 729
[43043-28-3]	1-(2,3,4-Trihydroxyphenyl)-1-octanone, 783
[43043-31-8]	1-[2,4,6-Trihydroxyphenyl]-1-heptanone, 729
[43043-32-9]	1-(2,4,6-Trihydroxyphenyl)-1-octanone, 783
[43221-42-7]	1-(2-Hydroxy-4-methoxyphenyl)-1-nonanone, 844
[43228-96-2]	5-Chloro-1-(2-methoxyphenyl)-1-pentanone, 567
[43228-97-3]	1-(2-Methoxyphenyl)-5-iodo-1-pentanone, 569
[47660-65-1]	1-(4-Hydroxyphenyl)-1-docosanone, 1104
[49572-23-8]	1-(4-Ethoxy-2-hydroxyphenyl)-1-dodecanone, 965
[49582-13-0]	Trisaspidinol BBB, 348
[49582-14-1]	Trisaspidinol PBB, 348
[49582-15-2]	Trisaspidinol PBP, 348
[49583-26-8]	1-(2,4,6-Trihydroxy-3-methylphenyl)-1-pentanone, 499
[49583-27-9]	3-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone, 194
[49710-85-2]	1-(4,7-Dimethoxy-2,3-dimethyl-6-benzofuranyl)-1-tetradecanone, 1018
[49710-86-3]	1-(4,7-Dimethoxy-2,3-dimethyl-6-benzofuranyl)-1-hexadecanone, 1048
[49710-89-6]	1-(4,7-Dihydroxy-2,3-dimethyl-6-benzofuranyl)-1-decanone, 894
[49710-91-0]	1-(2,5-Dimethoxyphenyl)-1-decanone, 873
[50113-09-5]	1-[3-[(Dimethylamino)methyl]-2,4,5-trihydroxyphenyl]-1-butanone, 85
[50342-14-8]	1-(2-hydroxy-4,5-dimethylphenyl)-1-heptanone, 743
[50444-92-3]	1-(4-Chloro-2-hydroxyphenyl)-1-hexanone, 624
[50444-95-6]	1,1′-[Sulfonylbis(6-chloro-4-hydroxy-3,1-phenylene)]bis-1-butanone, 300
[50444-96-7]	1,1′-[Sulfonylbis(6-chloro-4-hydroxy-3,1-phenylene)]bis-1-pentanone, 537
[50444-97-8]	1,1′-[Sulfonylbis(6-chloro-4-hydroxy-3,1-phenylene)]bis-1-hexanone, 693
[50652-74-9]	1-(2-Hydroxy-4-methylphenyl)-1-hexanone (Oxime), 639
[50652-75-0]	1-[2-Hydroxyphenyl]-3,5,5-trimethyl-1-hexanone (Oxime), 619
[50652-76-1]	1-(2-Hydroxy-5-methylphenyl)-1-dodecanone (Oxime), 959
[50766-16-0]	1,6-Bis(3,4-dimethoxyphenyl)-1,6-hexanedione, 675
[50766-17-1]	1,9-Bis(3,4-dimethoxyphenyl)-1,9-nonanedione, 852
[50766-18-2]	1,6-Bis(3,4-diethoxyphenyl)-1,6-hexanedione, 676
[50766-19-3]	1,6-Bis(3,4-dipropyloxyphenyl)-1,6-hexanedione, 676
[50766-20-6]	1,6-Bis(3,4-dibutyloxyphenyl)-1,6-hexanedione, 676
[50766-21-7]	1,6-Bis(4-ethoxy-3-methoxyphenyl)-1,6-hexanedione, 687
[50766-22-8]	1,6-Bis(4-benzyloxy-3-methoxyphenyl)-1,6-hexanedione, 688
[50766-25-1]	1,6-Bis(3,4-dimethoxyphenyl)-3-methyl-1,6-hexanedione, 682
[50766-27-3]	1,5-Bis(3,4-dimethoxyphenyl)-1,5-pentanedione (Dimethyloxime), 521
[50766-28-4]	1,6-Bis(3,4-dimethoxyphenyl)-1,6-hexanedione (Dioxime), 676
[50766-29-5]	1,7-Bis(3,4-dimethoxyphenyl)-1,7-heptanedione (Dioxime), 755
[50766-30-8]	1,8-Bis(3,4-dimethoxyphenyl)-1,8-octanedione (Dioxime), 813
[50766-31-9]	1,9-Bis(3,4-dimethoxyphenyl)-1,9-nonanedione (Dioxime), 852

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[50766-33-1]	1,6-Bis(3,4-dimethylenedioxyphenyl)-1,6-hexanedione (Dimethyloxime), 677
[50766-34-2]	1,6-Bis(3,4-diethoxyphenyl)-1,6-hexanedione (Dioxime), 676
[50766-35-3]	1,6-Bis(3,4-dipropyloxyphenyl)-1,6-hexanedione (Dioxime), 676
[50766-36-4]	1,6-Bis(3,4-dibutyloxyphenyl)-1,6-hexanedione (Dioxime), 676
[50766-37-5]	1,6-Bis(4-ethoxy-3-methoxyphenyl)-1,6-hexanedione (Dioxime), 688
[50766-38-6]	1,6-Bis(4-benzyloxy-3-methoxyphenyl)-1,6-hexanedione (Dioxime), 688
[50766-42-2]	1,6-Bis(3,4-dimethoxyphenyl)-3-methyl-1,6-hexanedione (Dioxime), 682
[50874-43-6]	1-[2,4,6-Trihydroxy-3,5-bis(3-methyl-2-buten-1-yl)phenyl]-1-pentanone, 537
[50874-48-1]	1-[2,4,6-Trihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-1-butanone, 119
[51067-61-9]	6-(4-Methoxyphenyl)-1-phenyl-1,6-hexanedione, 672
[51317-85-2]	4-Chloro-1-(2-hydroxy-5-methylphenyl)-1-butanone, 284
[51317-86-3]	6-Chloro-1-(2-hydroxy-5-methylphenyl)-1-hexanone, 706
[51528-14-4]	1-(2-Hydroxy-5-methylphenyl)-1-octanone (Oxime), 793
[51528-15-5]	2-Ethyl-1-(2-hydroxy-5-methylphenyl)-1-hexanone (Oxime), 657
[51528-16-6]	1-(2-Hydroxy-5-nonylphenyl)-1-octanone (Oxime), 824
[51621-21-7]	1-(2-Hydroxy[1,1′-biphenyl]-3-yl)-1-octanone, 814
[51686-50-1]	Methyl 4-(2,3,4-trimethoxyphenyl)-4-oxo-1-butanoate, 411
[51795-94-9]	6-Bromo-1-(2-methoxyphenyl)-1-hexanone, 698
[51821-14-8]	6-Bromo-1-(2-hydroxyphenyl)-1-hexanone, 697
[51830-11-6]	1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-octadecanone (Oxime), 1082
[51944-08-2]	1-(4-Hydroxyphenyl)-1,3-butanedione, 310
[51978-33-7]	1-(5-Chloro-2-hydroxyphenyl)-1-butanone, 30
[51995-88-1]	1-[5-(1-Hydroxyethyl)-2-methoxyphenyl]-3-methyl-1-butanone, 198
[51995-98-3]	1-(5-Acetyl-2-methoxyphenyl)-3-methyl-1-butanone, 379
[52016-63-4]	1,5-Bis(5-chloro-2-hydroxypheny)l-1,5-pentanedione, 516
[52016-87-2]	1-(4,6-Dichloro-2-hydroxyphenyl)-1-hexanone, 622
[52066-90-7]	1-(5-Dodecyl-2-methoxyphenyl)-1-dodecanone, 986
[52122-64-2]	1-(2-Hydroxy-4-methylphenyl)-3,5,5-trimethyl-1-hexanone (Oxime), 665
[52122-70-0]	1-(2-Hydroxy-4-methylphenyl)-1-hexanone, 639
[52122-73-3]	1-(2-Hydroxy-4-methylphenyl)-3,5,5-trimethyl-1-hexanone, 665
[52196-48-2]	1-(5-Chloro-2-hydroxyphenyl)-1-octanone, 787
[52245-99-5]	4-(4-Hydroxy-3,5-dimethylphenyl)-4-oxo-1-butanoic acid, 444
[52375-87-8]	1-(3,4-Dimethoxyphenyl)-1-hexanone, 610
[52376-23-5]	1-(4-Bromo-2,5-dihydroxyphenyl)-1-butanone, 28
[52376-24-6]	1-(4-Bromo-2,5-dihydroxyphenyl)-1-butanone (Semicarbazone), 28
[52376-25-7]	1-(4-Bromo-2,5-dihydroxyphenyl)-1-pentanone, 481
[52376-26-8]	1-(4-Bromo-2,5-dihydroxyphenyl)-1-pentanone (Semicarbazone), 481
[52672-75-0]	1-(2-Hydroxy-5-methylphenyl)-1-dodecanone (Oxime, nickel complex), 960
[52751-45-8]	1-[2,6-Dihydroxy-4-(phenylmethoxy)phenyl]-1,3-butanedione, 333
[52754-68-4]	1-(4-Methoxyphenyl)-1-nonanone, 837
[52780-68-4]	1-(4-Hydroxy-3-methylphenyl)-1-butanone, 51
[52852-89-8]	1,5-Bis(2-hydroxyphenyl)-3-methyl-1,5-pentanedione, 528
[52856-20-9]	1-(2,6-Dimethoxyphenyl)-3-methyl-1-butanone, 179

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[52856-31-2]	1-(2,6-Dimethoxyphenyl)-3-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 179
[52922-74-4]	1-(2-Ethyloxyphenyl)-1-heptanone, 720
[53107-50-9]	1-(2,3-Dichloro-4-methoxyphenyl)-3-methyl-1-butanone, 185
[53107-51-0]	1-(2,3-Dichloro-4-methoxyphenyl)-3-methyl-2-methylene-1-butanone, 188
[53107-64-5]	6-Bromo-1-(2,3-dichloro-4-methoxyphenyl)-1-hexanone, 702
[53107-72-5]	7-Bromo-1-(2,3-dichloro-4-methoxyphenyl)-1-heptanone, 764
[53270-35-2]	1-(2,4-Dimethoxy-6-methylphenyl)-1,3-butanedione, 318
[53347-08-3]	1-(5-Chloro-3-ethyl-2-hydroxyphenyl)-1-butanone, 63
[53347-27-6]	1-(5-Chloro-3-ethyl-2-hydroxyphenyl)-1-pentanone, 500
[53347-28-7]	1-(5-Chloro-3-ethyl-2-hydroxyphenyl)-1-hexanone, 647
[53623-37-3]	4-(4-Ethoxyphenyl)-4-oxo-1-butanoic acid, 401
[53771-36-1]	3-Methyl-1-(3,4-dihydro-5,7-dihydroxy-2,2-dimethyl-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-8-yl)-1-butanone, 233
[53903-58-5]	2-Bromo-1-(4-hydroxyphenyl)-1-butanone, 269
[54011-26-6]	Methyl 4-(4′-methoxybiphenyl)-4-oxo-1-butanoate, 452
[54103-36-5]	1-(4-Methoxyphenyl)-1,3-pentanedione, 460
[54103-37-6]	1-(4-Methoxyphenyl)-4-phenyl-1,3-butanedione, 354
[54109-33-0]	1-(3,5-Dimethoxyphenyl)-1-pentanone-1-14C, 475
[54289-79-1]	1-(2,4-Dihydroxy-3-quinolinyl)-1-hexanone, 654
[54343-87-2]	6-Chloro-1-(2,3-dichloro-4-methoxyphenyl)-2-methylene-1-hexanone, 705
[54419-21-5]	1-(3,4-Dimethoxyphenyl)-1-butanone, 14
[54419-64-6]	1-(2,5-Dimethoxyphenyl)-1-butanone, 11
[54419-69-1]	1-(2,5-Dimethoxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 12
[54535-83-0]	1-(3,4-Dihydroxyphenyl)-1-hexadecanone, 1037
[54556-08-0]	1-(3,5-Dihexyl)-2,4,6-(trihydroxyphenyl)-1-hexanone, 694
[54614-64-1]	3-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone, 215
[54685-34-6]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-eicosanone, 1100
[54696-06-9]	1-(4-Methoxy-2-methylphenyl)-1-butanone, 51
[54874-25-8]	1-(2,4-Dimethoxyphenyl)-3-methyl-1-butanone, 178
[54963-60-9]	1-[5-Acetyl-2-hydroxy-3-(3-hydroxy-3-methyl-1-butenyl)phenyl]-3-methyl-1-butanone *(E)*, 381
[54963-61-0]	1-[5-Acetyl-2-hydroxy-3-(1-hydroxy-3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone, 381
[55007-22-2]	4-(2-Methoxy-5-methylphenyl)-4-oxo-1-butanoic acid, 434
[55049-56-4]	1-(3,5-Dimethoxyphenyl)-1-dodecanone, 949
[55382-31-5]	1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-3-methyl-1-butanone, 199
[55382-32-6]	1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-2-methyl-1-butanone, 135
[55469-24-4]	1-(4-Methoxyphenyl)-1-tridecanone, 996
[55507-71-6]	1-(2,3-Dichloro-4-hydroxyphenyl)-3,3-dimethyl-1-butanone, 252
[55507-79-4]	1-(2,3-Dichloro-4-hydroxyphenyl)-1-pentanone, 479
[55507-84-1]	1-(2,3-Dichloro-4-hydroxyphenyl)-1-heptanone, 732
[55576-64-2]	1-[3-[(3-Acetyl-2,6-dihydroxy-4-methoxy-5-methylphenyl)methyl]-5-[[2,6-dihydroxy-4-methoxy-3-methyl-5-(2-methyl-1-oxopropyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone, 168

(continued)

[55576-65-3]	1-[3,5-Bis[[2,6-dihydroxy-4-methoxy-3-methyl-5-(2-methyl-1-oxopropyl) phenyl]methyl]-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone, 168
[55576-66-4]	1-[3,5-Bis[[2,6-dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl] methyl]-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone (2*S*), 169
[55576-68-6]	1-[3,5-Bis[[2,6-dihydroxy-4-methoxy-3-methyl-5-(1-acetyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone, 346
[55785-59-6]	1,1′-[[2,4,6-Trihydroxy-5-(1-oxobutyl)-1,3-phenylene]bis[methylene-(2,4-dihydroxy-6-methoxy-5-methyl-3,1-phenylene)]]bis-1-butanone, 348
[55813-81-5]	1-(2-Hydroxy-5-methylphenyl)-3-methyl-1-butanone, 190
[55896-05-4]	1-(2-Hydroxy-4-methoxyphenyl)-1-undecanone, 931
[55917-79-8]	1-(2-Hydroxyphenyl)-1-dodecanone (Oxime, nickel complex), 940
[56116-77-9]	1-(4′-Methoxy[1,1′-biphenyl]-4-yl)-1-pentanone, 525
[56116-78-0]	1-(4′-Methoxy[1,1′-biphenyl]-4-yl)-1-hexanone, 680
[56116-79-1]	1-(4′-Methoxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56116-80-4]	1,1′-(4′-Methoxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56116-81-5]	1-(4′-Methoxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[56116-82-6]	1-(4′-Methoxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56116-87-1]	1-(4′-Ethoxy[1,1′-biphenyl]-4-yl)-1-hexanone, 680
[56116-88-2]	1-(4′-Ethyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56116-89-3]	1-(4′-Ethyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56116-90-6]	1-(4′-Ethyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[56116-91-7]	1-(4′-Ethyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56116-95-1]	1-(4′-Propyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 680
[56116-96-2]	1-(4′-Propyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56116-97-3]	1-(4′-Propyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56116-98-4]	1-(4′-Propyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[56116-99-5]	1-(4′-Propyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56117-03-4]	1-(4′-Butyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 680
[56117-04-5]	1-(4′-Butyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56117-05-6]	1-(4′-Butyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56117-06-7]	1-(4′-Butyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[56117-07-8]	1-(4′-Butyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56117-12-5]	1-(4′-Pentyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 680
[56117-13-6]	1-(4′-Pentyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56117-14-7]	1-(4′-Pentyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56117-15-8]	1-(4′-Pentyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[56117-16-9]	1-(4′-Pentyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56117-21-6]	1-(4′-Hexyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 680
[56117-22-7]	1-(4′-Hexyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56117-23-8]	1-(4′-Hexyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56117-24-9]	1-(4′-Hexyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[56117-25-0]	1-(4′-Hexyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56117-30-7]	1-(4′-Heptyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 681
[56117-31-8]	1-(4′-Heptyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56117-32-9]	1-(4′-Heptyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815

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[56117-33-0]	1-(4′-Heptyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56117-37-4]	1-(4′-Octyloxy[1,1′-biphenyl]-4-yl)-1-pentanone, 525
[56117-38-5]	1-(4′-Octyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 681
[56117-39-6]	1-(4′-Octyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56117-40-9]	1,1′-(4′-Octyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56117-41-0]	1-(4′-Octyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[56117-42-1]	1-(4′-Octyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56117-47-6]	1-(4′-Nonyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 681
[56117-48-7]	1-(4′-Nonyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56117-49-8]	1-(4′-Nonyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56117-50-1]	1-(4′-Nonyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 854
[56117-51-2]	1-(4′-Nonyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56117-56-7]	1-(4′-Decyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 681
[56117-57-8]	1-(4′-Decyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56117-58-9]	1-(4′-Decyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56117-59-0]	1-(4′-Decyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 854
[56117-60-3]	1-(4′-Decyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56117-65-8]	1-(4′-Dodecyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 681
[56117-66-9]	1-(4′-Dodecyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 757
[56117-67-0]	1-(4′-Dodecyloxy[1,1′-biphenyl]-4-yl)-1-octanone, 815
[56117-68-1]	1-(4′-Dodecyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 854
[56117-69-2]	1-(4′-Dodecyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[56134-29-3]	1-(2-Hydroxy-5-methoxyphenyl)-1-dodecanone, 962
[56134-31-7]	1-(3-Dodecyl-2-hydroxy-5-methoxyphenyl)-1-dodecanone, 989
[56134-34-0]	1-(2-Hydroxy-4,5-dimethoxyphenyl)-1-dodecanone, 966
[56134-35-1]	1-(2,4,5-Trimethoxyphenyl)-1-dodecanone, 951
[56189-90-3]	1-(4′-Heptyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[56226-93-8]	1-[3-[[2,6-Dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxy-5-methylphenyl]-1-butanone, 340
[56290-52-9]	1-(2-Methoxy-5-methylphenyl)-1,3-butanedione, 317
[56290-53-0]	1-(2-Methoxyphenyl)-1,3-butanedione, 309
[56397-48-9]	1-(6-Methoxy-3-methyl-2-benzofuranyl)-1-butanone, 79
[56426-10-9]	1-[4-(1,1,2,2-Tetrafluoroethyloxy)phenyl]-1-heptanone, 724
[56490-66-5]	1-[4-Hydroxy-3-(methylsulfonylmethyl)phenyl]-1-butanone, 77
[56490-73-4]	1-[3-(Methylsulfonylmethyl)-4-(phenylmethoxy)phenyl]-1-butanone, 77
[56490-82-5]	2-Bromo-1-[3-(methylsulfonylmethyl)-4-phenylmethoxy)phenyl] butanone, 273
[56490-86-9]	1-[(3-Chloromethyl)-4-hydroxyphenyl]-1-butanone, 45
[56686-30-7]	1-(2-Hydroxy-3-methylphenyl)-1,3-butanedione (Dioxime), 317
[56686-34-1]	1-(2-Hydroxy-5-methylphenyl)-1,3-butanedione (Dioxime), 317
[56871-93-3]	Methyl 4-(2-hydroxyphenyl)-4-oxo-1-butanoate, 399
[56872-07-2]	4-(3-Hydroxyphenyl)-4-oxo-1-butanoic acid, 399
[56872-21-0]	4-(3-Chloro-4-hydroxyphenyl)-4-oxo-1-butanoic acid, 422
[56872-34-5]	4-(3-Hydroxy-4-methylphenyl)-4-oxo-1-butanoic acid, 435
[56872-39-0]	4-(4-Hydroxyphenyl)-4-oxo-1-butanoic acid, 400

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[56872-41-4]	4-(4-Hydroxy-3-nitrophenyl)-4-oxo-1-butanoic acid, 426
[56872-54-9]	1-(5-Amino-2-hydroxyphenyl)-4-oxo-1-butanoic acid, 428
[56872-60-7]	Ethyl 4-(3,4-dimethoxyphenyl)-4-oxo-1-butanoate, 409
[56872-61-8]	Ethyl 4-(3,4-dihydroxyphenyl)-4-oxo-1-butanoate, 410
[57010-67-0]	4-Chloro-1-(3,4-dimethoxyphenyl)-1-butanone, 282
[57073-43-5]	1-[2-Hydroxy-4-[(2,2,4-trimethylpentyl)oxy]phenyl]-1-nonanone (Oxime), 862
[57073-45-7]	1-[2-Hydroxy-5-(2,2,4-trimethylpentyl)phenyl]-1-nonanone (Oxime), 862
[57080-91-8]	2-Ethyl-1-[2-hydroxy-4-(1-methylethyl)phenyl]-1-hexanone (Oxime), 669
[57080-92-9]	2-Ethyl-1-[2-hydroxy-4-(1-methylethyl)phenyl]-1-hexanone, 669
[57080-94-1]	1-(2-Hydroxy-4-methylphenyl)-14-methyl-1-pentadecanone, 1030
[57080-95-2]	1-(5-Chloro-2-hydroxy-4-methylphenyl)-2-ethyl-1-hexanone (Oxime), 656
[57080-96-3]	1-(5-Chloro-2-hydroxy-4-methylphenyl)-2-ethyl-1-hexanone, 656
[57080-97-4]	2-Ethyl-1-(2-hydroxy-4-methylphenyl)-1-hexanone (Oxime), 657
[57080-99-6]	2-Ethyl-1-(2-hydroxy-4-methylphenyl)-1-hexanone, 657
[57125-28-7]	1-(2-Hydroxy-4-methylphenyl)-14-methyl-1-pentadecanone (Oxime), 1030
[57133-44-5]	1-[2-Hydroxy-3,5-di(1-methylethyl)phenyl]-1-pentanone (ion) (1-), (radical ion) (1-), 527
[57262-58-5]	7-(2-Hydroxyphenyl)-7-oxo-1-heptanoic acid, 766
[57314-80-4]	1-(2-Hydroxy-5-methoxyphenyl)-1-pentanone, 496
[57314-81-5]	1-(2-Hydroxy-5-methoxyphenyl)-1-butanone, 55
[57596-02-8]	4-(3,4-Dihydroxyphenyl)-4-oxo-1-butanoic acid, 408
[57640-96-7]	9-(3,4-Dimethoxyphenyl)-9-oxo-1-nonanoic acid, 864
[57641-18-6]	Methyl 6-(3,4-dimethoxyphenyl)-6-oxo-1-hexanoate, 714
[57641-19-7]	Ethyl 8-(3,4-dimethoxyphenyl)-8-oxo-1-octanoic acid, 831
[57641-20-0]	Ethyl 9-(3,4-dimethoxyphenyl)-9-oxo-1-nonanoate, 864
[57765-52-3]	1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-1-pentanone, 502
[57835-34-4]	1-(2-Hydroxyphenyl)-1-octanone (Oxime), 773
[57840-53-6]	6-Bromo-1-(4-Chloro-2-methoxyphenyl)-1-hexanone, 703
[57840-61-6]	6-Bromo-1-(4-methoxyphenyl)-1-hexanone, 698
[57863-94-2]	1-(2,4,5-Trihydroxyphenyl)-1-octadecanone, 1068
[57991-55-6]	1-(2,4-Dihydroxyphenyl)-1-pentanone (Oxime), 471
[58185-73-2]	6-(2-Hydroxy-3,4,6-trimethylphenyl)-6-oxo-1-hexanoic acid, 717
[58185-75-4]	7-(2-Hydroxy-3,4,6-trimethylphenyl)-7-oxo-1-heptanoic acid, 770
[58185-77-6]	10-(2-Hydroxy-3,4,6-trimethylphenyl)-10-oxo-1-decanone, 922
[58218-16-9]	1-(2-Hydroxy-4-methylphenyl)-1,3-butanedione, 317
[58218-17-0]	1-(2-Hydroxy-3-methylphenyl)-1,3-butanedione, 317
[58530-24-8]	1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1,3-butanedione, 322
[59010-46-7]	4-(2-Hydroxy-4-methylphenyl)-4-oxo-1-butanoic acid, 433
[59010-47-8]	Methyl 4-(2-hydroxy-4-methylphenyl)-4-oxo-1-butanoate, 434
[59010-62-7]	4-(2-Hydroxyphenyl)-3-methyl-4-oxo-1-butanoic acid, 414
[59043-82-2]	1-(2,3-Dichloro-4-methoxyphenyl)-2-methylene-1-butanone, 131
[59445-62-4]	1-(2-Acetyl-4-methoxy-7-benzofuranyl)-1-dodecanone, 971
[59445-63-5]	1-(2-Acetyl-4-methoxy-7-benzofuranyl)-1-octadecanone, 1081
[59445-72-6]	1-(2-Acetyl-7-methoxy-4-benzofuranyl)-1-hexanone, 661

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[59445-73-7]	1-(2-Acetyl-7-methoxy-4-benzofuranyl)-1-dodecanone, 971
[59445-74-8]	1-(2-Acetyl-7-methoxy-4-benzofuranyl)-1-octadecanone, 1081
[59445-81-7]	1-(2-Acetyl-7-hydroxy-4-benzofuranyl)-1-hexanone, 661
[59701-65-4]	4-(2,5-Dihydroxyphenyl)-4-oxo-1-butanoic acid, 405
[59701-66-5]	Methyl 4-(2-hydroxy-5-methoxyphenyl)-4-oxo-1-butanoate, 440
[60159-70-8]	1-(2-Ethoxyphenyl)-1,3-butanedione, 310
[60170-85-6]	1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-decanone, 896
[60202-03-1]	1-(2-Hydroxy-4-methylphenyl)-1-dodecanone (Oxime, cobalt alloys), 959
[60474-43-3]	1-(3-Chloro-2-hydroxyphenyl)-1-butanone, 29
[60488-53-1]	1-(2-Hydroxy-4-methoxy-5-methylphenyl)-1-dodecanone, 966
[60488-57-5]	1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1-dodecanone, 966
[60658-72-2]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-1,3-hexanedione, 647
[60697-65-6]	1-(8-Hydroxy-7-quinolinyl)-1-heptanone, 745
[60755-22-8]	1-(4-Methoxyphenyl)-4-phenyl-1,4-butanedione, 357
[60831-55-2]	1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-3-methyl-1-butanone, 207
[60985-68-4]	1-[4-(2-Bromoethyloxy)phenyl]-1-heptanone, 724
[61053-78-9]	4-Chloro-1-(4-fluoro-2-hydroxyphenyl)-1-butanone, 278
[61363-13-1]	1-(3,4-Methylenedioxyphenyl)-1,4-pentanedione, 487
[61468-98-2]	5-(4-Methoxyphenyl)-2,2-dimethyl-5-oxo-1-pentanoic acid, 584
[62036-46-8]	1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1,3-pentanedione, 499
[62036-47-9]	1-(2,4-Dimethoxy-6-methylphenyl)-1,3-pentanedione, 488
[62060-62-2]	1-(2,4,5-Trihydroxyphenyl)-1-pentanone, 476
[62153-16-6]	1-(8-Hydroxy-7-quinolinyl)-1-heptanone (Copper complex), 745
[62170-25-6]	1-(4-Methoxyphenyl)-1-octanone, 775
[62189-86-0]	1-(8-Ethyloxy-7-quinolinyl)-1-heptanone, 745
[62189-88-2]	1-(8-Hydroxy-5-quinolinyl)-1-heptanone, 745
[62406-99-9]	1-(2,4,5-Trimethoxyphenyl)-1,3-butanedione, 314
[62407-00-5]	1-(2,4,5-Trimethoxyphenyl)-2-methyl-1,3-butanedione, 315
[62439-32-1]	1-(4-Hydroxyphenyl)-3-methyl-1-pentanone (+), 554
[62458-64-4]	1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone, 378
[62545-32-8]	1-[4-(Acetyloxy)-2,6-dihydroxyphenyl]-3-methyl-1-butanone, 196
[62545-33-9]	1-[2-(Acetyloxy)-4,6-dihydroxyphenyl]-3-methyl-1-butanone, 195
[62596-41-2]	1-(4-Methoxyphenyl)-1,4-hexanedione, 597
[62643-23-6]	7-(2,4-Dimethoxy-6-methylphenyl)-3,5,7-trioxo-1-heptanoic acid, 768
[62643-36-1]	1-(2,4-Dimethoxy-6-methylphenyl)-1,3,5-hexanetrione, 629
[62643-39-4]	1-(2-Benzyloxy-4-methoxy-6-methylphenyl)-1,3,5-hexanetrione, 645
[62643-41-8]	Methyl 7-(2-benzyloxy-4-methoxy-6-methylphenyl)-3,5,7-trioxo-1-heptanoate, 770
[62810-51-9]	1-(3-Hydroxyphenyl)-1-pentanone, 464
[62893-18-9]	4-(3-Hydroxy-4-nitrophenyl)-4-oxo-1-butanoic acid, 426
[62903-11-1]	4-(3,5-Dichloro-2-hydroxy-4-methylphenyl)-4-oxo-1-butanoic acid, 430
[62903-21-3]	4-(5-Chloro-2-hydroxy-4-methylphenyl)-4-oxo-1-butanoic acid, 432
[62903-22-4]	4-(3,5-Dichloro-2-hydroxyphenyl)-4-oxo-1-butanoic acid, 420
[62903-23-5]	4-(5-Chloro-2-hydroxyphenyl)-4-oxo-1-butanoic acid, 423
[62903-25-7]	4-(3,5-Dichloro-4-hydroxyphenyl)-4-oxo-1-butanoic acid, 420

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[63023-50-7]	Methyl 5-(2-hydroxy-4-methylphenyl)-5-oxo-1-pentanoate, 591
[63134-27-0]	1-(2,5-Dihydroxy-4-octylphenyl)-1-octanone, 823
[63171-82-4]	Tert-Butyl 4-(2,5-dimethoxyphenyl)-4-oxo-1-butanoate, 407
[63213-25-2]	4-(2,4,6-Trimethoxyphenyl)-4-oxo-1-butanoic acid, 414
[63213-26-3]	Ethyl 4-(2,4,5-triethoxyphenyl)-4-oxo-1-butanoate, 413
[63213-28-5]	4-(2,4,5-Trihydroxyphenyl)-4-oxo-1-butanoic acid, 412
[63213-31-0]	1-(2,4,5-Triethoxyphenyl)-1-butanone, 18
[63213-32-1]	4-(2,4,5-Triethoxyphenyl)-2-methyl-4-oxo-1-butanoic acid, 418
[63213-33-2]	5-(2,4,5-Triethoxyphenyl)-5-oxo-1-pentanoic acid, 583
[63213-34-3]	4-(2,4,5-Triethoxyphenyl)-2,4-dioxo-1-butanoic acid, 398
[63213-39-8]	4-(2,4,5-Tripropoxyphenyl)-4-oxo-1-butanoic acid, 413
[63213-40-1]	4-(5-Bromo-2,4-dimethoxyphenyl)-4-oxo-1-butanoic acid, 421
[63213-41-2]	4-(2,3,4-Trimethoxyphenyl)-4-oxo-1-butanoic acid, 411
[63213-42-3]	4-(3,4-Diethoxyphenyl)-4-oxo-1-butanoic acid, 409
[63213-44-5]	Ethyl 4-(2,4,5-triethoxyphenyl)-2,4-dioxo-1-butanoate, 398
[63213-45-6]	4-(4,5-Diethoxy-2-hydroxyphenyl)-4-oxo-1-butanoic acid, 450
[63213-46-7]	4-(2,5-Diethoxyphenyl)-4-oxo-1-butanoic acid, 407
[63213-94-5]	4-(5-Chloro-2-methoxyphenyl)-4-oxo-1-butanoic acid, 424
[63335-23-9]	1-(2,6-Dihydroxyphenyl)-9-phenyl-1-nonanone, 855
[63335-24-0]	1-(2,6-Dihydroxyphenyl)-9-(4-hydroxyphenyl)-1-nonanone, 855
[63335-25-1]	1-(2,6-Dihydroxyphenyl)-9-(3,4-dihydroxyphenyl)-1-nonanone, 856
[63335-26-2]	9-(1,3-Benzodioxol-5-yl)-1-(2,6-dihydroxyphenyl)-1-nonanone, 857
[63411-80-3]	1-(2,6-Dihydroxyphenyl)-1-pentanone, 472
[63424-82-8]	3-Amino-1-(4-hydroxyphenyl)-1-dodecanone (Hydrochloride), 953
[63424-84-0]	2-Bromo-1-(4-methoxyphenyl)-1-dodecanone, 993
[63442-82-0]	1-(3-Methoxyphenyl)-1-decanone, 869
[63442-83-1]	1-(3-Methoxyphenyl)-1-dodecanone, 941
[63442-84-2]	1-(3-Methoxyphenyl)-1-hexadecanone, 1032
[63442-85-3]	1-(3-Methoxyphenyl)-1-octadecanone, 1063
[63442-86-4]	1-(3-Hydroxyphenyl)-1-dodecanone, 941
[63442-87-5]	1-(3-Hydroxyphenyl)-1-hexadecanone, 1032
[63442-88-6]	1-(3-Hydroxyphenyl)-1-octadecanone, 1063
[63467-20-9]	5-(2,5-Dimethoxyphenyl)-5-oxo-1-pentanoic acid, 581
[63471-88-5]	4-(4-Butoxyphenyl)-4-oxo-1-butanoic acid, 402
[63480-88-6]	1-(3-Hydroxyphenyl)-1-decanone, 869
[63494-45-1]	1-(2-Hydroxy-5-pentylphenyl)-1-pentanone, 513
[63828-97-7]	2-Bromo-1-(3,4-dimethoxyphenyl)-1-dodecanone, 993
[63829-15-2]	1-[3-(Dimethylaminomethyl)-4-methoxyphenyl]-1-dodecanone, 971
[63829-20-9]	1-(4-Methoxyphenyl)-1-dodecanone, 943
[63861-11-0]	2,4,6-Trihydroxy-3-methyl-5-(3-methyl-1-oxobutyl)benzaldehyde, 389
[63861-20-1]	2,4-Dihydroxy-6-methoxy-5-methyl-3-(3-methyl-1-oxobutyl) benzaldehyde, 390
[63861-21-2]	2,6-Dihydroxy-4-methoxy-5-methyl-3-(3-methyl-1-oxobutyl) benzaldehyde, 390
[64142-23-0]	1-(4-Hydroxy-3-methoxyphenyl)-1-butanone, 56

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[64779-96-0]	5-Butyryl-2-methoxybenzoic acid, 44
[64808-71-5]	Methyl 5-butyryl-2-methoxybenzoate, 44
[64808-72-6]	5-(1-Oxobutyl)-2-methoxybenzoyl chloride, 41
[64957-70-6]	1-(2-Methoxyphenyl)-1-pentanone (2,4-Dinitrophenylhydrazone), 463
[65240-03-1]	2,2,3,3,4,4,4-Heptafluoro-1-(2,4-dihydroxyphenyl)-1-butanone, 289
[65240-04-2]	2,2,3,3,4,4,4-Heptafluoro-1-(2,4-dihydroxy-3-methylphenyl)-1-butanone, 290
[65240-06-4]	1-(2,4-Dihydroxy-3-methylphenyl)-2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-1-octanone, 829
[65242-00-4]	4-Chloro-1-(2-hydroxy-4-methoxyphenyl)-1-butanone, 285
[65547-46-8]	1-(2,3,6-Trimethoxyphenyl)-1,3-butanedione, 324
[65547-48-0]	1-(2,3,4-Trimethoxyphenyl)-1,3-butanedione, 323
[65547-50-4]	1-(2,5-Dimethoxyphenyl)-1,3-butanedione, 313
[65547-52-6]	1-(2,3-Dimethoxyphenyl)-1,3-butanedione, 312
[65547-54-8]	1-(2,4-Dimethoxyphenyl)-1,3-butanedione, 312
[65547-60-6]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-1,3-butanedione, 324
[65547-62-8]	1-(2-Hydroxy-3,6-dimethoxyphenyl)-1,3-butanedione, 323
[65547-63-9]	1-(2-Hydroxy-6-methoxyphenyl)-1,3-butanedione, 320
[65547-68-4]	1-(2-Hydroxy-4,5-dimethoxyphenyl)-1,3-butanedione, 324
[65547-70-8]	1-[4,5-Dimethoxy-2-(phenylmethoxy)phenyl]-1,3-butanedione, 324
[65547-71-9]	1-(6-Hydroxy-2,3-dimethoxyphenyl)-1,3-butanedione, 325
[65547-75-3]	1-(2-Hydroxy-3,4-dimethoxyphenyl)-1,3-butanedione, 323
[65547-78-6]	1-(2-Hydroxy-3-methoxyphenyl)-1,3-butanedione, 319
[65547-81-1]	1-(2-Hydroxy-5-methoxyphenyl)-1,3-butanedione, 320
[65547-83-3]	1-[5-methoxy-(2-phenylmethoxy)phenyl]-1,3-butanedione, 320
[65687-21-0]	1-(3′-Chloro-4′-methoxy[1,1′-biphenyl]-4-yl)-1-octanone, 814
[65792-31-6]	2-Methyl-1-(2,4,6-trihydroxy-3,5-dimethylphenyl)-1-butanone, 136
[65897-66-7]	1-(5-Chloro-2-hydroxyphenyl)-1,3-butanedione, 316
[66053-97-2]	1-(3,4-Dimethoxyphenyl)-1-pentanone, 473
[66123-43-1]	Ethyl 4-(4-hydroxyphenyl)-4-oxo-1-butanoate, 402
[66123-78-2]	Ethyl 5-(4-hydroxyphenyl)-5-oxo-1-pentanoate, 580
[66333-82-2]	1-(4-Methoxyphenyl)-3-methyl-1-pentanone, 554
[66346-51-8]	1-(2,4-Dimethoxy-6-methylphenyl)-1,3-hexanedione, 633
[66468-51-7]	1-(4-Ethoxy-2-hydroxyphenyl)-1-decanone (Copper complex), 888
[66475-97-6]	1-(3-Decanoyloxy-4-methoxyphenyl)-1-decanone, 885
[66476-00-4]	1-(3-Hydroxy-4-methoxyphenyl)-1-decanone, 885
[66476-01-5]	1-(4-Hydroxy-3-methoxyphenyl)-1-decanone, 885
[66711-56-6]	1-[2,4,6-Trihydroxy-3-(2-methylpropyl)phenyl]-1-hexanone, 666
[66757-68-4]	5-(2,4-Dimethoxy-6-methylphenyl)-3,5-dioxo-1-pentanoic acid, 589
[66832-64-2]	Methyl 5-(2-hydroxy-4-methoxyphenyl)-5-oxo-1-pentanoate, 594
[66832-66-4]	5-Chloro-1-(2-hydroxy-4-methoxyphenyl)-1-pentanone, 575
[67049-69-8]	1-(3,4-Dihydroxyphenyl)-2-methyl-1-butanone, 128
[67049-70-1]	1-(3,4-Dimethoxyphenyl)-2-methyl-1-butanone, 128
[67114-29-8]	1-(3,4-Dihydroxyphenyl)-2-ethyl-3-methyl-1-butanone, 184
[67188-50-5]	1-(5,8-Dimethoxy-4-methyl-2-quinolinyl)-1-nonanone, 847

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[67231-33-8]	1-(2,3,4,6-Tetramethoxyphenyl)-1,3-butanedione, 328
[67231-43-0]	1-(2,3,4,5-Tetramethoxyphenyl)-1,3-butanedione, 328
[67231-44-1]	1-(2,3,4,5,6-Pentamethoxyphenyl)-1,3-butanedione, 331
[67231-46-3]	1-(2-Hydroxy-3,4,5-trimethoxyphenyl)-1,3-butanedione, 328
[67231-48-5]	1-(2-Hydroxy-3,4,5,6-tetramethoxyphenyl)-1,3-butanedione, 331
[67239-25-2]	1-(3,4-Dihydroxyphenyl)-3-methyl-1-butanone, 179
[67405-48-5]	4-(4-Methoxy-2-methylphenyl)-4-oxo-1-butanoic acid, 435
[67548-60-1]	1-(4-Chloro-2-hydroxyphenyl)-1-nonanone, 842
[67548-61-2]	1-(3-Bromo-4-hydroxyphenyl)-1-pentanone, 480
[67548-62-3]	1-(5-Bromo-2-hydroxyphenyl)-1-pentanone, 481
[67756-15-4]	1-(4-Methoxyphenyl)-1,4-decanedione, 867
[67756-16-5]	1-(4-Chlorophenyl)-4-(4-methoxyphenyl)-1,4-butanedione, 357
[67756-19-8]	1-(2,4-Dimethoxyphenyl)-1,4-pentanedione, 461
[67756-20-1]	1-(2,4-Dimethoxyphenyl)-1,4-hexanedione, 597
[67756-21-2]	1-(2,4-Dimethoxyphenyl)-1,4-decanedione, 867
[67756-23-4]	1-(3,4-Dimethoxyphenyl)-1,4-hexanedione, 597
[67756-24-5]	1-(3,4-Dimethoxyphenyl)-1,4-decanedione, 868
[67756-25-6]	1-(3,4-Dimethoxyphenyl)-4-phenyl-1,4-butanedione, 357
[68223-30-3]	1,1′-[Methylenebis(2,4,6-trihydroxy-3,5-phenylene)]bis-1-butanone, 345
[68223-33-6]	1,1′,1″,1‴-[Methylenebis(2,4,6-trihydroxy-5,1,3-benzenetriyl)] bis-3-methyl-1-butanone, 346
[68223-34-7]	1,1′-Methylenebis(2,4,6-trihydroxy-3,5,1-phenylene)bis-1-hexanone, 695
[68223-37-0]	1,1′-[Methylenebis(2,4,6-trihydroxy-3-acetyl-5,1-phenylene)] bis-1-butanone, 341
[68223-39-2]	1-[3-[(3,5-Dipropionyl)-2,4,6-trihydroxyphenylmethyl]-2,4,6-trihydroxy-5-methylphenyl]-1-butanone, 339
[68223-50-7]	1-[3-(3-Acetyl-5-butyryl-2,4,6-trihydroxyphenylmethyl)-2,4,6-trihydroxy-5-methylphenyl]-1-butanone, 338
[68436-75-9]	1-[(4-methoxy-6-methyl-2-phenylmethoxy)phenyl]-1,3-butanedione, 322
[68436-79-3]	1-[4,6-Dimethoxy-2-(phenylmethoxy)phenyl]-1,3-butanedione, 325
[68486-75-9]	1-(2-Hydroxy-3,4-dimethoxyphenyl)-4-oxo-1-butanoic acid, 446
[68754-16-5]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-methyl-1-butanone, 199
[69271-91-6]	1-(4-Hydroxy-3,5-dimethoxyphenyl)-1-butanone, 76
[69287-13-4]	1-(4-Methoxyphenyl)-1-heptanone, 723
[69299-76-9]	Uliginosin A-iBiV, 346
[69480-05-3]	1-(2,6-Dihydroxy-4-methoxyphenyl)-1-pentanone, 498
[69480-08-6]	1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-1-butanone, 84
[69618-10-6]	1,4-Bis(2-acetyloxy-5-methylphenyl)-1,4-butanedione, 366
[69618-11-7]	1,4-Bis(2-methoxy-5-methylphenyl)-1,4-butanedione, 367
[69639-78-7]	1-(5-Bromo-2-methoxyphenyl)-4-chloro-1-butanone, 277
[69639-79-8]	1-(5-Bromo-2-hydroxyphenyl)-4-chloro-1-butanone, 277
[69657-35-8]	1-[3-(Chloromethyl)-4-methoxyphenyl]-1-undecanone, 930
[69657-36-9]	1-(4-Methoxyphenyl)-1-undecanone, 924
[69916-08-1]	1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone, 97
[69916-09-2]	1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-pentanone, 512

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[69916-10-5]	1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-hexanone, 668
[69916-11-6]	1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-heptanone, 751
[69916-12-7]	1-(2,4,6-Trihydroxy-3-pentylphenyl)-1-pentanone, 515
[70079-24-2]	1-(4-Hydroxy-3-nitrophenyl)-1-dodecanone, 956
[70079-25-3]	1-(4-Hydroxy-3-nitrophenyl)-1-hexanone, 627
[70079-26-4]	1-(4-Hydroxy-3-nitrophenyl)-1-octanone, 788
[70079-27-5]	1-(4-Hydroxy-3-nitrophenyl)-1-decanone, 881
[70079-28-6]	1-(4-Hydroxy-3-nitrophenyl)-1-hexadecanone, 1040
[70079-29-7]	1-(4-Hydroxy-3-nitrophenyl)-1-octadecanone, 1072
[70206-42-7]	3-[4-(2-Chloroethyl)phenyl]-1-(2-hydroxyphenyl)-1-hexanone, 688
[70206-43-8]	3-[4-(2-Chloroethyl)phenyl]-2-hydroxy-1-(2-hydroxyphenyl)-1-hexanone, 688
[70219-82-8]	1-[2,6-Dihydroxy-4-[(3-methyl-2-butenyl)oxy]phenyl]-2-methyl-1-butanone, 142
[70219-89-5]	1-[2,4-Dihydroxy-3,6-dimethoxy-5-(3-methyl-2-butenyl)phenyl]-1-butanone, 111
[70219-90-8]	1-[2,4-Diacetyloxy-3,6-dimethoxy-5-(3-methyl-2-butenyl)phenyl]-1-butanone, 111
[70233-75-9]	3,4-Dihydro-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one, 149
[70627-61-1]	1-(3,5-Dihydroxyphenyl)-1-pentanone, 473
[70977-53-6]	N-(3-Butanoyl-2-hydroxy-5-methylphenyl)-1*H*-tetrazole-5-carboxamide, 80
[70978-14-2]	N-(3-Butanoyl-2-hydroxy-5-methylphenyl)-1-phenylmethyltetrazole-5-carboxamide, 118
[70978-45-9]	1-(2-Hydroxy-5-methyl-3-nitrophenyl)-1-butanone, 46
[70978-64-2]	1-(3-Amino-2-hydroxy-5-methylphenyl)-1-butanone, 60
[71248-64-1]	1,6-Bis(4-methoxyphenyl)-2,5-dibromo-1,6-hexanedione, 671
[71290-02-3]	1-(4,5-Dichloro-2-hydroxyphenyl)-1-butanone, 25
[71354-31-9]	5-(3-Chloro-4-methoxyphenyl)-5-oxo-1-pentanoic acid, 587
[71354-32-0]	Methyl 5-(3-chloro-4-methoxyphenyl)-5-oxo-1-pentanoate, 587
[71354-33-1]	5-(2-Chloro-5-methoxyphenyl)-5-oxo-1-pentanoic acid, 587
[71354-34-2]	Methyl 5-(2-chloro-5-methoxyphenyl)-5-oxo-1-pentanoate, 587
[71354-35-3]	5-(2-Chloro-4-methoxyphenyl)-5-oxo-1-pentanoic acid, 586
[71354-36-4]	Methyl 5-(2-chloro-4-methoxyphenyl)-5-oxo-1-pentanoate, 586
[71491-29-7]	1-(2-Hydroxy-5-methylphenyl)-1-decanone (Oxime), 883
[71539-60-1]	2-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone, 142
[71539-61-2]	2-Methyl-1-[2,4,6-tris(acetyloxy)-3-(3-methyl-2-butenyl)phenyl]-1-butanone, 142
[71539-62-3]	1-[2,4-Dihydroxy-6-methoxy-3-(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone, 144
[71539-64-5]	1-[2,4-Diacetyloxy-6-methoxy-3-(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone, 145
[71539-67-8]	1-[4-[(3,7-Dimethyl-2,6-octadienyl)oxy]-2,6-dihydroxyphenyl]-2-methyl-1-butanone (*E*), 151

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[71539-68-9]	1-[4-[(3,7-Dimethyl-2,6-octadienyl)oxy]-2,6-diacetyloxyphenyl]-2-methyl-1-butanone (*E*), 151
[71539-70-3]	1-(3,4-Dihydro-5-hydroxy-7-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-2-methyl-1-butanone, 145
[71898-88-9]	1-(2-Methoxy-4-methylphenyl)-3-methyl-1-butanone, 190
[72008-04-9]	1-[3-(3,7-Dimethyl-2,6-octadienyl)-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone (*E*), 151
[72008-09-4]	1-[3-(3,7-Dimethyl-2,6-octadienyl)-2,4,6-tris(acetyloxy)phenyl]-2-methyl-1-butanone, 152
[72046-93-6]	1-(2,5-Dihexadecyloxy-4-methylphenyl)-1-dodecanone, 961
[72047-09-7]	1-(2,5-Didodecyloxyphenyl)-1-dodecanone, 947
[72057-94-4]	1-(4′-Hexanoyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 681
[72236-93-2]	5-Bromo-1-[4-methoxy-2-methyl-5-(1-methylethyl)phenyl]-1-pentanone, 576
[72236-94-3]	6-Bromo-1-[4-methoxy-2-methyl-5-(1-methylethyl)phenyl]-1-hexanone, 708
[72236-95-4]	10-Bromo-1-[4-methoxy-2-methyl-5-(1-methylethyl)phenyl]-1-decanone, 917
[72247-02-0]	1-(5-Ethyl-2-methoxyphenyl)-3-methyl-1-butanone, 197
[72306-95-7]	1-(2-Hydroxy-5-methoxy-3-octadecylphenyl)-1-octadecanone, 1088
[72306-96-8]	1-(2,5-Dihydroxy-3-octadecylphenyl)-1-octadecanone, 1087
[72306-97-9]	1-(2,5-Dihydroxy-4-octadecylphenyl)-1-octadecanone, 1088
[72327-93-6]	1-(2,4,6-Tribenzyloxyphenyl)-1,3,5,7-octanetetraone, 771
[72327-96-9]	1-(2,4,6-Trihydroxyphenyl)-1,3,5,7-octanetetraone, 771
[72424-10-3]	1-(3-Methoxyphenyl)-1-undecanone, 923
[72674-91-0]	Methyl 9-(3,4-methylenedioxyphenyl)-9-oxo-1-nonanoate, 864
[72724-26-6]	1-(2-Hydroxy-4-methylphenyl)-1-dodecanone, 958
[72782-46-8]	1-[2-Hydroxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-octanone (Oxime), 822
[72793-41-0]	3-[4-(2-Chloroethyl)phenyl]-2-hydroxy-1-(2-hydroxyphenyl)-1-hexanone, 688
[72793-42-1]	3-[4-(2-Chloroethyl)phenyl]-2-hydroxy-1-(2-hydroxyphenyl)-1-hexanone, 688
[72935-10-5]	2-(5,7-Dihydroxy-8-isovaleryl-2,2-dimethyl-2*H*-chromen-6-ylmethyl)-3,5-dihydroxy-6-isobutyryl-4,4-dimethyl-2,5-cyclohexadiene-1-one, 345
[72935-11-6]	2-(5,7-Dihydroxy-6-isovaleryl-2,2-dimethyl-2*H*-chromen-8-ylmethyl)-3,5-dihydroxy-6-isobutyryl-4,4-dimethyl-2,5-cyclohexadiene-1-one, 345
[73213-21-5]	1-(4,6-Dimethoxy-1,3-benzodioxol-5-yl)-2-methyl-1-butanone, 133
[73694-18-5]	1-(4,6-Dihydroxy-2,3-dimethoxyphenyl)-2-methyl-1-butanone, 137
[73694-27-6]	1-(4,6-Diacetyloxy-2,3-dimethoxyphenyl)-2-methyl-1-butanone, 137
[73991-79-4]	1-[2-Hydroxy-3,5-di(1-methylethyl)phenyl]-1-pentanone, 527
[74061-22-6]	1-(2,3-Dihydroxy-5-octadecylphenyl)-1-octadecanone, 1087
[74261-29-3]	1-[4-(4-Bromophenyloxy)phenyl]-1-nonanone, 837
[74277-78-4]	4-(4′-Hydroxybiphenyl)-4-oxo-1-butanoic acid, 451
[74362-69-9]	4-(4-Ethoxy-3-nitrophenyl)-4-oxo-1-butanoic acid, 426
[74477-96-6]	1-(2,4,6-Trihydroxy-3-pentylphenyl)-1-butanone, 100
[74477-97-7]	1-[2,4,6-Trihydroxy-3-(3-methylbutyl)phenyl]-1-butanone, 100

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[74477-98-8]	1-[2,4,6-Trihydroxy-3-(3-methylbutyl)phenyl]-1-pentanone, 514
[74477-99-9]	1-[2,4,6-Trihydroxy-3-(2-propenyl)phenyl]-1-pentanone, 504
[74478-03-8]	3-Methyl-1-(2,4,6-trihydroxy-3-pentylphenyl)-1-butanone, 217
[74478-04-9]	1-(2,4,6-Trihydroxy-3-pentylphenyl)-1-hexanone, 671
[74478-05-0]	1-[2,4,6-Trihydroxy-3-(3-methylbutyl)phenyl]-1-hexanone, 670
[74478-06-1]	1-[2,4,6-Trihydroxy-3-(2-propenyl)phenyl]-1-hexanone, 655
[74478-07-2]	1-[3-(2-Butenyl)-2,4,6-trihydroxyphenyl]-1-hexanone, 662
[74478-08-3]	1-[2,4,6-Trihydroxy-3-(2-methyl-2-propenyl)phenyl]-1-hexanone, 663
[74478-09-4]	4-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-buten-1-yl)phenyl]-1-pentanone, 550
[74478-10-7]	1-[2,4,6-Trihydroxy-3-methylphenyl]-1-octanone, 797
[74478-11-8]	1-(2,4,6-Trihydroxyphenyl)-1-nonanone, 840
[74478-12-9]	1-(2,4,6-Trihydroxy-3-pentylphenyl)-1-decanone, 898
[74478-13-0]	1-[2,4,6-Trihydroxy-3-(3-methylbutyl)phenyl]-1-decanone, 898
[74478-14-1]	1-(2,4,6-Trihydroxyphenyl)-1-undecanone, 928
[74571-50-9]	1-(5-Methoxy-2-methylphenyl)-1-pentanone, 494
[74571-52-1]	1-(5-Methoxy-2-methylphenyl)-1-pentanone (2,4-Dinitrophenylhydrazone), 495
[74604-06-1]	1-(2-Hydroxy-5-methylphenyl)-1-heptanone (Oxime), 739
[74604-07-2]	1-(2-Hydroxy-5-methyl-3-nitrophenyl)-1-octanone (Oxime), 791
[74604-08-3]	1-(3-Chloro-2-hydroxy-5-methylphenyl)-1-octanone (Oxime), 790
[74604-11-8]	1-(2-Hydroxy-5-octylphenyl)-1-octanone (Oxime), 822
[74604-13-0]	1-(2-Hydroxy-5-methylphenyl)-1-heptanone, 738
[74604-14-1]	1-(2-Hydroxy-5-methyl-3-nitrophenyl)-1-octanone, 791
[74604-16-3]	1-(3-Chloro-2-hydroxy-5-methylphenyl)-1-octanone, 790
[74604-17-4]	2-Ethyl-1-(2-hydroxy-5-methylphenyl)-1-hexanone, 657
[74604-21-0]	1-(2-Hydroxy-5-octylphenyl)-1-octanone, 822
[74832-95-4]	1-(3,5-Dichloro-2-hydroxyphenyl)-1-octanone (Oxime), 786
[74832-96-5]	1-(3,5-Dibromo-2-hydroxyphenyl)-1-octanone (Oxime), 785
[74882-02-3]	Methyl 1-(2-hydroxy-3,4-dimethoxyphenyl)-4-oxo-1-butanoate, 446
[74882-03-4]	4-(2,3-Dihydroxy-4-methoxyphenyl)-4-oxo-1-butanoic acid, 441
[74882-04-5]	4-(2,3,4-Trihydroxyphenyl)-4-oxo-1-butanoic acid, 410
[74965-90-5]	4-Hydroxy-3-(1-oxohexadecyl)-2*H*-1-benzopyran-2-one, 1045
[75058-74-1]	1-(3′-Bromo-4′-methoxy[1,1′-biphenyl]-4-yl)-1-octanone, 814
[75060-45-6]	1-[5-(1,1-Dimethylethyl)-2-methoxyphenyl]-1-pentanone, 508
[75060-46-7]	1-[5-(1,1-Dimethylethyl)-2-methoxyphenyl]-1-butanone, 90
[75060-52-5]	1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-pentanone, 508
[75060-53-6]	1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-butanone, 90
[75060-70-7]	1-[(3-Aminomethyl)-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-pentanone (Hydrochloride), 515
[75060-71-8]	1-[3-(Aminomethyl)-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-butanone (Hydrochloride), 101
[75060-95-6]	1-[(3-Aminomethyl)-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-pentanone, 515
[75160-39-3]	1-(2-Allyloxy-4,6-dimethoxyphenyl)-1,3-butanedione, 325

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[75160-45-1]	1-(2-Allyloxy-4-methoxy-6-methylphenyl)-1,3-butanedione, 322
[75218-94-9]	1-(2-Hydroxy-3,4-dimethoxyphenyl)-1-butanone, 74
[75343-08-7]	4-Chloro-1-(4-ethoxyphenyl)-1-butanone, 280
[75343-28-1]	4-Chloro-1-(4-ethoxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 280
[75349-76-7]	4-Chloro-1-(4-methoxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 280
[75487-43-3]	1-(2-Hydroxy-5-methylphenyl)-1-nonanone, 844
[75487-44-4]	1-(2-Hydroxy-5-methylphenyl)-1-dodecanone, 959
[75501-54-1]	4-(2-Hydroxy-5-methoxyphenyl)-4-oxo-1-butanoic acid, 440
[75656-31-4]	1-(2,4,6-Trihydroxyphenyl)-12,14-dihydroxyoctadecanone, 1069
[75679-83-3]	1-(2,4,6-Trimethoxyphenyl)-12,14-dimethoxyoctadecanone, 1069
[76092-85-8]	1-(3,5-Dibromo-2,4-dihydroxyphenyl)-1-octanone, 785
[76092-86-9]	1-(3,5-Dibromo-2,4-dihydroxyphenyl)-1-nonanone, 841
[76115-96-3]	1-(2-Hydroxy-5-methylphenyl)-1-decanone, 883
[76402-07-8]	1-(2,5-Dihydroxy-3,4-dimethylphenyl)-1-tetradecanone, 1015
[76402-08-9]	1-[5-Hydroxy-3,4-dimethyl-2-(2-propenyloxy)phenyl]-1-tetradecanone, 1019
[76402-09-0]	1-[2,5-Dihydroxy-3,4-dimethyl-6-(2-propenyl)phenyl]-1-tetradecanone, 1019
[76402-10-3]	1-(2,5-Dihydroxy-3,4-dimethyl-6-propylphenyl)-1-tetradecanone, 1019
[76402-12-5]	1-[2-Hydroxy-4-methyl-5-(2-propenyloxy)phenyl]-1-hexadecanone, 1049
[76402-13-6]	1-[3,6-Dihydroxy-4-methyl-2-(2-propenyl)phenyl]-1-hexadecanone, 1048
[76402-14-7]	1-(3,6-Dihydroxy-4-methyl-2-propylphenyl)-1-hexadecanone, 1050
[76569-40-9]	1-(2,4,6-Trimethoxyphenyl)-1-butanone, 19
[76631-00-0]	1-(2,4-Dimethoxy-6-hydroxyphenyl)-1,3,5-hexanetrione, 645
[76631-01-1]	1-(2,4,6-Trimethoxyphenyl)-1,3,5-hexanetrione, 596
[76631-02-2]	1-(2,4,6-Tribenzyloxyphenyl)-1,3,5-hexanetrione, 596
[76631-04-4]	1-(2,4-Dimethoxy-6-hydroxyphenyl)-1,3,5,7-octanetetraone, 798
[76631-05-5]	1-(2,4,6-Trimethoxyphenyl)-1,3,5,7-octanetetraone, 771
[76750-11-3]	1-(2-Ethoxy-4-hydroxyphenyl)-1-octadecanone, 1078
[76752-90-4]	1-(4-Methoxy-3-nitrophenyl)-1-dodecanone, 956
[77007-22-8]	1-(3′-Bromo-4′-methoxy[1,1′-biphenyl]-4-yl)-1-heptanone, 756
[77132-64-0]	1-(4-Chloro-2-hydroxyphenyl)-1-hexanone (Phenylhydrazone), 624
[77311-66-1]	1-[5-(Acetyloxyethyl)-2-methoxyphenyl]-3-methyl-1-butanone, 208
[77346-69-1]	1-(5-Ethyl-2-hydroxyphenyl)-3-methyl-1-butanone, 197
[77346-70-4]	1-(5-Ethyl-2-hydroxyphenyl)-3-methyl-1-butanone (Isovalerate), 197
[77346-71-5]	1,1′-(5-Ethyl-2-hydroxy-1,3-phenylene)bis-3-methyl-1-butanone, 304
[77346-72-6]	1,1′-(5-Ethyl-2-methoxy-1,3-phenylene)bis-3-methyl-1-butanone, 304
[77464-71-2]	1-(2,6-Dihydroxy-4-methoxyphenyl)-6,9,12,15-tetraen-1-octadecanone, 1073
[77711-94-5]	Methyl 22-(2-Hydroxy-3,4-dimethoxy-6-methylphenyl)-22-oxo-1-docosanoate, 1109
[77712-02-8]	18-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-octadecanone, 1081

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[77712-07-3]	11-Acetyloxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-undecanone, 931
[77712-08-4]	11-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-undecanone, 931
[77712-21-1]	12-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-dodecanone, 970
[77794-62-8]	Euglobal-IIc, 393
[77942-74-6]	1-(4-Hydroxyphenyl)-2-methyl-1-butanone *(R)*, 127
[78334-92-6]	4-(5-Methoxy-2,4-dimethylphenyl)-4-oxo-1-butanoic acid, 444
[78417-95-5]	Methyl 5-hexanoyl-2-hydroxybenzoate, 634
[78417-96-6]	Methyl 2-hydroxy-5-octanoylbenzoate, 789
[78417-97-7]	Methyl 2-hydroxy-5-decanoylbenzoate, 881
[78417-98-8]	Methyl 2-Hydroxy-5-tetradecanoylbenzoate, 1011
[78418-00-5]	5-Hexanoyl-2-hydroxybenzoic acid, 634
[78418-01-6]	2-Hydroxy-5-octanoylbenzoic acid, 789
[78418-02-7]	2-Hydroxy-5-decanoylbenzoic acid, 881
[78418-03-8]	2-Hydroxy-5-dodecanoylbenzoic acid, 956
[78418-04-9]	2-Hydroxy-5-tetradecanoylbenzoic acid, 1011
[78423-49-1]	2,4,6-Trihydroxy-3-(3-methyl-1-oxobutyl)benzaldehyde, 387
[78432-96-9]	Methyl 2-Hydroxy-5-dodecanoylbenzoate, 957
[78481-50-2]	1-(5-Methoxy-2,3-diphenyl-6-benzofuranyl)-1,3-butanedione, 334
[79111-54-9]	1-(8-Hydroxy-7-quinolinyl)-1-nonanone, 846
[79111-55-0]	1-(8-Hydroxy-5-quinolinyl)-1-nonanone (Hydrochloride), 846
[79111-56-1]	1-(8-Hydroxy-5-quinolinyl)-1-nonanone, 845
[79214-31-6]	4-Chloro-1-(5-fluoro-2-hydroxyphenyl)-1-butanone, 278
[79330-93-1]	22-(2-Hydroxy-3,4-dimethoxy-6-methylphenyl)-22-oxo-1-docosanoic acid, 1108
[79381-16-1]	6-(2,5-Dimethoxyphenyl)-6-oxo-1-hexanoic acid, 713
[79553-90-5]	1-(2,4,6-Trihydroxyphenyl)-5,8,11,14,17-eicosapentaen-1-one (all *Z*), 1097
[79553-91-6]	1-(2,4,6-Trihydroxyphenyl)-1-eicosanone, 1098
[79619-25-3]	1-(4-Trifluoromethyloxyphenyl)-1-pentanone, 469
[79744-63-1]	3-Methyl-1-[2,4,5-trihydroxyphenyl]-1-butanone, 181
[80081-75-0]	Ethyl 4-(2,4-dimethoxyphenyl)-2,4-dioxo-1-butanoate, 397
[80222-34-0]	1-(4-Fluoro-2-methoxyphenyl)-1-pentanone, 484
[80222-35-1]	1-(2-Fluoro-4-methoxyphenyl)-1-pentanone, 483
[80269-97-2]	4-Chloro-1-(2,4-dimethoxyphenyl)-1-butanone, 281
[80356-11-2]	1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-pentanone, 509
[80356-12-3]	1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-3-methyl-1-butanone, 208
[80356-13-4]	1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-2-methyl-1-butanone, 139
[80427-32-3]	1-(5-Hydroxy-2-methoxyphenyl)-1-decanone, 885
[80427-37-8]	1-(2-Hydroxy-5-methoxyphenyl)-1-decanone, 884
[80752-03-0]	5,7-Dihydroxy-6-(1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 115
[80848-70-0]	1-[4-(2-Ethylhexyloxy-2-hydroxyphenyl]-1-hexanone (Oxime, nickel complex), 689

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[80848-71-1]	1-[4-(2-Ethylhexyloxy)-2-hydroxyphenyl]-1-decanone (Oxime, nickel complex), 912
[80848-72-2]	1-[4-(2-Ethylhexyloxy)-2-hydroxyphenyl]-1-octanone (Oxime, nickel complex), 823
[80849-31-6]	1-(2-Hydroxy-4-methylphenyl)-1-dodecanone (Nickel complex), 958
[80851-64-5]	1-[4-(2-Ethylhexyloxy)-2-hydroxyphenyl]-1-hexanone, 689
[80856-35-5]	1-(2-Hydroxyphenyl)-1,3-hexanedione, 596
[80856-36-6]	1-(2-Hydroxyphenyl)-4-methyl-1,3-hexanedione, 615
[80904-51-4]	4-Chloro-1-(2,4,6-trimethoxyphenyl)-1-butanone, 283
[80986-13-6]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-pentanone, 502
[81096-36-8]	1,4-Bis(4-methoxyphenyl)-2,3-dimethyl-1,4-butanedione, 367
[81141-14-2]	1-(3,5-Dichloro-2-hydroxyphenyl)-1-butanone, 24
[81321-89-3]	1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-dodecanone (Oxime, nickel complex), 973
[81515-08-4]	1-(2,4-Dichloro-6-hydroxyphenyl)-1-tetradecanone, 1010
[81515-09-5]	1-(4,6-Dichloro-2-hydroxy-3-nitrophenyl)-1-tetradecanone, 1010
[81515-10-8]	1-[4,6-Bis(butylthio)-2-hydroxy-3-nitrophenyl]-1-tetradecanone, 1021
[81515-11-9]	1-[4,6-Bis(butylsulfonyl)-2-hydroxy-3-nitrophenyl]-1-tetradecanone, 1021
[82307-87-7]	1-(2,4-Dihydroxy-5-octylphenyl)-1-hexanone (Oxime, nickel complex), 689
[82322-05-2]	1-[5-(1,1-Dimethylethyl)-2,4-dihydroxyphenyl]-1-decanone (Oxime, nickel complex), 896
[82350-83-2]	1-(4-Hydroxy-3-nitrophenyl)-1-butanone, 35
[82427-57-4]	1-(2,6-Dihydroxyphenyl)-11-phenyl-1-undecanone, 932
[82460-89-7]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-hexadecanone, 1045
[82460-90-0]	1-(2-Acetyloxy-4,6-dimethoxyphenyl)-1-hexadecanone, 1045
[82460-91-1]	1-(2,4,6-Triacetyloxyphenyl)-1-hexadecanone, 1038
[82461-11-8]	1-(2,4,6-Trihydroxyphenyl)-1-hexadecanone, 1038
[82652-25-3]	1-(6,7-Dimethoxy-5-propyl-1,3-benzodioxol-4-yl)-1-pentanone, 507
[82652-26-4]	1-(6,7-Dimethoxy-5-propyl-1,3-benzodioxol-4-yl)-1-hexanone, 663
[82652-27-5]	1-(6,7-Dimethoxy-5-propyl-1,3-benzodioxol-4-yl)-1-heptanone, 748
[82652-28-6]	1-(6,7-Dimethoxy-5-propyl-1,3-benzodioxol-4-yl)-1-octanone, 805
[82652-29-7]	1-(6,7-Dimethoxy-5-propyl-1,3-benzodioxol-4-yl)-1-nonanone, 848
[82652-30-0]	1-(6,7-Dimethoxy-5-propyl-1,3-benzodioxol-4-yl)-1-decanone, 894
[82652-35-5]	1-(6,7-Dihydro-4-methoxy-6-methylfuro[2,3-f]-1,3-benzodioxol-8-yl)-1-heptanone, 747
[82652-36-6]	1-(6,7-Dihydro-4-methoxy-6-methylfuro[2,3-f]-1,3-benzodioxol-8-yl)-1-octanone, 805
[82652-37-7]	1-(6,7-Dihydro-4-methoxy-6-methylfuro[2,3-f]-1,3-benzodioxol-8-yl)-1-decanone, 894
[82684-67-1]	1-[4-(2-Hydroxyethyloxy)phenyl]-1-decanone, 871
[82883-60-1]	1-(2,4-Diphenylmethoxy-6-methylphenyl)-1,3-butanedione, 319
[82938-20-3]	1-(4-Methoxyphenyl)-3-methyl-1-butanone, 175
[82944-57-8]	1-[4-(2-Acetoxyethyloxy)phenyl]-1-decanone, 871
[82961-09-9]	Methyl 4-(2,4,5-trimethoxyphenyl)-4-oxo-1-butanoate, 412
[83162-76-9]	13-Hydroxy-1-(2,4,6-Trihydroxyphenyl)-1-hexadecanone, 1039
[83162-77-0]	14-Hydroxy-1-(2,4,6-Trihydroxyphenyl)-1-hexadecanone, 1039

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[83212-56-0]	1-(2,4,6-Trimethoxyphenyl)-12,14-dimethoxyoctadecanone, 1069
[83212-66-2]	1-(2,4,6-Trihydroxyphenyl)-12,14-dihydroxyoctadecanone, 1069
[83213-39-2]	1-(2,4,6-Trihydroxyphenyl)-12,14-dihydroxyoctadecanone, 1069
[83258-17-7]	1-(3′-Bromo-4′-methoxy[1,1′-biphenyl]-4-yl)-1-hexanone, 678
[83481-33-8]	4-(2-Hydroxy-3,4-dimethylphenyl)-4-oxo-1-butanoic acid, 443
[83671-25-4]	1-(2,4-Dihydroxyphenyl)-2-ethyl-1-hexanone, 618
[83805-59-8]	1-(3,4-Dihydro-7-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1,3-butanedione, 332
[83805-61-2]	1-[2-Hydroxy-6-methoxy-4-(phenylmethoxy)phenyl]-1,3-butanedione, 333
[83805-67-8]	1-(3,4-Dihydro-7-hydroxy-5-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1,3-butanedione, 332
[83882-87-5]	5-Chloro-1-(4-hydroxyphenyl)-1-pentanone, 568
[83882-88-6]	5-Chloro-1-(4-difluoromethyloxyphenyl)-1-pentanone, 568
[83893-20-3]	1-(2,5-Dimethoxy-4-methylphenyl)-1-butanone, 54
[83893-22-5]	1-(2,5-Dimethoxy-4-methylphenyl)-1-pentanone, 496
[83893-24-7]	1-(2,5-Dimethoxy-4-methylphenyl)-1-hexanone, 641
[84498-20-4]	1-(2-Hydroxy-4-methylphenyl)-1-octanone (Oxime), 792
[84498-21-5]	1-(4-Hydroxyphenyl)-1-octanone (Oxime), 775
[84633-05-6]	1-[3,5-Bis[[2,4,6-trihydroxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-1-butanone, 347
[84633-06-7]	1-[3-(5-methyl-3-propionyl-2,4,6-trihydroxyphenylmethyl)-2,4,6-trihydroxy-5-methylphenyl]-1-butanone, 336
[84633-27-2]	1-(2,4,6-Trihydroxy-3,5-dimethylphenyl)-1-butanone, 77
[84836-32-8]	2-Ethyl-1-(4-methoxyphenyl)-1-butanone, 170
[84978-10-9]	22-(2-Methoxy-3,4-dimethoxy-6-methylphenyl)-22-oxo-1-docosanoic acid, 1108
[84978-12-1]	4-(2-Hydroxy-3,4,6-trimethylphenyl)-4-oxo-1-butanoic acid, 447
[84978-13-2]	5-(2-Hydroxy-3,4,6-trimethylphenyl)-5-oxo-1-pentanoic acid, 594
[84978-14-3]	1,5-Bis(2-hydroxy-3,4,6-trimethylphenyl)-1,5-pentanedione, 538
[84978-15-4]	1,6-Bis(2-hydroxy-3,4,6-trimethylphenyl)-1,6-hexanedione, 693
[84978-16-5]	1,10-Bis(2-hydroxy-3,4,6-trimethylphenyl)-1,10-decanedione, 915
[84978-19-8]	7-(2-Hydroxy-3,4,5-trimethylphenyl)-7-oxo-1-heptanoic acid, 770
[84978-21-2]	10-(2-Hydroxy-3,4,5-trimethylphenyl)-10-oxo-1-decanone, 922
[84978-22-3]	1,10-Bis(2-hydroxy-3,4,5-trimethylphenyl)-1,10-decanedione, 915
[85052-18-2]	1-(5-Chloro-2-hydroxyphenyl)-1-heptanone, 734
[85052-25-1]	1-(5-Chloro-2-hydroxy-3-nitrophenyl)-1-heptanone, 732
[85052-34-2]	1-[5-(1,1-Dimethylethyl)-2-hydroxyphenyl]-1-heptanone, 749
[85052-35-3]	1-[5-(1,1-Dimethylethyl)-2-hydroxy-3-nitrophenyl]-1-heptanone, 748
[85052-45-5]	1-(3-Amino-5-chloro-2-hydroxyphenyl)-1-heptanone (Hydrochloride), 735
[85052-49-9]	1-[3-Amino-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-hexanone (Hydrochloride), 667
[85052-50-2]	1-[3-Amino-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-1-hexanone, 667
[85052-73-9]	1-(3-Amino-5-chloro-2-hydroxyphenyl)-1-heptanone, 735
[85157-92-2]	1-(4-Methoxyphenyl)-3,3-dimethyl-1-butanone, 251
[85298-88-0]	1-(2,6-Dihydroxyphenyl)-1-undecanone, 926

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[85298-89-1]	1-(3-Chloro-2,6-dihydroxyphenyl)-1-undecanone, 929
[85298-90-4]	1-(3,5-Dihydroxyphenyl)-1-undecanone, 927
[85298-94-8]	1-(3,5-Dichloro-2,6-dihydroxyphenyl)-1-undecanone, 929
[85298-95-9]	1-(2,6-Dimethoxyphenyl)-1-undecanone, 926
[85485-53-6]	4-Chloro-1-(4-fluoro-2-hydroxyphenyl)-1-butanone (Oxime) (1*E*), 278
[85602-20-6]	1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-nonanone, 849
[85602-21-7]	1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-octanone, 809
[85602-25-1]	4-Methyl-1-[2,4,6-trihydroxy-3-(2-propenyl)phenyl]-1-pentanone, 549
[85602-31-9]	4-Methyl-1-[2,4,6-trihydroxy-3-(phenylmethyl)phenyl]-1-pentanone, 551
[85602-33-1]	1-[2,4,6-Trihydroxy-3-(phenylmethyl)phenyl]-1-nonanone, 857
[85602-35-3]	4-Methyl-1-[2-hydroxy-4,6-dimethoxy-3-(3-methyl-2-buten-1-yl)phenyl]-1-pentanone, 551
[85602-40-0]	1-(3,4-Dihydro-5,7-dihydroxy-2*H*-1-benzopyran-6-yl)-1-octanone, 804
[85602-44-4]	4-Methyl-1-(2,4,6-trihydroxyphenyl)-1-pentanone (Monosodium salt), 546
[86360-63-6]	1-(2,4,6-Trimethoxyphenyl)-1-hexanone, 613
[87035-85-6]	2-Methyl-1-(2,4,6-trihydroxy-3,5-dimethylphenyl)-1-butanone, 136
[87035-88-9]	1-(4-Hydroxy-2,6-dimethoxy-3,5-dimethylphenyl)-2-methyl-1-butanone, 140
[87338-25-8]	4-(3-Bromo-2-hydroxy-5-methoxyphenyl)-4-oxo-1-butanoic acid, 432
[87364-84-9]	4-(4,5-Dimethoxy-2-nitrophenyl)-4-oxo-1-butanoic acid, 427
[87364-85-0]	Ethyl 4-(2-amino-4,5-dimethoxyphenyl)-4-oxo-1-butanoate, 429
[87374-67-2]	Ethyl 4-(4,5-dimethoxy-2-nitrophenyl)-4-oxo-1-butanoate, 427
[87667-31-0]	1-(3,4,5-Trihydroxyphenyl)-1-nonadecanone, 1094
[87961-41-9]	5-(3,4-Methylenedioxyphenyl)-5-oxo-1-pentanoic acid, 582
[88167-05-9]	1,6-Bis(4-ethoxyphenyl)-1,6-hexanedione, 674
[88555-60-6]	1-(2-Hydroxy-4-methylphenyl)-5-methyl-1-hexanone, 650
[88555-61-7]	1-(2-Methoxy-4-methylphenyl)-5-methyl-1-hexanone, 650
[88559-37-9]	1-(8-Hydroxy-5-quinolinyl)-1-decanone, 889
[88559-38-0]	1-(8-Hydroxy-7-quinolinyl)-1-decanone, 890
[88559-39-1]	1-(5-Chloro-8-hydroxy-7-quinolinyl)-1-decanone, 889
[88559-43-7]	1-(8-Hydroxy-7-quinolinyl)-1-nonanone (Hydrazone), 846
[88559-44-8]	1-(8-Hydroxy-7-quinolinyl)-1-decanone (Hydrazone), 890
[88559-45-9]	1-(5-Chloro-8-hydroxy-7-quinolinyl)-1-decanone (Hydrazone), 889
[88580-91-0]	1,1′-(2-Hydroxy-5-methyl-1,3-phenylene)bis-1-butanone, 299
[88858-34-8]	1-(4-Ethoxyphenyl)-1-butanone (Semicarbazone), 8
[88924-67-8]	1-(2,4-Dihydroxy-3,5-dimethylphenyl)-1-hexanone, 651
[89647-61-0]	1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-2-methyl-1-butanone, 135
[90033-66-2]	1-(2-Amino-5-methoxyphenyl)-1-pentanone, 486
[90269-45-7]	1-[2-Methyl-(4-phenoxyphenyl)-1-butanone, 127
[90269-46-8]	1-(4-Methoxyphenyl)-2-methyl-1-butanone, 126
[90834-05-2]	1-(2,4,5-Trimethoxyphenyl)-1-pentanone, 476
[90834-06-3]	1-(2,4,5-Trimethoxyphenyl)-1-hexanone, 612
[90834-07-4]	2-Bromo-1-(2,4,5-trimethoxyphenyl)-1-butanone, 271
[90834-08-5]	2-Bromo-1-(2,4,5-trimethoxyphenyl)-1-pentanone, 566
[90834-09-6]	2-Bromo-1-(2,4,5-trimethoxyphenyl)-1-hexanone, 700

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[90841-48-8]	2-Bromo-1-(3-hydroxyphenyl)-1-butanone, 269
[90919-46-3]	1-(5-Chloro-2,4-dihydroxyphenyl)-1-butanone, 31
[90922-78-4]	1-(2-Hydroxy-4-nitrophenyl)-1-butanone, 34
[91065-87-1]	2-Bromo-1-(4-methoxyphenyl)-1,3-butanedione, 308
[91142-94-8]	1-(4-Hydroxyphenyl)-2-methyl-1,3-butanedione, 314
[91143-26-9]	1-(4-Hydroxyphenyl)-1,3-pentanedione, 460
[91335-45-4]	2-Bromo-1-(3-methoxyphenyl)-1-butanone, 269
[91453-24-6]	1,5-Bis(2,5-dihydroxyphenyl)-1,5-pentanedione, 520
[91453-25-7]	1,5-Bis(2,5-dihydroxy-4-methylphenyl)-1,5-pentanedione, 533
[91453-26-8]	1,6-Bis(2,5-dihydroxyphenyl)-1,6-hexanedione, 675
[91453-27-9]	1,6-Bis(2,5-dihydroxy-4-methylphenyl)-1,6-hexanedione, 687
[91497-29-9]	1-[4-(Acetyloxy)-2-hydroxyphenyl]-1-butanone, 61
[91497-61-9]	4-(2-Methoxy-4-methylphenyl)-4-oxo-1-butanoic acid, 433
[91541-03-6]	4-(4-Hydroxy-3-methylphenyl)-4-oxo-1-butanoic acid, 436
[91555-33-8]	1-(2,6-Dihydroxy-4-methoxyphenyl)-3-methyl-1-butanone, 194
[91555-34-9]	1-(2-Hydroxy-4,5-dimethoxyphenyl)-1-butanone, 74
[91646-56-9]	1-(4-Methoxyphenyl)-1-butanone (Semicarbazone), 7
[91667-38-8]	1-(2-Hydroxy-4,5-dimethylphenyl)-1-butanone, 66
[91767-62-3]	4-Chloro-1-(2,5-dimethoxyphenyl)-1-butanone, 282
[91963-55-2]	1-(4-Acetyloxyphenyl)-1,3-butanedione, 311
[91964-06-6]	1-(4-Carboxy-3-methoxyphenyl)-4-oxo-1-butanoic acid, 431
[91970-63-7]	1-(2,3-Dihydroxy-5-methylphenyl)-1-butanone, 53
[91970-65-9]	1-(3-Hydroxy-4-methoxyphenyl)-1-butanone, 55
[91992-00-6]	1-(2-Hydroxy-3-nitrophenyl)-1-butanone, 34
[92016-84-7]	1-(4-Hydroxy-3-methylphenyl)-1,3-butanedione, 318
[92017-91-9]	Methyl 4-(4-methoxyphenyl)-2,3-dibromo-4-oxo-1-butanoate, 397
[92019-26-6]	1-(2-Chloro-4-hydroxy-3-methylphenyl)-2-ethyl-1-butanone, 172
[92019-28-8]	4-Chloro-1-(4-propoxyphenyl)-1-butanone, 281
[92019-50-6]	4-Chloro-1-(2,3,4-trimethoxyphenyl)-1-butanone, 283
[92035-99-9]	1-(4-Ethoxyphenyl)-3-methyl-1-butanone, 176
[92050-07-2]	1-(4-Methoxyphenyl)-4-methyl-4-nitro-1-pentanone, 541
[92050-08-3]	1-(4-Methoxyphenyl)-4-methyl-4-nitro-2-sulfinyl-1-pentanone, 541
[92120-37-1]	1-(4-Methoxyphenyl)-4-methyl-1,3,5-hexanetrione, 614
[92120-60-0]	1-(2,4-Dimethoxy-6-methylphenyl)-1-pentanone (D), 495
[92120-78-0]	1-[2,4-Dimethoxy-6-[(trimethylsilyl)methyl]phenyl]-1-pentanone, 510
[92300-78-2]	1-(4-Methoxyphenyl)-5-methyl-1-hexanone, 616
[92301-09-2]	1-(3,5-Dimethyl-4-hydroxyphenyl)-2-methyl-1-pentanone, 561
[92317-86-7]	1-(4-Butoxy-4-chlorophenyl)-1-butanone, 281
[92422-41-8]	1-(4-Amino-3-methoxyphenyl)-4-oxo-1-butanoic acid, 428
[92532-18-8]	1-(3-Benzyloxyphenyl)-1-hexanone, 601
[92655-68-0]	1-(3-Butyryloxy-4-methoxyphenyl)-1-butanone, 56
[92730-14-8]	1-(3,4-Dimethoxyphenyl)-2-ethyl-3-methyl-1-butanone, 185
[92730-24-0]	1-(2-Hydroxy-4-propoxyphenyl)-1-hexanone, 659
[92755-95-8]	1-(2-Hydroxy-4-methoxy-3-methylphenyl)-1-butanone, 71

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[92755-96-9]	1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1-butanone, 71
[92757-66-9]	1-(5-Acetyl-2-hydroxyphenyl)-1-butanone, 377
[92757-67-0]	1-(5-Acetyl-2-hydroxyphenyl)-1-hexanone, 646
[92844-55-4]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-(1-methylpropyl)-2*H*-1-benzopyran-2-one (*R,R*), 156
[92865-60-6]	5-(2,4,5-Trimethoxyphenyl)-5-oxo-1-pentanoic acid, 583
[92907-10-3]	1-(5-Chloro-2,4-dihydroxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 31
[93041-47-5]	1-(4-Cyano-3-methoxyphenyl)-4-oxo-1-butanoic acid, 430
[93156-87-7]	1-(4-Pentyloxyphenyl)-1-pentanone, 468
[93157-10-9]	1-(3,4-Dimethoxyphenyl)-1-octanone, 782
[93175-38-3]	2-Bromo-1-(2,5-dimethoxyphenyl)-1-butanone, 271
[93249-83-3]	1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-decanone, 904
[93249-88-8]	1-(4′-Acetyloxy[1,1′-biphenyl]-4-yl)-1-decanone, 905
[93429-81-3]	1-(2-Hydroxy-5-methylphenyl)-4-methyl-1-pentanone, 547
[93534-71-5]	4-(3-Methoxy-4-nitrophenyl)-4-oxo-1-butanoic acid, 426
[93542-23-5]	1-(4-Hexyloxyphenyl)-1-pentanone, 468
[93542-41-7]	1-[2-Hydroxy-4-(isopentyloxy)phenyl]-1-hexanone, 670
[93650-62-5]	1-(2-Hydroxyphenyl)-3-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 174
[93762-01-7]	1-(4-Methoxyphenyl)-5-methyl-1-hexanone (Semicarbazone), 616
[93796-34-0]	3-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)-5-(3-methylbutyl) phenyl]-1-butanone, 233
[93970-90-2]	1-(3,4-Dihydro-7,8-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone, 97
[93970-91-3]	1-(3,4-Dihydro-5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone, 96
[93970-92-4]	1-(3,4-Dihydro-7-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone, 96
[93970-93-5]	1-(2,4-Dihydroxy-3-methylphenyl)-1-butanone, 53
[93970-94-6]	1-(3,4-Dihydro-7-hydroxy-2,2,8-trimethyl-2*H*-1-benzopyran-6-yl)-1-butanone, 106
[93970-95-7]	1-(3,4-Dihydro-7-hydroxy-8-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-1-butanone, 107
[94119-33-2]	5-(2,5-Diethoxyphenyl)-5-oxo-1-pentanoic acid, 582
[94413-27-1]	1-[5-Acetyl-2-hydroxy-3-(1-hydroxy-3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone, 381
[94413-28-2]	1,1′-[5-Acetyl-2-hydroxy-1,3-phenylene]bis-3-methyl-1-butanone, 382
[94432-99-2]	1-(2,4-Dihydroxy-3-quinolinyl)-1-decanone, 890
[94613-09-9]	1-[2-Hydroxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-decanone (Oxime), 911
[94613-10-2]	1-[2-Methoxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-decanone (Oxime), 912
[94708-70-0]	1-(2-Hydroxy-4-nitrophenyl)-1-butanone (Phenylhydrazone), 35
[94711-66-7]	1-(2,4-Dihydroxyphenyl)-3-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 178
[94759-02-1]	1-(2,4-Dihydroxyphenyl)-1-octanone (2,4-Dinitrophenylhydrazone), 779

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[94899-67-9]	1-[2-Methoxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-decanone, 911
[94899-68-0]	1-[2-Hydroxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-decanone, 911
[94960-09-5]	4-(4-Phenoxyphenyl)-4-oxo-1-butanoic acid (Semicarbazone), 402
[95002-59-8]	1,5-Bis(2,4-dimethoxyphenyl)-1,5-pentanedione, 520
[95102-14-0]	1-(2,4-Dihydroxy-5-methylphenyl)-1-dodecanone, 961
[95102-15-1]	1-(4-Hydroxy-3-methylphenyl)-1-tetracosanone, 1114
[95102-16-2]	1-(2,4-Dihydroxy-5-methylphenyl)-1-tetradecanone, 1012
[95102-17-3]	1-(5-Ethyl-2,4-dihydroxyphenyl)-1-hexanone, 652
[95102-18-4]	1-(4-Hydroxy-3-(1-methylethyl)phenyl)-1-heptanone, 747
[95102-20-8]	1-(4-Hydroxy-2,3-dimethylphenyl)-1-octanone, 800
[95102-21-9]	1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-octanone, 807
[95102-22-0]	1-(2-Hydroxy[1,1′-biphenyl]-5-yl)-1-octanone, 814
[95102-23-1]	1-(4-Hydroxy-2,5-dimethylphenyl)-1-decanone, 888
[95102-27-5]	1-(4-Hydroxy-3-methylphenyl)-1-heptanone, 739
[95102-30-0]	1-(4-Hydroxy-2,5-dimethylphenyl)-1-hexanone, 651
[95102-32-2]	1-[3-(1,1-Dimethylethyl)-4-hydroxyphenyl]-1-octanone, 806
[95102-33-3]	1-[1,1′-Biphenyl]-5-yl-2-hydroxy-1-pentanone, 524
[95102-34-4]	1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-hexanone, 665
[95102-35-5]	1-(6-Hydroxy[1,1′-biphenyl]-3-yl)-1-heptanone, 758
[95102-36-6]	1-[4-Hydroxy-3-(1-methylethyl)phenyl]-1-hexanone, 658
[95102-37-7]	1-[4-Hydroxy-3-(1-methylethyl)phenyl]-1-pentanone, 505
[95102-38-8]	1-(4-Hydroxy-2,5-dimethylphenyl)-1-nonanone, 845
[95102-39-9]	1-(4-Hydroxy-2,5-dimethylphenyl)-1-heptanone, 744
[95102-41-3]	1-(4-Hydroxy-3-methylphenyl)-1-octanone, 793
[95102-42-4]	1-(6-Hydroxy[1,1′-biphenyl]-3-yl)-1-hexanone, 680
[95149-08-9]	1-(2,4-Dihydroxy-3-methylphenyl)-1-octanone, 794
[95185-58-3]	1-(2,4-Dihydroxy-5-methylphenyl)-1-octanone, 795
[95185-59-4]	1-(5-Ethyl-2,4-dihydroxyphenyl)-1-octanone, 802
[95185-60-7]	1-(2,4-Dihydroxy-5-methylphenyl)-1-octadecanone, 1076
[95185-61-8]	1-(4-Hydroxy-2,5-dimethylphenyl)-1-docosanone, 1107
[95185-62-9]	1,1′-(2-Hydroxy[1,1′-biphenyl]-5-yl)-1-butanone, 260
[95185-63-0]	1-[3-(1,1-Dimethylethyl)-4-hydroxyphenyl]-1-pentanone, 508
[95185-65-2]	1-[3-(1,1-Dimethylethyl)-4-hydroxyphenyl]-1-heptanone, 749
[95185-66-3]	1-(3-Ethyl-4-hydroxyphenyl)-1-heptanone, 742
[95185-67-4]	1-(4-Hydroxy-2,5-dimethylphenyl)-1-octanone, 800
[95185-68-5]	1-(4-Hydroxy-2,5-dimethylphenyl)-1-hexadecanone, 1043
[95185-69-6]	1-(4-Hydroxy-2,5-dimethylphenyl)-1-octadecanone, 1077
[95185-70-9]	1-(4-Hydroxy-3-methylphenyl)-1-docosanone, 1107
[95185-72-1]	1-[4-Hydroxy-2-methyl-5-(1-methylethyl)phenyl]-1-butanone, 91
[95185-73-2]	1-[4-Hydroxy-3-(1-methylethyl)phenyl]-3-methyl-1-butanone, 206
[95269-86-6]	5-(1-Octadecanoyl)-2-hydroxybenzoic acid, 1074
[95269-91-3]	5-(1-Octadecanoyl)-2-hydroxybenzoic acid (Na salt), 1074
[95269-96-8]	5-(1-Octadecanoyl)-2-hydroxybenzoic acid (Tris(2-hydroxyethyl)amine salt), 1075

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[95269-97-9]	5-(1-Octadecanoyl)-2-hydroxybenzoic acid (N-methylmorpholine salt), 1075
[95282-26-1]	1-(2,4-Dihydroxyphenyl)-1-nonanone (2,4-Dinitrophenylhydrazone), 838
[95302-59-3]	5-(1-Octadecanoyl)-2-hydroxybenzoic acid (Lysine salt), 1075
[95807-67-3]	1-(2,5-Dihydroxyphenyl)-1-hexadecanone, 1036
[95809-40-8]	1-(2,4-Dihydroxyphenyl)-1-decanone (2,4-Dinitrophenylhydrazone), 872
[95869-30-0]	1-(4-Methoxyphenyl)-1-octadecanone, 1064
[95869-36-6]	1-(2-Hydroxy-4-methoxyphenyl)-1-octadecanone, 1077
[95958-93-3]	1-(2,4-Dihydroxyphenyl)-1-undecanone (2,4-Dinitrophenylhydrazone), 925
[96070-21-2]	1-(2,3,4-Trihydroxyphenyl)-1-eicosanone, 1098
[96123-20-5]	1-(4′-Octyloxy[1,1-biphenyl]-4-yl)-3-methyl-1-pentanone, 563
[96251-00-2]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1,2-hexanedione, 688
[96251-01-3]	1-[3,5-(1,1-Dimethylethyl)-4-hydroxyphenyl]-3,3-dimethyl-1,2-butanedione, 308
[96271-43-1]	1,5-Bis(5-bromo-2,4-dihydroxyphenyl)-2,4-diphenyl-1,5-pentanedione, 539
[96271-44-2]	1,5-Bis(2,4-dihydroxyphenyl)-2,4-di-(4-bromophenyl)-1,5-pentanedione, 539
[96271-50-0]	1,5-Bis(5-chloro-2,4-dihydroxyphenyl)-2,4-diphenyl-1,5-pentanedione, 539
[96273-02-8]	1,5-Bis(2,4-dihydroxyphenyl)-1,5-pentanedione (Di-2,4-Dinitrophenyl-hydrazone), 520
[96273-22-2]	1,5-Bis(2,4-dihydroxyphenyl)-2,4-diphenyl-1,5-pentanedione, 540
[96358-74-6]	4-(2-Hydroxy-4,6-dimethylphenyl)-4-oxo-1-butanoic acid, 444
[96573-30-7]	2,4,6-Trihydroxy-3-(1-oxobutyl)benzaldehyde, 387
[96573-31-8]	2,4,6-Trihydroxy-3-(1-oxopentyl)benzaldehyde, 490
[96573-32-9]	2,4,6-Trihydroxy-3-(1-oxohexyl)benzaldehyde, 634
[96573-33-0]	2,4,6-Trihydroxy-3-(1-oxoheptyl)benzaldehyde, 737
[96573-34-1]	3-Ethyl-2,4,6-trihydroxy-5-(3-methyl-1-oxobutyl)benzaldehyde, 391
[96573-35-2]	2,4,6-Trihydroxy-3-(3-methyl-1-oxobutyl)-5-propylbenzaldehyde, 392
[96573-36-3]	3-Butyl-2,4,6-trihydroxy-5-(3-methyl-1-oxobutyl)benzaldehyde, 392
[96573-40-9]	1-[2,4,6-Trihydroxy-3-(1-oxopropyl)phenyl]-1-butanone, 385
[96573-43-2]	2,4,6-Trihydroxy-5-(3-methyl-1-oxobutyl)-1,3-benzenedicarboxaldehyde, 388
[96590-58-8]	1,5-Bis(2,4-dihydroxyphenyl)-2,4-di-(4-methoxyphenyl)-1,5-pentanedione, 540
[96676-42-5]	1,5-Bis(2,4-dimethoxyphenyl)-2,4-diphenyl-1,5-pentanedione, 540
[96710-34-8]	1,5-Bis(5-bromo-2,4-diacetyloxyphenyl)-2,4-diphenyl-1,5-pentanedione, 539
[96710-35-9]	1,5-Bis(5-chloro-2,4-diacetyloxyphenyl)-2,4-diphenyl-1,5-pentanedione, 539
[96809-09-5]	1,5-Bis(5-chloro-2,4-dihydroxypheny)l-1,5-pentanedione (Di-2,4-Dinitro-phenylhydrazone), 516
[96820-25-6]	1-(2,6-Dihydroxyphenyl)-1-hexadecanone, 1037
[96853-73-5]	3-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-2,4,6-trihydroxy-5-[(3,3-dimethylallyl)phenyl]-1-butanone, 343
[96966-45-9]	1-(3,4-Dimethoxyphenyl)-1-dodecanone, 949
[96968-05-7]	1-(2,4-Diacetyloxyphenyl)-1-hexadecanone, 1035

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[97023-54-6]	1-[4-Hydroxy-3-(2-propenyl)phenyl]-1-butanone, 80
[97037-81-5]	1-(2-Acetyloxyphenyl)-1-pentanone, 463
[97153-67-8]	1-(3,4-Dihydroxyphenyl)-1-dodecanone (2,4-Dinitrophenylhydrazone), 948
[97271-30-2]	5-(2,4-Dibenzyloxy-6-methylphenyl)-3,5-dioxo-1-pentanoic acid, 589
[97582-34-8]	1-[4-[(Dimethylamino)methyl]-2-hydroxy-3-propylphenyl]-1-pentanone, 528
[97582-39-3]	1-[4-(Chloromethyl)-2-hydroxy-3-propylphenyl]-1-pentanone, 507
[97744-24-6]	2-Bromo-3,5,5-trimethyl-1-(4-pentyloxyphenyl)-1-hexanone, 707
[97744-27-9]	2-Bromo-1-(4-tert-butyloxyphenyl)-1-heptanone, 764
[97911-40-5]	9-Chloro-1-(3,4-dihydroxyphenyl)-1-octadecanone, 1091
[97911-41-6]	10-Chloro-1-(3,4-dihydroxyphenyl)-1-octadecanone, 1091
[97924-31-7]	1,5-Bis(2,4-diacetyloxyphenyl)-2,4-di-(4-methoxyphenyl)-1,5-pentanedione, 540
[98192-57-5]	5,7-Dihydroxy-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 228
[98192-58-6]	5,7-Dihydroxy-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 149
[98192-60-0]	5,7-Dihydroxy-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one, 148
[98192-61-1]	5,7-Dihydroxy-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 220
[98192-62-2]	5,7-Dihydroxy-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 104
[98192-64-4]	5,7-Dihydroxy-8-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 229
[98192-65-5]	5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 150
[98192-67-7]	5,7-Dihydroxy-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 220
[98192-68-8]	5,7-Dihydroxy-8-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 104
[98192-70-2]	5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*-1-benzopyran-2-one, 159
[98192-74-6]	5,7-Dihydroxy-8-(2-methyl-1-oxobutyl)-4-(1-methylpropyl)-2*H*-1-benzopyran-2-one, 146
[98193-78-3]	5-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7-hydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 165
[98230-17-2]	3-Methyl-1-[2,4,5-trimethoxyphenyl]-1-butanone, 181
[98244-54-3]	6-(3,7-Dimethyl-2,6-octadienyl)-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 165
[98244-56-6]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-(1-methylpropyl)-2*H*-1-benzopyran-2-one (*R,S*), 156
[98244-57-6]	5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one (S) isomer, 154
[98314-46-6]	1-(2,5-Dimethoxyphenyl)-1-dodecanone, 947
[98333-38-1]	1,10-Bis(2,4,6-trihydroxyphenyl)-1,10-decanedione, 904
[98357-89-2]	1-[2-Hydroxy-5-(2-propenyloxy)phenyl]-1-hexadecanone, 1046
[98357-90-5]	1-[3,6-Dihydroxy-2-(2-propenyl)phenyl]-1-hexadecanone, 1046
[98498-56-7]	2-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone (Racemic), 129

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[98498-59-0]	4-(1-Bromopropyl)-5,7-dihydroxy-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (racemic), 219
[98498-60-3]	4-(Chloromethyl)-5,7-dihydroxy-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one, 87
[98498-64-7]	5,7-Diacetyloxy-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 104
[98498-67-0]	5,7-Dimethoxy-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 104
[98498-69-2]	4-[1-(Acetyloxy)propyl]-5,7-dimethoxy-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one, 113
[98498-77-2]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 147
[98498-78-3]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (racemic), 227
[98498-79-4]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one Stereoisomer (1′RS,2″S), 147
[98498-80-7]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one Stereoisomer (1′RS,2″S), 147
[98498-81-8]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (racemic), 242
[98574-77-7]	4-[1-(Acetyloxy)propyl]-6-(3,7-dimethyl-2,6-octadienyl)-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (R,R), 167
[98574-78-8]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one Stereoisomer (1′RS,2″S), 147
[98574-79-9]	4-[1-(Acetyloxy)propyl]-6-(3,7-dimethyl-2,6-octadienyl)-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (R-R,S), 167
[98574-80-2]	4-[1-(Acetyloxy)propyl]-6-(3,7-dimethyl-2,6-octadienyl)-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (S-R,R), 167
[98574-81-3]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one Stereoisomer (1′RS,2″S), 147
[98575-56-5]	4-[1-(Acetyloxy)propyl]-6-(3,7-dimethyl-2,6-octadienyl)-5,7-dihydroxy-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (R,S), 167
[98631-68-6]	1-(3,5-Dimethoxyphenyl)-1-pentanone-1-13C, 475
[98813-29-7]	1-(5-Chloro-2-hydroxyphenyl)-1-decanone, 879
[98813-30-9]	1-(5-Chloro-2-hydroxyphenyl)-1-dodecanone, 955
[98813-31-1]	1-(5-Chloro-2-hydroxyphenyl)-1-tetradecanone, 1011
[98841-70-4]	1-(4-Ethyl-5-fluoro-2-hydroxyphenyl)-1-butanone, 63
[99046-13-6]	Methyl 4-(2-methoxyphenyl)-4-oxo-1-butanoate, 399
[99070-24-3]	1-(3-Bromo-2,6-dihydroxyphenyl)-1-butanone, 27
[99070-35-6]	1-(3,5-Dibromo-2-hydroxyphenyl)-1-butanone (Oxime), 21
[99070-83-4]	1-(3-Chloro-2,6-dihydroxyphenyl)-1-butanone, 31
[99075-34-0]	1-(5-Amino-2-hydroxyphenyl)-1-butanone, 39
[99245-46-2]	1-(6-Hydroxy-3-methyl-2-benzofuranyl)-1-butanone, 79
[99283-86-0]	1-(2-Hydroxy-5-methylphenyl)-1-hexanone (Oxime), 640
[99783-83-2]	2-Bromo-1-(3-hydroxy-4-methoxyphenyl)-3-methyl-1-butanone, 294
[99783-85-4]	1-(3-Hydroxy-4-methoxyphenyl)-3-methyl-1-butanone, 193
[99853-34-6]	1-[5-Bromo-2,4-dihydroxy-3-(1-oxobutyl)]benzoic acid, 40
[99854-21-4]	Methyl 4-(5-chloro-2-hydroxyphenyl)-4-oxo-1-butanoate, 424
[99854-28-1]	1-[5-Chloro-2,4-dihydroxy-3-(1-oxobutyl)]benzoic acid, 41

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[99865-80-2]	4-(2-Hydroxyphenyl)-2-methyl-4-oxo-1-butanoic acid, 414
[100059-66-3]	1-(2,3,4,6-Tetrahydroxyphenyl)-3-methyl-1-butanone, 184
[100079-25-2]	1-(3,4,5-Trihydroxyphenyl)-1-heptanone, 729
[100079-26-3]	1-(3,4,5-Trihydroxyphenyl)-1-nonanone, 840
[100079-28-5]	1-(3,4,5-Tribenzyloxyphenyl)-1-heptanone, 730
[100116-12-9]	Methyl 1-[5-bromo-2,4-dihydroxy-3-(1-oxobutyl)]benzoate (Oxime), 41
[100116-82-3]	Methyl 1-[5-chloro-2,4-dihydroxy-3-(1-oxobutyl)]benzoate (Oxime), 41
[100118-19-2]	6-(2-Hydroxyphenyl)-6-oxo-1-hexanoic acid, 709
[100121-89-9]	6-(3,5-Dibromo-4-hydroxyphenyl)-6-oxo-1-hexanoic acid, 714
[100130-01-6]	1-(3-Chloro-2-hydroxyphenyl)-1-butanone (Semicarbazone), 29
[100137-55-1]	1-(2,4-Dimethoxy-5-nitrophenyl)-1-butanone, 36
[100256-47-1]	2-Ethyl-1-(4-hydroxyphenyl)-1-butanone, 169
[100256-99-3]	1-(2,6-Dihydroxy-3-ethylphenyl)-1-butanone, 69
[100257-43-0]	1-(3,5-Dihydroxyphenyl)-4-methyl-1-pentanone, 545
[100257-71-4]	2-Ethyl-1-(2,4,5-trihydroxyphenyl)-1-butanone, 170
[100370-41-0]	1-(5-Amino-2,4-dimethoxyphenyl)-1-butanone, 40
[100380-49-2]	1-(5-Bromo-6-hydroxy-3-methyl-7-benzofuranyl)-1-butanone (Oxime), 78
[100388-73-6]	1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-butanone, 63
[100391-90-0]	6-(2-Hydroxyphenyl)-6-oxo-1-hexanoic acid (Oxime), 709
[100397-26-0]	1-(6-Hydroxy-3-methyl-7-benzofuranyl)-1,3-butanedione, 326
[100486-17-7]	1-(2-Hydroxyphenyl)-1-pentadecanone, 1025
[100486-26-8]	1-(2,4-Dihydroxyphenyl)-1-pentadecanone, 1027
[100559-74-8]	9,10,12,13,15,16-Hexabromo-1-(3,4-dimethoxyphenyl)-1-octadecanone, 1090
[100559-75-9]	9,10,12,13,15,16-Hexabromo-1-(3,4-dihydroxyphenyl)-1-octadecanone, 1090
[100559-77-1]	9,10,12,13-Tetrabromo-1-(3,4-dimethoxyphenyl)-1-octadecanone, 1090
[100559-78-2]	9,10,12,13-Tetrabromo-1-(3,4-dihydroxyphenyl)-1-octadecanone, 1090
[100559-80-6]	9,10,12,13,15,16-Hexabromo-1-(3,4-dihydroxyphenyl)-1-heneicosanone, 1102
[100568-25-0]	9,10,12,13,15,16-Hexabromo-1-(3,4-dimethoxyphenyl)-1-heneicosanone, 1102
[100607-74-7]	1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-pentanone, 499
[100619-32-7]	1-(3,4-Dimethoxyphenyl)-1-pentanone (Oxime), 473
[100696-99-9]	1,1′-[Ethylidenebis(2-fluoro-5-hydroxy-4,1-phenylene)]bis-1-butanone, 336
[100697-01-6]	1-(4-Butyryl-2-fluoro-5-hydroxyphenyl)-1-(3-butyryl-5-fluoro-2-hydroxyphenyl)ethane, 335
[100697-02-7]	1-(5-Fluoro-2-hydroxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 33
[100706-52-3]	6-(2-Hydroxyphenyl)-6-oxo-1-hexanoic acid (Semicarbazone), 709
[100712-42-3]	1-(5-Chloro-6-hydroxy-3-methyl-7-benzofuranyl)-1-butanone, 78
[100792-29-8]	1-[3-Bromo-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-butanone, 89
[100792-79-8]	1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-hexanone, 647
[100794-83-0]	1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-pentanone (Semicarbazone), 499
[100863-37-4]	1-(3-Methoxyphenyl)-1-heptanone, 721

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[100864-00-4]	1-(2-Hydroxy-5-methoxyphenyl)-1-heptanone, 740
[100864-42-4]	1-(2,4,5-Trihydroxyphenyl)-2-ethyl-1-hexanone, 619
[100884-40-0]	1-(3,5-Diacetyloxyphenyl)-1-butanone, 15
[100952-80-5]	1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-hexanone (Semicarbazone), 647
[100972-54-1]	1-[4-(Acetyloxy)-2-hydroxyphenyl]-1-hexanone, 646
[100972-66-5]	1-(4-Methoxy-3-propylphenyl)-4-oxo-1-butanoic acid, 447
[100972-91-6]	4-(2,4-Dimethoxy-5-ethylphenyl)-4-oxo-1-butanoic acid, 445
[100972-92-7]	4-(4,5-Dimethoxy-2-ethylphenyl)-4-oxo-1-butanoic acid, 446
[100976-33-8]	1-(6-Acetyloxy-3-methyl-2-benzofuranyl)-1-butanone, 79
[101002-14-6]	1-(3-Chloro-2-hydroxyphenyl)-1-hexanone (Oxime), 624
[101002-19-1]	1-[2-Hydroxy-4-(pentyloxy)phenyl]-1-hexanone (Oxime), 670
[101002-20-4]	1-[4-(Decyloxy)-2-hydroxyphenyl]-1-hexanone (Oxime), 692
[101002-21-5]	1-[2-Hydroxy-4-(octyloxy)phenyl]-1-dodecanone (Oxime), 983
[101002-23-7]	1-(3-Chloro-2-hydroxyphenyl)-1-dodecanone (Oxime), 954
[101002-24-8]	1-(5-Chloro-2-hydroxyphenyl)-1-dodecanone (Oxime), 955
[101002-27-1]	1-[4-(Decyloxy)-2-hydroxyphenyl]-1-dodecanone (Oxime), 985
[101002-28-2]	1-(2-Hydroxy-5-methylphenyl)-1-hexanone, 640
[101002-32-8]	1-[2-Hydroxy-4-(pentyloxy)phenyl]-1-hexanone, 670
[101002-33-9]	1-[4-(Decyloxy)-2-hydroxyphenyl]-1-hexanone, 692
[101002-34-0]	1-[2-Hydroxy-4-(octyloxy)phenyl]-1-dodecanone, 983
[101032-04-6]	3-Methyl-1-(2,4,6-trimethoxyphenyl)-1-butanone, 183
[101043-59-8]	1-(5-Chloro-2,4-dihydroxyphenyl)-1-pentanone, 483
[101088-95-3]	1-(5-Ethyl-6-hydroxy-3-methyl-7-benzofuranyl)-1-butanone, 94
[101100-37-2]	1-(2-Hydroxy-5-pentylphenyl)-1-butanone, 99
[101100-66-7]	1-(4-Butyloxyphenyl)-1-pentanone, 468
[101100-86-1]	1-(3,4-Dimethoxyphenyl)-1-heptanone, 727
[101103-45-1]	1-(3,5-Diacetyloxyphenyl)-1-pentanone, 474
[101109-36-8]	1-(3,4-Dimethoxyphenyl)-1-hexanone (Semicarbazone), 610
[101117-26-4]	4-(3,5-Dimethoxyphenyl)-3-methyl-4-oxo-1-butanoic acid (Semicarbazone), 417
[101253-68-3]	10-(2-Hydroxyphenyl)-10-oxo-1-decanoic acid, 918
[101254-34-6]	1-[3-Bromo-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-hexanone, 663
[101254-66-4]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-hexanone, 664
[101267-59-8]	1-(4-Hydroxy-3-methylphenyl)-4-methyl-1-pentanone, 547
[101268-53-5]	1-(2,4,6-Trihydroxy-3-methylphenyl)-1-hexanone, 644
[101271-65-2]	1-(2-Hydroxy-4,6-dimethylphenyl)-1-octanone, 799
[101375-31-9]	1-(2,3-Dichloro-4-methoxyphenyl)-1-pentanone, 479
[101375-32-0]	1-(4-Methoxy-2,3-dimethylphenyl)-1-pentanone, 500
[101375-33-1]	1-(2,3-Dichloro-4-methoxyphenyl)-2-methylene-1-pentanone, 556
[101375-34-2]	1-(4-Methoxyphenyl)-2-methylene-1-pentanone, 477
[101375-35-3]	1-(4-Methoxy-2,3-dimethylphenyl)-2-methylene-1-pentanone, 559
[101394-53-0]	1,4-Bis(3,4,5-trimethoxyphenyl)-1,4-butanedione, 364
[101396-06-9]	1-(2-Methoxy-5-methylphenyl)-1-hexadecanone (Oxime), 1041
[101396-10-5]	1-(2-Methoxy-5-methylphenyl)-1-decanone (Oxime), 884

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[101396-11-6]	1-(2-Hydroxy-4-methoxyphenyl)-1,3-butanedione, 319
[101427-26-3]	1-(3,4-Dimethoxyphenyl)-1-heptanone (Semicarbazone), 727
[101430-14-2]	2,4-Dimethoxy-5-isovalerylcinnamic acid, 205
[101430-19-7]	1-(3,5-Diacetyloxyphenyl)-1-hexanone, 610
[101430-33-5]	1-(3,5-Diacetyloxyphenyl)-4-methyl-1-pentanone, 545
[101499-61-0]	4-[4-Methoxy-2-methyl-5-(1-methylethyl)phenyl]-4-oxo-1-butanoic acid, 450
[101499-71-2]	Ethyl 5-(3,4-dimethoxyphenyl)-5-oxo-1-pentanoate, 582
[101577-83-7]	1-[3-Bromo-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-heptanone, 748
[101593-65-1]	1-(3,5-Dihydroxyphenyl)-3-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 180
[101593-70-8]	1-(3,5-Dihydroxyphenyl)-1-pentanone (2,4-Dinitrophenylhydrazone), 474
[101597-59-5]	1-(2-Hydroxyphenyl)-5-(4-hydroxyphenyl)-1,5-pentanedione, 519
[101598-23-6]	1-(3-Chloro-6-allyloxy-2,4-dimethylphenyl)-1-hexanone, 647
[101602-22-6]	1-(3,5-Dibromo-2-benzoyloxyphenyl)-1-butanone, 21
[101649-67-6]	1-(2,5-Dihydroxy-4-methylphenyl)-1-octadecanone, 1076
[101684-67-7]	1,5-Bis(4-ethoxyphenyl)-1,5-pentanedione, 519
[101684-68-8]	1,5-Bis(4-propyloxyphenyl)-1,5-pentanedione, 519
[101684-69-9]	1,5-Bis(4-butyloxyphenyl)-1,5-pentanedione, 519
[101684-71-3]	1,5-Bis(4-pentyloxyphenyl)-1,5-pentanedione, 519
[101720-12-1]	1-(4-Hydroxyphenyl)-1-hexanone (iso-Nicotinylhydrazone), 602
[101728-14-7]	1-(5-Bromo-2-hydroxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 623
[101735-99-3]	1,6-Bis-(5-chloro-2-hydroxyphenyl)-1,6-hexanedione, 671
[101737-37-5]	1,4-Bis(5-methoxy-2-nitrophenyl)-2-bromo-1,4-butanedione, 355
[101741-01-9]	1-(4-Methoxyphenyl)-1-decanone, 870
[101741-11-1]	1-(2,5-Dimethoxyphenyl)-1-nonanone, 839
[101741-97-3]	1-(3,5-Dihydroxyphenyl)-4-methyl-1-pentanone (2,4-Dinitrophenylhydrazone), 545
[101777-85-9]	1-(4-Methoxyphenyl)-1-hexanone (Semicarbazone), 604
[101778-04-5]	1-(3,4-Dimethoxyphenyl)-3-methyl-1-butanone (Semicarbazone), 180
[101778-12-5]	1-(3,4-Dimethoxyphenyl)-1-pentanone (Semicarbazone), 473
[101784-96-7]	1-(2-Hydroxy-4-methylphenyl)-3-methyl-1-butanone (Phenylhydrazone), 190
[101789-78-0]	1-(5-Benzoyl-2-hydroxy-3-methylphenyl)-1-butanone, 386
[101790-34-5]	1-(2-Hydroxyphenyl)-6-(4-hydroxyphenyl)-1,6-hexanedione, 674
[101790-57-2]	1-[2-Hydroxy-4-methoxy-5-(phenylmethoxy)phenyl]-1,3-butanedione, 333
[101829-84-9]	1-(8-Hydroxy-5-quinolinyl)-1-dodecanone, 968
[101873-66-9]	1-(4-Heptyl-2-hydroxyphenyl)-3-methyl-1-butanone, 225
[101873-69-2]	1-(2-Hydroxy-4,6-dimethylphenyl)-1-decanone, 887
[101873-72-7]	1-[3-Hydroxy-4-(3-methylbutyl)phenyl]-1-heptanone, 752
[101874-06-0]	1-[2-Hydroxy-4,6-dimethoxy-3-(3-methylbutyl)phenyl]-3-methyl-1-butanone, 226
[101874-19-5]	1-[2,4-Dihydroxy-3,6-dimethoxy-5-(3-methylbutyl)phenyl]-3-methyl-1-butanone, 226

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[101876-10-2]	1-(5-Bromo-2-hydroxyphenyl)-1-pentanone (2,4-Dinitrophenylhydrazone), 481
[101892-45-9]	1-(6-Allyloxy-3-chloro-2,4-dimethylphenyl)-1-heptanone, 741
[102003-68-9]	1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-heptanone, 741
[102003-73-6]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-pentanone, 507
[102011-49-4]	1-(4-Hydroxyphenyl)-1-heptanone (Nicotinylhydrazone), 722
[102020-37-1]	1-[6-Methoxy-2-methyl-3-(1-methylethyl)phenyl]-1-octanone, 807
[102020-42-8]	1-(4-Heptyl-2-hydroxy-5-methoxyphenyl)-3-methyl-1-butanone, 228
[102075-11-6]	1-(3-Chloro-6-allyloxy-2,4-dimethylphenyl)-1-pentanone, 500
[102158-27-0]	1-(3,5-Diacetyloxyphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 15
[102159-08-0]	1-(2-Acetyloxy-5-benzoyl-3-methylphenyl)-1-butanone, 386
[102161-19-3]	1-(4-Methoxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 604
[102161-23-9]	1-(3,5-Dihydroxyphenyl)-1-heptanone (2,4-Dinitrophenylhydrazone), 728
[102166-29-0]	13-(2-Hydroxyphenyl)-13-oxo-1-tridecanoic acid, 1001
[102172-04-3]	1-(2,4-Dimethoxy-6-methylphenyl)-4-phenyl-1,3-butanedione, 355
[102222-55-9]	Ethyl 4-(2,3,4-trimethoxyphenyl)-4-oxo-1-butanoate, 411
[102240-70-0]	1-(4-Hydroxyphenyl)-1-octanone (isoNicotinylhydrazone), 775
[102240-72-2]	1-(4-Hydroxyphenyl)-1-octanone (Nicotinylhydrazone), 775
[102370-52-5]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-decanone, 895
[102447-83-6]	1,5-Bis(4-methoxyphenyl)-3,3-dimethyl-1,5-pentanedione, 533
[102456-07-5]	1-[2-Hydroxy-5,6-dimethyl-3-(1-methylethyl)phenyl]-1-decanone, 897
[102456-30-4]	1-(4-Methoxyphenyl)-1-tetradecanone, 1004
[102457-90-9]	4-(2-Hydroxy-3,5-dimethylphenyl)-4-oxo-1-butanoic acid (S-Benzylthiuronium salt), 443
[102458-44-6]	1-(3-Methoxyphenyl)-1-heptanone (2,4-Dinitrophenylhydrazone), 722
[102458-53-7]	3-Methyl-1-[2,4,5-trimethoxyphenyl]-1-butanone (2,4-Dinitrophenylhydrazone), 181
[102462-84-0]	1-[4-(N-Diethylaminoethyloxy)phenyl]-1-octanone (Hydrochloride), 777
[102465-47-4]	1-[3-Bromo-2-allyloxy-5-(1,1-dimethylethyl)phenyl]-1-heptanone, 748
[102474-24-8]	1,5-Bis(4-acetyloxyphenyl)-1,5-pentanedione, 518
[102475-97-8]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-hexanone (2,4-Dinitrophenylhydrazone), 664
[102596-47-4]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-pentanone (2,4-Dinitrophenylhydrazone), 507
[102655-30-1]	1-(3,5-Diacetyloxyphenyl)-1-heptanone (2,4-Dinitrophenylhydrazone), 728
[102661-34-7]	1-(3,5-Diacetyloxyphenyl)-3-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 181
[102665-28-1]	1-(3-Chloro-2,6-dibenzoyloxyphenyl)-1-butanone, 31
[102701-26-8]	1-(4-Hydroxyphenyl)-1-decanone (iso-Nicotinylhydrazone), 870
[102701-83-7]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-dodecanone, 972
[102709-19-3]	1-(3,4-Dimethoxyphenyl)-1-decanone (Semicarbazone), 874
[102753-19-5]	1-(4-Methoxyphenyl)-1-decanone (iso-Nicotinylhydrazone), 871
[102758-43-0]	1,10-Bis(2-hydroxyphenyl)-1,10-decanedione (Oxime), 900
[102758-82-7]	1-(3,4-Dimethoxyphenyl)-1-octanone (2,4-Dinitrophenylhydrazone), 782
[102810-66-2]	1-(3,5-Diacetyloxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 611

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[102810-70-8]	1-(3,5-Diacetyloxyphenyl)-4-methyl-1-pentanone (2,4-Dinitrophenylhydrazone), 545
[102812-21-5]	1-(4-Heptyl-2-hydroxyphenyl)-3-methyl-1-butanone (p-Nitrophenylhydrazone), 225
[102897-71-2]	1-(4-Heptyl-2-hydroxyphenyl)-3-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 225
[102898-52-2]	1-(2-Hydroxy-5-pentylphenyl)-1-dodecanone, 975
[102898-55-5]	1-(4-Methoxyphenyl)-1-hexadecanone, 1033
[102898-63-5]	1-(2-Hydroxy-5-methoxyphenyl)-1-hexadecanone, 1043
[102898-66-8]	1-(2-Hydroxy-5-methoxy-3-octylphenyl)-1-octanone, 825
[102904-17-6]	1-[3-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-2,4,6-trihydroxy-5-(2-hydroxy-3-methyl-3-butenyl)phenyl]-1-butanone, 344
[102946-00-9]	1-(4-Capryloxyphenyl)-1-octanone, 776
[102946-84-9]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-decanone (2,4-Dinitrophenylhydrazone), 895
[102947-41-1]	1-(3,4-Dimethoxyphenyl)-1-dodecanone (2,4-Dinitrophenylhydrazone), 949
[102949-16-6]	Methyl 1-[5-chloro-2,4-dibenzoyloxy-3-(1-oxobutyl)]benzoate, 42
[102955-19-1]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-octanone (2,4-Dinitrophenylhydrazone), 806
[102957-05-1]	1,8-Bis(4-acetyloxyphenyl)-1,8-octanedione, 811
[103033-88-1]	5,7-Dimethoxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 246
[103040-41-1]	2-Chloro-1-(2-hydroxyphenyl)-1-butanone, 276
[103044-77-5]	1-(2,5-Dimethoxyphenyl)-1-heptadecanone, 1056
[103045-61-0]	1-(8-Hydroxy-5-quinolinyl)-1-hexadecanone, 1046
[103048-59-5]	1-(2,5-Dimethoxyphenyl)-1-octadecanone, 1066
[103098-69-7]	Methyl 1-[5-ethyl-2,4-dibenzoyloxy-3-(1-oxobutyl)]benzoate, 81
[103099-04-3]	1-(2,5-Dimethoxyphenyl)-1-nonadecanone, 1093
[103119-13-7]	1-(3-Hydroxyphenyl)-1-hexanone, 600
[103119-42-2]	1-(3-Benzyloxyphenyl)-2,2-dimethyl-1-hexanone, 617
[103159-09-7]	1-(4-Hydroxyphenyl)-1-hexadecanone (iso-Nicotinylhydrazone), 1033
[103161-22-4]	1,13-Bis(4-acetyloxyphenyl)-1,13-tridecanedione, 1000
[103168-03-2]	1-(2-Hydroxy-5-methoxy-3-methylphenyl)-1-hexadecanone, 1044
[103170-10-1]	1,18-Bis(2,4-dihydroxyphenyl)-1,18-octadecanedione, 1084
[103204-42-8]	1-(2,4-Dihydroxy-5-nitrophenyl)-1-butanone, 36
[103204-43-9]	1-(2,6-Dihydroxy-3-nitrophenyl)-1-butanone, 37
[103205-61-4]	1-(2,4-Dihydroxy-3-nitrophenyl)-1-butanone, 36
[103209-07-0]	1,13-Bis(2,4-dimethoxyphenyl)-1,13-tridecanedione, 1001
[103209-93-4]	5,7-Diacetyloxy-8-(3-methylbutyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 248
[103273-98-9]	1-(5-Bromo-2,4-dihydroxy-3-nitrophenyl)-1-butanone, 21
[103274-59-5]	1-(3-Bromo-2,4-dihydroxy-5-nitrophenyl)-1-butanone, 21
[103279-18-1]	1-(2,3,4-Trihydroxyphenyl)-1-docosanone, 1105
[103323-29-1]	1-(3-Hydroxyphenyl)-1-butanone, 3
[103323-62-2]	1-(3,5-Dihydroxyphenyl)-1-butanone, 15
[103324-17-0]	1-(2,3-Dihydroxyphenyl)-1-butanone, 8

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[103325-22-0]	1-(2,5-Dimethoxyphenyl)-1-nonadecanone (2,4-Dinitrophenylhydrazone), 1093
[103326-23-4]	1,4-Bis(4-methoxyphenyl)-2,3-(4-methoxyphenyl)-1,4-butanedione, 375
[103330-25-2]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-dodecanone (2,4-Dinitrophenylhydrazone), 973
[103396-94-7]	1-(4-Hydroxyphenyl)-1-docosanone (iso-Nicotinylhydrazone), 1104
[103398-74-9]	1-(2-Methoxy-5-methylphenyl)-1-docosanone, 1107
[103398-77-2]	1-(2,5-Dihydroxy-4-dodecylphenyl)-1-dodecanone, 987
[103449-09-8]	2-Hexyl-1-(6-hydroxy-1,3-benzodioxol-5-yl)-1-decanone, 905
[103449-10-1]	2-Hexyl-1-(2,4,5-trihydroxyphenyl)-1-decanone, 877
[103449-14-5]	1-(2,3,4-Trihydroxyphenyl)-1-octadecanone, 1067
[103509-18-8]	1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)bis-1-butanone, 334
[103567-06-2]	3-Methyl-1-[2,3,4,6-tetrabenzoyloxy-5-(3-methylbutyl)phenyl]-1-butanone, 218
[103582-37-2]	1-(2-Hydroxy-5-methylphenyl)-1-butanone (Oxime), 49
[103582-39-4]	1-(2-Hydroxy-5-methylphenyl)-1-octanone (Oxime) (*E*), 793
[103582-40-7]	1-(2-Hydroxy-5-methylphenyl)-1-decanone (Oxime) (*E*), 883
[103582-41-8]	1-(2-Hydroxy-5-methylphenyl)-1-dodecanone (E) (Oxime), 959
[103646-41-9]	4-(3-Methoxy-2-nitrophenyl)-4-oxo-1-butanoic acid, 425
[103650-06-2]	1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-pentanone, 537
[103758-73-2]	1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-hexanone, 693
[103766-18-3]	3-[[2,4-Dihydroxy-6-methoxy-3-(2-methyl-1-oxobutyl)phenyl]methyl]-6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one, 150
[103771-69-3]	1-[2,6-Dihydroxy-4-methoxy-3-(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone, 145
[103771-71-7]	3-[[2,4-Dihydroxy-6-methoxy-5-(3-methyl-2-butenyl)-3-(2-methyl-1-oxobutyl)phenyl]-methyl]-6-ethyl-4-hydroxy-5-methyl-2H-pyran-2-one, 163
[103771-75-1]	1-[2,3-Dihydro-4,6-dihydroxy-2-(1-methylethenyl)-5-benzofuranyl]-2-methyl-1-butanone, 141
[103771-76-2]	3-[[5,7-Dihydroxy-2,2-dimethyl-6-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-8-yl]methyl]-6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one, 162
[103797-90-6]	1-(5-Bromo-2-hydroxyphenyl)-1-hexanone, 623
[103798-50-1]	1-(2,5-Dihydroxy-4-octylphenyl)-1-pentanone, 535
[103834-39-5]	3-[[2,3-Dihydro-4,6-dihydroxy-2-(1-methylethenyl)-5-(2-methyl-1-oxobutyl)-7-benzo-furanyl]methyl]-6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one, 162
[103862-60-8]	4-(4-Methoxyphenyl)-2,3-dibromo-4-oxo-1-butanoic acid, 397
[103981-28-8]	1-[2-Hydroxy-4-[(3-nitrophenyl)methoxy]phenyl]-1-hexanone, 683
[103981-30-2]	1-[2-Methoxy-4-[(3-nitrophenyl)methoxy]phenyl]-1-hexanone, 683
[103987-16-2]	4-(2-Methoxyphenyl)-4-oxo-1-butanoic acid, 399
[103987-17-3]	4-(2-Hydroxy-5-methylphenyl)-4-oxo-1-butanoic acid, 434
[104008-42-6]	1-(4-Hydroxy-3,5-dimethylphenyl)-1-butanone, 68
[104008-48-2]	1-(3,5-Diethyl-4-hydroxyphenyl)-1-butanone, 92
[104008-49-3]	1-(4-Methoxy-3,5-dimethylphenyl)-1-hexanone, 651
[104098-36-4]	1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-heptanone, 763

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[104129-16-0]	1-[3-(Aminomethyl)-5-bromo-4-hydroxyphenyl]-1-pentanone (O-Methyloxime), 491
[104145-15-5]	1-[3-(Aminomethyl)-5-bromo-4-hydroxyphenyl]-1-pentanone (Oxime), 491
[104174-31-4]	1-(4-Hydroxy-2-methylphenyl)-1-butanone, 50
[104192-31-6]	1,5-Bis(4-hexyloxyphenyl)-1,5-pentanedione, 519
[104216-24-2]	1-(2,3-Dihydroxyphenyl)-3-methyl-1-butanone, 176
[104216-80-0]	1-(3,5-Dihydroxyphenyl)-3-methyl-1-butanone, 180
[104295-23-0]	1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-nonanone, 863
[104325-46-4]	1-(3-Hydroxyphenyl)-2,2-dimethyl-1-hexanone, 617
[104325-65-7]	6,6,6-Trifluoro-1-(3-hydroxyphenyl)-1-hexanone, 702
[104325-67-9]	5,5,5-Trifluoro-1-(3-hydroxyphenyl)-1-pentanone, 564
[104341-05-1]	1-(3-Phenoxymethyloxyphenyl)-2,2-dimethyl-1-hexanone, 617
[104397-43-5]	1-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)-1-octanone, 826
[104440-88-2]	1,1′-(4,4′-Dihydroxy[1,1′-biphenyl]-3,3′-diyl)bis-1-dodecanone, 991
[104516-35-0]	1-(2-Hydroxy-5-methylphenyl)-1,3-pentanedione, 488
[104516-36-1]	1-(2-Hydroxy-3,5-dimethylphenyl)-1,3-butanedione, 321
[104780-38-3]	Methyl 1-[5-bromo-2,4-dihydroxy-3-(1-oxobutyl)]benzoate, 40
[104783-89-3]	1-(2-Hydroxy-4-methoxy-6-methylphenyl)-2-(methylsulfinyl)-1-ethanone, 60
[104783-90-6]	1-[2-Hydroxy-4-(β-methoxyethoxymethoxy)-6-methylphenyl]-2-(methylsulfinyl)-1-ethanone, 93
[104851-85-6]	Methyl 1-[5-chloro-2,4-dihydroxy-3-(1-oxobutyl)]benzoate, 41
[104966-92-9]	10-(Acetyloxy)-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-decanone, 893
[104966-93-0]	12-Acetyloxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-dodecanone, 971
[104966-94-1]	20-Acetyloxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-eicosanone, 1100
[104966-97-4]	10-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-decanone, 892
[104966-98-5]	20-Hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-eicosanone, 1100
[104967-07-9]	10-(Acetyloxy)-1-(2,3,4-trimethoxy-6-methylphenyl)-1-decanone, 893
[104967-08-0]	10-(Acetyloxy)-1-(2,4-dihydroxy-3-methoxy-6-methylphenyl)-1-decanone, 895
[104967-09-1]	10-(Acetyloxy)-1-(2,3-dihydroxy-4-methoxy-6-methylphenyl)-1-decanone, 895
[104988-70-7]	18-Acetyloxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl)-1-octadecanone, 1081
[105041-43-8]	1-(3,5-Dibromo-2-hydroxyphenyl)-1-butanone (Semicarbazone), 21
[105133-00-4]	4-Chloro-1-(3,4-dihydroxyphenyl)-1-butanone, 282
[105174-43-4]	4-Bromo-1-(3,4-dihydroxyphenyl)-1-butanone, 275
[105174-45-6]	4-Bromo-1-(2,4-dihydroxyphenyl)-1-butanone, 274
[105174-47-8]	4-Bromo-1-(2,3,4-trihydroxyphenyl)-1-butanone, 275
[105174-48-9]	4-Bromo-1-(3,4-dimethoxyphenyl)-1-butanone, 275
[105174-49-0]	4-Chloro-1-(2,4-dihydroxyphenyl)-1-butanone, 281
[105174-51-4]	4-Chloro-1-(2,3,4-trihydroxyphenyl)-1-butanone, 282

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[105174-55-8]	1-(3,4-Dimethoxyphenyl)-4-iodo-1-butanone, 291
[105174-58-1]	4-Iodo-1-(2,3,4-trihydroxyphenyl)-1-butanone, 291
[105174-61-6]	1-(3,4-Dihydroxyphenyl)-4-iodo-1-butanone, 291
[105211-80-1]	1-(5-Bromo-2-hydroxyphenyl)-1-butanone, 27
[105306-66-9]	1-(3,4-Dihydro-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-1-butanone, 96
[105334-08-5]	1-(3,4-Dihydro-5,7-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-4-methyl-1-pentanone, 550
[105337-38-0]	1-(2-Hydroxy-4-methylphenyl)-3-methyl-1-butanone, 189
[105337-39-1]	1-(4-Hydroxy-3-methylphenyl)-3-methyl-1-butanone, 191
[105337-84-6]	1-(2-Hydroxy-3-methylphenyl)-3-methyl-1-butanone, 189
[105401-56-7]	1-(3,5-Dihydroxyphenyl)-1-hexanone, 610
[105465-02-9]	1-(5-Bromo-2-hydroxyphenyl)-1-octanone, 786
[105475-33-0]	4-(5-Chloro-2-ethoxyphenyl)-4-oxo-1-butanoic acid, 424
[105475-57-8]	1-(5-Hydroxy-2,4-dimethoxyphenyl)-1-butanone, 76
[105476-01-5]	1-(4-Hydroxy-2,5-dimethoxyphenyl)-1-butanone, 75
[105476-10-6]	1-(2,4,5-Trihydroxyphenyl)-1-hexanone, 612
[105701-23-3]	1-(5-Ethyl-2-hydroxyphenyl)-1-tetradecanone (Oxime), 1014
[105701-24-4]	1-(4-Ethyl-2-hydroxyphenyl)-1-tetradecanone, 1013
[105932-66-9]	1-(2-4-Dihydroxyphenyl)-2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-1-octanone, 828
[106141-14-4]	1-(2-Hydroxyphenyl)-2,2-dimethyl-1-butanone, 131
[106141-15-5]	1-(2-Hydroxy-5-methylphenyl)-2,2-dimethyl-1-butanone, 135
[106163-57-9]	1-(3,4-Dimethoxyphenyl)-1-butanone (Semicarbazone), 14
[106214-14-6]	1-[5-Ethyl-2,4-dihydroxy-3-(1-oxobutyl)]benzoic acid, 81
[106276-13-5]	1-(2,4-Dihydroxy-3,6-dimethoxyphenyl)-3-methyl-1-butanone, 202
[106320-28-9]	1-(5-Bromo-6-hydroxy-3-methyl-7-benzofuranyl)-1-butanone, 78
[106321-41-9]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-butanone, 89
[106393-53-7]	5-Butyryl-2-hydroxybenzoic acid, 43
[106393-54-8]	5-(2-Ethylbutyryl)-2-hydroxybenzoic acid, 171
[106476-93-1]	1-[2-Hydroxy-3-(1-methylethyl)-6-methylphenyl]-1-butanone, 91
[106591-86-0]	1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-4-oxo-1-butanoic acid, 450
[107076-65-3]	1-[4-Hydroxy-3-[[[3-(trifluoromethyl)phenyl]amino]methyl]phenyl]-1-octanone, 818
[107151-39-3]	6-(2-Methoxyphenyl)-6-oxo-1-hexanoic acid, 710
[107151-50-8]	1-(3-Chloro-6-hydroxy-2,4-dimethylphenyl)-1-heptanone (Semicarbazone), 741
[107152-23-8]	3-Methyl-1-[2,3,4,6-tetrahydroxy-5-(3-methylbutyl)phenyl]-1-butanone, 218
[107259-36-9]	1,12-Bis(4-hydroxyphenyl)-1,12-dodecanedione, 977
[107259-37-0]	1,10-Bis(4-hydroxy-2,6-dimethylphenyl)-1,10-decanedione, 913
[107276-31-3]	1-(2,4-Dihydroxy-3-quinolinyl)-1-octanone, 803
[107327-65-1]	4-(5-Ethoxy-2-methoxyphenyl)-4-oxo-1-butanoic acid, 407
[107327-72-0]	4-(2-Ethoxy-5-methoxyphenyl)-4-oxo-1-butanoic acid, 407
[107522-52-1]	1,1′-(4,6-Dihydroxy-5-nitro-1,3-phenylene)bis-1-butanone, 297

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[107623-54-1]	1-(6-Hydroxy-3-methyl-7-benzofuranyl)-1-butanone, 79
[107771-42-6]	1-(2-Hydroxy-3,6-dimethylphenyl)-1-hexanone, 649
[107772-24-7]	1-(2-Hydroxy-3,5-dimethylphenyl)-1-hexanone, 649
[107778-10-9]	1-(3,4-Dimethoxyphenyl)-1-octanone (Semicarbazone), 782
[107778-29-0]	1,1′-(4,6-Diacetyloxy-5-nitro-1,3-phenylene)bis-1-butanone, 298
[107821-60-3]	1-(2,4,5-Trihydroxyphenyl)-1-octanone, 783
[108080-61-1]	1-[2,4,6-Trihydroxyphenyl]-1-heptanone (Polymer with formaldehyde), 729
[108111-23-5]	1-(2-Hydroxy-4-methylphenyl)-1-octanone (Oxime, nickel complex), 792
[108111-24-6]	1-[2-Hydroxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-dodecanone (Oxime, nickel complex), 982
[108111-25-7]	1-[4-[(2-Ethylhexyl)oxy]-2-hydroxyphenyl]-1-dodecanone (Oxime, nickel complex), 983
[108125-65-1]	Methyl 1-[5-ethyl-2,4-dihydroxy-3-(1-oxobutyl)]benzoate, 81
[108300-00-1]	1-[3-Chloro-2-hydroxy-5-(1,1-dimethylethyl)phenyl]-1-octanone, 806
[108401-78-1]	1-(2,3,4-Trimethoxyphenyl)-1-butanone, 16
[108515-73-7]	6-(2,5-Dihydroxyphenyl)-6-oxo-1-hexanoic acid, 712
[108623-73-0]	1-(2-Methoxy-4,5-dimethylphenyl)-1-decanone, 887
[108666-97-3]	1-(2-Hydroxy-4-methylphenyl)-1-octanone, 792
[108667-53-4]	1-(2-Hydroxy-3-methylphenyl)-1-octanone, 791
[108715-26-0]	1-(3,5-Diacetyloxyphenyl)-3-methyl-1-butanone, 180
[108719-92-2]	1-[3-Bromo-2-allyloxy-5-(1,1-dimethylethyl)phenyl]-1-hexanone, 663
[108791-64-6]	1,4-Bis(4-hydroxyphenyl)-1,4-butanedione, 359
[108919-66-0]	1-[4-(2-Propenyloxy)phenyl]-1-pentanone, 469
[108919-67-1]	1-[4-(3-Pentenyloxy)phenyl]-1-pentanone, 469
[108919-68-2]	1-[4-(5-Methyl-4-hexenyloxy)phenyl]-1-pentanone, 469
[108919-69-3]	1-[4-(3-Butenyloxy)phenyl]-1-pentanone, 469
[108919-70-6]	1-[4-(3-Methyl-3-butenyloxy)phenyl]-1-pentanone, 469
[108919-71-7]	1-[4-(3-Pentenyloxy)phenyl]-1-pentanone (Z), 469
[108919-72-8]	1-[4-(4-Methyl-3-pentenyloxy)phenyl]-1-pentanone, 469
[108919-73-9]	1-[4-(4-Pentenyloxy)phenyl]-1-pentanone, 469
[108919-74-0]	1-[4-(5-Hexenyloxy)phenyl]-1-pentanone, 469
[108919-75-1]	1-[4-(10-Undecenyloxy)phenyl]-1-pentanone, 469
[108955-15-3]	5-Bromo-6-hydroxy-3-methyl-7-(1-oxobutyl)-2-benzofurancarboxylic acid, 86
[108978-55-8]	1-(2,4,5-Trihydroxyphenyl)-1-decanone, 875
[108984-69-6]	1-(4-Hydroxyphenyl)-1-heptanone (isoNicotinylhydrazone), 723
[108991-24-8]	3-Methyl-1-(2,4,6-trihydroxyphenyl)-1-pentanone (S), 555
[109068-12-4]	7-Methoxy-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 204
[109103-09-5]	6-Chloro-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one, 86
[109103-12-0]	5-Chloro-6-hydroxy-3-methyl-7-(1-oxobutyl)-2-benzofurancarboxylic acid, 87
[109175-98-6]	1-(3,4-Dibutyloxyphenyl)-1-tridecanone, 998
[109248-77-3]	1-(4-Hydroxy-3-methylphenyl)-3-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 191
[109248-78-4]	1-(3,5-Dihydroxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 610

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[109250-84-2]	1-(2-Hydroxy-4-methylphenyl)-1-decanone, 882
[109250-85-3]	1-(4-Hydroxy-3-methylphenyl)-1-decanone, 884
[109251-96-9]	1-(2-Hydroxy-3-methylphenyl)-1-decanone, 882
[109252-17-7]	1-(2-Hydroxy-3-methylphenyl)-3-methyl-1-butanone (2,4-Dinitrophenylhydrazone), 189
[109252-18-8]	1-(2,4-Dihydroxyphenyl)-1-hexanone (2,4-Dinitrophenylhydrazone), 607
[109262-64-8]	6-Bromo-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one (Semicarbazone), 86
[109441-87-4]	5-Ethyl-6-hydroxy-3-methyl-7-(1-oxobutyl)-2-benzofurancarboxylic acid, 103
[109471-10-5]	1,6-Bis(2-hydroxyphenyl)-1,6-hexanedione, 672
[109473-68-9]	6-Ethyl-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one, 103
[109558-46-5]	1-(3,4-Dimethoxyphenyl)-1-decanone, 874
[109559-39-9]	1-(2,4,5-Trihydroxyphenyl)-1-dodecanone, 951
[109564-87-6]	6-Hydroxy-7-(1-oxobutyl)-3-methylcoumarilic acid, 88
[109602-86-0]	6-Bromo-7-acetyloxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one, 86
[109641-80-7]	6-Methoxy-7-(1-oxobutyl)-3-methylcoumarilic acid, 88
[109720-03-8]	1-[4-(4-Hydroxyphenylethyloxy)phenyl]-1-pentanone, 468
[109720-05-0]	1-[4-(4-Methoxyphenylethyloxy)phenyl]-1-pentanone, 469
[109966-03-2]	7-Hydroxy-8-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 203
[109966-52-1]	7-Hydroxy-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 203
[110029-30-6]	6-Bromo-7-hydroxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one, 86
[110051-30-4]	1-(3-Hydroxyphenyl)-1-heptanone (2,4-Dinitrophenylhydrazone), 721
[110055-35-1]	6-Ethyl-7-acetyloxy-4-methyl-8-(1-oxobutyl)-2*H*-1-benzopyran-2-one, 103
[110351-70-7]	1-[2-Hydroxy-5-(1,1,3,3-tetramethylbutyl)phenyl]-1-dodecanone (Oxime, nickel complex), 982
[110581-80-1]	1-(3,5-Dichloro-4-hydroxyphenyl)-1-tridecanone, 999
[110593-81-2]	1-(8-Hydroxy-5-quinolinyl)-1-octadecanone, 1079
[110593-82-3]	1-(8-Hydroxy-5-quinolinyl)-1-octanone, 803
[110647-47-7]	1-[4-(Dodecyloxy)-2-hydroxyphenyl]-1-hexanone (Oxime), 694
[110662-32-3]	1-(4-Hydroxyphenyl)-1-pentadecanone, 1026
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[116588-92-2]	1,4-Bis(3,4-dimethoxyphenyl)-2,3-dimethyl-1,4-butanedione (Monophenyl-hydrazone) (racemic), 368
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[117285-75-3]	Methyl 3-(2-hydroxy-5-isovaleroyl-4-methoxyphenyl)propanoate, 216
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[117482-22-1]	2,2,3,3,4,4,4-Heptafluoro-1-(4-methoxyphenyl)-1-butanone, 289
[117692-92-9]	1-(4-Benzyloxyphenyl)-2,6-dimethyl-1-heptanone, 731
[117692-93-0]	1-(4-Hydroxyphenyl)-2,6-dimethyl-1-heptanone, 731
[117693-01-3]	1-(4′-Benzyloxy[1,1′-biphenyl]-4-yl)-2,6-dimethyl-1-heptanone, 762
[117693-02-4]	1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-2,6-dimethyl-1-heptanone, 762
[117706-06-6]	5-[5-Hydroxy-4-(1-oxodecyl)-2-(2-propenyl)phenoxy]pentanenitrile, 911
[118018-78-4]	6-Bromo-1-(2,4-dimethoxyphenyl)-1-hexanone, 699
[118108-79-5]	6-Bromo-1-(2-chloro-4-methoxyphenyl)-1-hexanone, 702
[118191-27-8]	1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-pentanone, 487
[118191-28-9]	1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-hexanone, 631
[118191-29-0]	1-(3,5-Dibromo-2,4-dihydroxy-6-methoxyphenyl)-1-hexanone, 630
[118191-30-3]	1-(3,5-Dibromo-2,6-dihydroxy-4-methoxyphenyl)-1-hexanone, 630
[118191-31-4]	1-(3,5-Dichloro-2,4-dihydroxy-6-methylphenyl)-1-hexanone, 630
[118191-32-5]	1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-heptanone, 735
[118191-33-6]	1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-heptanone, 736
[118191-34-7]	1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-octanone, 789
[118191-35-8]	1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-nonanone, 843
[118191-36-9]	1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-nonanone, 843
[118222-70-1]	1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-1-butanone, 42
[118222-71-2]	1-(3,5-Dichloro-2,4,6-trihydroxyphenyl)-1-hexanone, 622
[118222-72-3]	1-(3,5-Dichloro-2,4-dihydroxy-6-methoxyphenyl)-1-octanone, 788
[118469-84-4]	1-(2-Hydroxy-5-tetradecylphenyl)-1-hexanone, 695
[118469-92-4]	1-(2-Hydroxy-4-tetradecylphenyl)-1-hexanone, 694
[118476-18-9]	1-(2-Methoxyphenyl)-1-heptanone, 720
[118683-27-5]	4-[3-Hydroxy-4-(1-hexanoyl)-2-propylphenoxymethyl]-3-methoxybenzoic acid, 693
[119039-35-9]	1,18-Bis-(4-hydroxy-3-methylphenyl)-1,18-octadecanedione, 1085
[119039-36-0]	1,18-Bis-(2-hydroxy-5-methylphenyl)-1,18-octadecanedione, 1085
[119039-37-1]	1,18-Bis-(4-hydroxy-2-methylphenyl)-1,18-octadecanedione, 1085
[119039-38-2]	1,18-Bis-(2-hydroxy-4-methylphenyl)-1,18-octadecanedione, 1085
[119039-49-5]	1,18-Bis-(2-hydroxy-3-methylphenyl)-1,18-octadecanedione, 1085
[119042-58-9]	5,7-Dimethoxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 237
[119348-65-1]	Ethyl 6-(4-hydroxyphenyl)-6-oxo-1-hexanoate, 712
[119348-66-2]	Ethyl 5-(4-hydroxyphenyl)-3,3-dimethyl-5-oxo-1-pentanoate, 585
[119531-08-7]	1-(4-Hydroxyphenyl)-1-tetradecanone (Myristate), 1005
[119691-93-9]	1-(2,4,6-Trihydroxy-3-nitrophenyl)-1-butanone, 37
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[119691-95-1]	1-(2,4,6-Trihydroxy-3-nitrophenyl)-1-pentanone, 485
[119691-96-2]	1-(2,4,6-Trihydroxy-3-nitrophenyl)-1-hexanone, 628
[119691-97-3]	1-(2,4,6-Trihydroxy-3-nitrophenyl)-1-heptanone, 735
[119691-99-5]	1-(2,4,6-Trihydroxy-3-nitro-5-propylphenyl)-1-butanone, 82
[119692-00-1]	3-Methyl-1-(2,4,6-trihydroxy-3-nitro-5-propylphenyl)-1-butanone, 206
[119692-01-2]	1-(2,4,6-Trihydroxy-3-nitro-5-propylphenyl)-1-pentanone, 505
[119692-02-3]	1-(2,4,6-Trihydroxy-3-nitro-5-propylphenyl)-1-hexanone, 657
[119748-12-8]	1-(4-Methoxyphenyl)-2-propyl-1-pentanone, 556
[119998-59-3]	1-[3-Acetyl-2,4,6-trihydroxy-5-(2-hydroxy-3-methyl-3-butenyl)phenyl]-3-methyl-1-butanone, 383
[119998-60-6]	1-[5-Acetyl-2,3-dihydro-4,6-dihydroxy-2-(1-hydroxy-1-methylethyl)-7-benzofuranyl]-3-methyl-1-butanone, 382
[119998-61-7]	1-[7-Acetyl-2,3-dihydro-4,6-dihydroxy-2-(1-hydroxy-1-methylethyl)-5-benzofuranyl]-3-methyl-1-butanone, 382
[119998-63-9]	1-(8-Acetyl-3,4-dihydro-3,5,7-trihydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-3-methyl-1-butanone, 383
[119998-64-0]	1-(6-Acetyl-3,4-dihydro-3,5,7-trihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-3-methyl-1-butanone, 383
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[119998-66-2]	1-[5-Acetyl-2,3-dihydro-4,6-dihydroxy-2-(1-methylethenyl)-7-benzofuranyl]-3-methyl-1-butanone, 381
[120058-71-1]	1-(3-Chloro-2,6-dihydroxy-5-propylphenyl)-1-butanone, 81
[120259-64-5]	1-(4-Fluoro-2-hydroxy-5-nitrophenyl)-1-butanone, 25
[120292-07-1]	1-(4-Fluoro-2-hydroxy-5-nitrophenyl)-3-methyl-1-butanone, 185
[120363-73-7]	5,7-Dimethoxy-6-(3-methylbutyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 239
[120363-74-8]	5,7-Diacetyloxy-6-(3-methylbutyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 239
[120363-75-9]	5,7-Dimethoxy-8-(3-methylbutyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 240
[120529-47-7]	1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-1-pentanone, 491
[120716-96-3]	3-Methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-pentanone (S), 559
[120716-97-4]	2,4,6-Trihydroxy-3-(3-methyl-1-oxopentyl)benzaldehyde (S), 558
[120836-88-2]	1-(4-Hydroxyphenyl)-2-methyl-1-butanone, 126
[120836-99-9]	1-(4-Hydroxyphenyl)-2-methyl-1-butanone (2*S*), 126
[120837-00-5]	1-(4-Hydroxyphenyl)-2-methyl-1-octanone (*S*), 794
[120837-01-6]	1-(4-Hydroxyphenyl)-2-methyl-1-decanone (*S*), 876
[120837-02-7]	1-(4-Hydroxyphenyl)-2-methyl-1-heptanone (+), 730
[120837-03-8]	1-(4-Hydroxyphenyl)-2-methyl-1-nonanone (+), 840
[120837-04-9]	2-Ethyl-1-(4-hydroxyphenyl)-1-octanone (+), 784
[120837-05-0]	1-(4-Hydroxyphenyl)-2-propyl-1-decanone (*S*), 876
[120837-08-3]	1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-2-methyl-1-butanone (S), 262
[120837-09-4]	1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-2-methyl-1-octanone (+), 817
[120837-13-0]	1-(4-Methoxyphenyl)-2-methyl-1-octanone (+), 794
[120837-31-2]	1-(4-Hydroxyphenyl)-2-methyl-1-nonanone, 840

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[120857-41-2]	1-(4-Hydroxyphenyl)-1-hexadecanone (Palmitate), 1035
[121079-06-9]	4-Chloro-1-(2-hydroxy-4,6-dimethoxyphenyl)-1-butanone, 287
[121426-03-7]	3-Methyl-1-[2,4,6-tribenzoyloxy-3,5-bis(3-methyl-2-butenyl)phenyl]-1-butanone, 232
[121586-48-9]	1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[121586-49-0]	1-(4′-Acetyloxy[1,1′-biphenyl]-4-yl)-1-nonanone, 853
[121693-16-1]	1-[3-[(3-Acetyl-2,6-dihydroxy-4-methoxy-5-methylphenyl)methyl]-5-[[2,6-dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl]methyl]-2,4,6-trihydroxyphenyl]-1-butanone, 347
[122214-67-9]	1-(4-Lauryloxyphenyl)-1-dodecanone, 943
[122427-50-3]	1,4-Bis(2-hydroxy-4-methylphenyl)-1,4-butanedione, 365
[122492-61-9]	1-(4-Stearoyloxyphenyl)-1-octadecanone, 1064
[122585-49-3]	1-[2,6-Dihydroxy-4-[(3-methyl-2-butenyl)oxy]phenyl]-1-butanone, 97
[122585-50-6]	1-[2,6-Dihydroxy-4-[(4-hydroxy-3-methyl-2-butenyl)oxy]phenyl]-1-butanone *(E)*, 98
[122585-51-7]	1-[4-[[4-(Acetyloxy)-3-methyl-2-butenyl]oxy]-2,6-dihydroxyphenyl]-1-butanone *(E)*, 110
[122585-54-0]	1-[2,6-Dihydroxy-4-[(4-hydroxy-3-methyl-2-butenyl)oxy]phenyl]-2-methyl-1-butanone (*E*), 143
[122585-55-1]	1-[4-[[(4-Acetyloxy)-3-methyl-2-butenyl]oxy]-2,6-dihydroxyphenyl]-2-methyl-1-butanone *(E)*, 146
[122585-56-2]	4-[3,5-Dihydroxy-4-(1-oxobutyl)phenoxy]-2-methyl-1-butanoic acid, 98
[122585-61-9]	1-[3-[4-(Acetyloxy)-3-methyl-2-butenyl]-2,4,6-trihydroxyphenyl]-1-butanone *(E)*, 110
[122585-96-0]	1-[2,6-Diacetyloxy-4-[(4-acetyloxy-3-(acetyloxymethyl)-2-butenyl)oxy]phenyl]-1-butanone, 98
[122616-67-5]	1-[2,6-Dihydroxy-4-[[4-hydroxy-3-(hydroxymethyl)-2-butenyl]oxy]phenyl]-1-butanone, 98
[123014-46-0]	6-Bromo-1-(3,4-dimethoxyphenyl)-1-hexanone, 699
[123015-21-4]	6-Bromo-1-[3,4-dimethoxy-2-methyl-5-(1-methylethyl)phenyl]-1-hexanone, 708
[123015-22-5]	6-Bromo-1-(3,4-dimethoxy-2,5-dimethylphenyl)-1-hexanone, 707
[123015-34-9]	6-Bromo-1-(2-fluoro-4,5-dimethoxyphenyl)-1-hexanone, 704
[123015-39-4]	6-Bromo-1-(3,4-dimethoxy-2,5,6-trimethylphenyl)-1-hexanone, 708
[123020-85-9]	1-(2,4-Dihydroxyphenyl)-2-methyl-1-butanone (2S), 127
[123020-88-2]	1-(4-Hydroxyphenyl)-2-methyl-1-butanone (+), 126
[123059-72-3]	1-(3,4,5-Trimethoxyphenyl)-1-tridecanone, 998
[123127-70-8]	5,7-Dihydroxy-8-(3-methylbutyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 240
[123172-47-4]	1-(4-Amino-3-hydroxyphenyl)-1-butanone, 39
[123172-48-5]	1-(3-Hydroxy-4-methylaminophenyl)-1-butanone, 60
[123387-95-1]	1,5-Bis(3,4-dibutyloxyphenyl)-1,5-pentanedione, 521
[123387-96-2]	1,5-Bis(3,4-didecyloxyphenyl)-1,5-pentanedione, 521
[123471-86-3]	Methyl 4-(2-hydroxy-5-methylphenyl)-4-oxo-1-butanoate, 435
[123471-91-0]	Methyl 4-(2-hydroxy-3,5-dimethylphenyl)-4-oxo-1-butanoate, 444
[123687-72-9]	1-(2,4,5-Trihydroxyphenyl)-16-methyl-1-heptadecanone, 1060

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[124016-88-2]	6-(3-Hydroxy-4-methylphenyl)-6-oxo-1-hexanoic acid, 716
[124135-37-1]	1,4-Bis[2-hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1,4-butanedione, 373
[124141-66-8]	1,9-Bis(2,4-dihydroxyphenyl)-1,9-nonanedione (Di-2,4-dinitrophenyl-hydrazone), 851
[124210-60-2]	1-(3,5-Dimethoxyphenyl)-1-pentadecanone, 1028
[124210-61-3]	1-(3,5-Dihydroxyphenyl)-1-pentadecanone, 1028
[124259-63-8]	1-(2,4-Dimethoxy-3-methylphenyl)-1,3-butanedione, 318
[124557-51-3]	1-(2,5-Dimethoxyphenyl)-3-methyl-1-butanone, 179
[124557-52-4]	1-(2,5-Dihydroxyphenyl)-3-methyl-1-butanone, 178
[124598-07-8]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-2-methyl-1-butanone (S), 136
[124598-08-9]	1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-2-methyl-1-butanone (S)-(+), 136
[124598-11-4]	2-Methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-butanone (S), 134
[124598-12-5]	2-Methyl-1-(2,4,6-trimethoxyphenyl)-1-butanone (S), 130
[124598-13-6]	1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-2-methyl-1-butanone (S), 138
[124598-14-7]	2-Methyl-1-(2,4,6-trimethoxy-3-methylphenyl)-1-butanone (S), 134
[124598-15-8]	1-[2,4-Bis(acetyloxy)-6-hydroxyphenyl]-2-methyl-1-butanone (S), 139
[124598-16-9]	2-Methyl-1-[2,4,6-tris(acetyloxy)phenyl]-1-butanone (S), 130
[124598-17-0]	1-(4,6-Diacetyloxy-2-methoxy-3-methylphenyl)-2-methyl-1-butanone (S)-(+), 136
[124598-18-1]	2-Methyl-1-[2,4,6-tris(acetyloxy)-3-methylphenyl]-1-butanone (S), 134
[124598-19-2]	1-(2-Acetyloxy-4,6-dimethoxy-3-methylphenyl)-2-methyl-1-butanone, 138
[124960-73-2]	1-[2-(β-D-Glucopyranosyloxy)-4,6-dihydroxyphenyl]-2-methyl-1-butanone, 145
[125009-82-7]	1-(2,6-Dihydroxyphenyl)-1-dodecanone, 947
[125074-06-8]	2-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone, 129
[125292-98-0]	1-[3,5-Bis[[2,6-dihydroxy-4-methoxy-3-methyl-5-(1-oxobutyl)phenyl] methyl]-2,4,6-trihydroxyphenyl]-2-methyl-1-butanone, 169
[125304-88-3]	1,4-Bis(2,4-dimethoxyphenyl)-1,4-butanedione (E,E)-Di-O-methyl oxime, 362
[125500-45-0]	1-(4-Chloro-8-hydroxy-3-quinolinyl)-1-butanone, 77
[125500-46-1]	1-[8-Hydroxy-4-[(2-methylphenyl)amino]-3-quinolinyl]-1-butanone, 118
[125628-93-5]	1-(3,4-Dihydroxy-5-nitrophenyl)-1-pentanone, 485
[125628-94-6]	1-(3,4-Dihydroxy-5-nitrophenyl)-1-decanone, 881
[125697-50-9]	1-(2,5-Dimethoxyphenyl)-2-octadecyl-1-eicosanone, 1099
[126163-53-9]	1-(2′,3′-Difluoro-4′-octyloxy[1,1′-biphenyl]-4-yl)-1-hexanone, 667
[126211-12-9]	1-(6-Hydroxy-2,4-dimethoxy-3-methylphenyl)-3-methyl-1-butanone, 207
[126516-15-2]	1-(4′-Acetyloxy[1,1′-biphenyl]-4-yl)-1-heptanone, 756
[127154-56-7]	1-(2-Benzyloxyphenyl)-1-pentanone, 463
[127275-13-2]	Methyl 4-(2,5-dihydroxyphenyl)-4-oxo-1-butanoate, 408
[127275-14-3]	Methyl 4-(5-chloro-2-hydroxy-4-methylphenyl)-4-oxo-1-butanoate, 432
[127313-53-5]	1-[2-Hydroxy-4-(sec-octyloxy)phenyl]-1-hexanone (Oxime), 689
[127313-65-9]	1-[2-Hydroxy-4-(sec-octyloxy)phenyl]-1-hexanone, 689
[127699-71-2]	1-(2-Hydroxy-5-methylphenyl)-1-butanone (2,4-Dinitrophenylhydrazone), 49

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[127699-72-3]	1-(2-Hydroxy-5-methylphenyl)-1-octanone (2,4-Dinitrophenylhydrazone), 793
[127699-73-4]	1-(2-Hydroxy-5-methylphenyl)-1-dodecanone (2,4-Dinitrophenylhydrazone), 960
[127789-29-1]	1-[2-Hydroxy-4-(1-methylheptyloxy)phenyl]-1-octanone, 823
[127789-31-5]	1-[2-Hydroxy-4-(1-methylheptyloxy)phenyl]-1-octanone (Oxime) (*E*), 823
[127789-34-8]	1-[2-Hydroxy-4-(1-methylheptyloxy)phenyl]-1-octanone (Oxime) (*Z*), 823
[127928-53-4]	1-(3-Fluoro-4-hydroxyphenyl)-2-methyl-1-octanone (+), 791
[127928-54-5]	1-(2-Fluoro-4-hydroxyphenyl)-2-methyl-1-octanone, 791
[127928-56-7]	1-(3-Fluoro-4-methoxyphenyl)-2-methyl-1-octanone (+), 791
[127928-60-3]	1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-2-methyl-1-octanone (S), 817
[127928-64-7]	1-(2-Fluoro-4-methoxyphenyl)-2-methyl-1-octanone (+), 791
[128733-94-8]	1,4-Bis(3-bromo-2-hydroxy-5-methylphenyl)-1,4-butanedione, 364
[129201-57-6]	4-(2-Ethoxy-4-methoxy-5-ethylphenyl)-4-oxo-1-butanoic acid, 445
[129218-86-6]	3-Chloro-1-(2-hydroxyphenyl)-1-butanone, 276
[129227-94-7]	1-[2,4,6-Trihydroxy-3-(1-oxopropyl)phenyl]-1-heptanone, 746
[129375-11-7]	1-[2-Hydroxy-4-methyl-5-(1-methylethyl)phenyl]-1-heptanone, 749
[129375-14-0]	1-[3-(1,1-Dimethylethyl)-2-hydroxy-6-methyl-5-(1-methylethyl)phenyl]-1-heptanone, 762
[129375-15-1]	1-[6-Hydroxy-2-methyl-3-(1-methylethyl)phenyl]-1-heptanone, 750
[129399-52-6]	1-[6-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-3,4-dihydro-3,5,7-trihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-1-butanone, 343
[129527-09-9]	1-(3,5-Dichloro-4-hydroxyphenyl)-1-butanone, 25
[129527-10-2]	1-(3,5-Dichloro-4-hydroxyphenyl)-1-butanone (Na salt), 25
[129684-20-4]	1-(2,4,6-Trihydroxyphenyl)-11-phenyl-1-undecanone, 933
[130907-67-4]	6-Acetyloxy-7-(1-oxobutyl)-3-methylcoumarilic acid, 88
[131033-26-6]	1-(4-Hydroxyphenyl)-2-methyl-1-octanone (+), 794
[131252-71-6]	1,1′-(3-Hydroxy[1,1′-biphenyl]-4-yl)-1-butanone, 260
[131427-27-5]	1-(3,5-Dichloro-4-hydroxyphenyl)-1-octanone, 786
[131427-28-6]	1-(3,5-Dichloro-4-hydroxyphenyl)-1-hexanone, 621
[131427-29-7]	1-(3,5-Dichloro-2-hydroxyphenyl)-1-octanone, 786
[131699-22-4]	Methyl 5-(3,4-dimethoxyphenyl)-5-oxo-1-pentanoate, 582
[131868-27-4]	4-Methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-pentanone, 548
[132041-56-6]	1-(4′-Methoxy[1,1′-biphenyl]-4-yl)-2-methyl-1-butanone, 262
[132180-62-2]	4-Cyclohexyl-1-(2-hydroxy-4-methylphenyl)-1-butanone, 257
[132180-63-3]	4-Cyclohexyl-1-(4-hydroxy-2-methylphenyl)-1-butanone, 258
[132330-85-9]	2-Ethyl-4-(2,5-dimethoxyphenyl)-4-oxo-1-butanoic acid, 419
[132341-31-2]	2,4,6-Trihydroxy-3-methyl-5-(3-methyl-1-oxopentyl)benzaldehyde, 560
[132858-47-0]	1-(3,4-Dimethoxyphenyl)-3-methyl-1-butanone, 180
[132858-49-2]	1-(3-Hydroxyphenyl)-1-heptanone, 720
[132858-60-7]	1-(2-Hydroxy-3-methylphenyl)-1-hexanone, 638
[132858-61-8]	1-(4-Hydroxy-2-methylphenyl)-1-hexanone, 640
[132858-62-9]	1-(4-Hydroxy-3-methylphenyl)-1-hexanone, 641
[132859-07-5]	1-(2,5-Dimethoxyphenyl)-1-octanone, 780

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[133101-50-5]	4-(2-Methoxyphenyl)-3-methyl-4-oxo-1-butanoic acid, 414
[133101-52-7]	4-[(2-Methoxymethyl)phenyl]-3-methyl-4-oxo-1-butanoic acid, 414
[133406-99-2]	1-(3-Hydroxy-4′-methoxy[1,1′-biphenyl]-4-yl)-2-methyl-1-octanone (S), 820
[133407-00-8]	1-(3,4′-Dihydroxy[1,1′-biphenyl]-4-yl)-2-methyl-1-octanone (S), 817
[133455-19-3]	1-[4-(3-Bromopropoxy)-3-methoxyphenyl]-1-pentanone, 504
[133535-19-0]	Methyl 7-(2-hydroxyphenyl)-7-oxo-1-heptanoate, 766
[133535-20-3]	6-(2,4-Dihydroxyphenyl)-6-oxo-1-hexanoic acid, 712
[133535-21-4]	Ethyl 4-(2,4-dihydroxyphenyl)-4-oxo-1-butanoate, 405
[133559-45-2]	1-(3-Methoxyphenyl)-4-(4-methoxyphenyl)-1,4-butanedione, 359
[133831-11-5]	1-(2,5-Dihydroxy-4-methoxyphenyl)-1-octanone, 797
[133839-66-4]	3-Hydroxy-1-(2-hydroxyphenyl)-1-dodecanone, 949
[134081-63-3]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-hexanone, 659
[134081-64-4]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-octanone, 804
[134081-65-5]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-decanone, 892
[134081-66-6]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-dodecanone, 970
[134081-67-7]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-tetradecanone, 1017
[134081-68-8]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-hexadecanone, 1047
[134081-69-9]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-octadecanone, 1080
[134081-70-2]	1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-hexanone, 660
[134081-71-3]	1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-octanone, 805
[134081-72-4]	1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-decanone, 892
[134081-73-5]	1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-dodecanone, 970
[134081-74-6]	1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-tetradecanone, 1017
[134081-75-7]	1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-hexadecanone, 1048
[134081-76-8]	1-(6-Hydroxy-2,3,4-trimethoxyphenyl)-1-octadecanone, 1080
[134081-78-0]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1-hexanone (p-Toluenesulfonate), 660
[134081-79-1]	1-[2-(p-Toluenesulfonyloxy)-3,4,6-trimethoxyphenyl]-1-octanone, 804
[134081-80-4]	1-[2-(p-Toluenesulfonyloxy)-3,4,6-trimethoxyphenyl]-1-decanone, 892
[134081-81-5]	1-[2-(4-Toluenesulfonyloxy)-3,4,6-trimethoxyphenyl)-1-dodecanone, 970
[134081-82-6]	1-[2-(4-Toluenesulfonyloxy)-3,4,6-trimethoxyphenyl]-1-tetradecanone, 1017, 1022
[134081-83-7]	1-[2-(p-Toluenesulfonoxy)-3,4,6-trimethoxyphenyl]-1-hexadecanone, 1048
[134081-84-8]	1-[2-(p-Toluenesulfonyloxy)-3,4,6-trimethoxyphenyl]-1-octadecanone, 1080
[134081-86-0]	1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-hexanone, 690
[134081-87-1]	1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-octanone, 824
[134081-88-2]	1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-decanone, 913
[134081-89-3]	1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-dodecanone, 984
[134081-90-6]	1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-tetradecanone, 1022

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[134081-91-7]	1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-hexadecanone, 1052
[134081-92-8]	1-[6-Hydroxy-3,4-dimethoxy-2-(4-methylphenylsulfonyloxy)phenyl]-1-octadecanone, 1087
[134081-94-0]	1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-hexanone, 653
[134081-95-1]	1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-octanone, 803
[134081-96-2]	1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-decanone, 889
[134081-97-3]	1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-dodecanone, 967
[134081-98-4]	1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-tetradecanone, 1016
[134081-99-5]	1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-hexadecanone, 1045
[134082-00-1]	1-(2,6-Dihydroxy-3,4-dimethoxyphenyl)-1-octadecanone, 1079
[134082-02-3]	1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-hexanone, 690
[134082-03-4]	1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-octanone, 823
[134082-04-5]	1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-decanone, 912
[134082-05-6]	1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-dodecanone, 984
[134082-06-7]	1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-tetradecanone, 1021
[134082-07-8]	1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-hexadecanone, 1051
[134082-08-9]	1-[2-Hydroxy-3,4-dimethoxy-6-(phenylmethoxy)phenyl]-1-octadecanone, 1086
[134179-54-7]	1-(2-Methoxyphenyl)-4-(4-methoxyphenyl)-1,4-butanedione, 358
[134179-55-8]	1,4-Bis(2-methoxyphenyl)-1,4-butanedione, 358
[134364-70-8]	1-(2,3-Difluoro-4-methoxyphenyl)-1-pentanone, 480
[134610-35-8]	1-(4-Hydroxy-3-methoxy-5-nitrophenyl)-1-butanone, 47
[134610-36-9]	1-(3,4-Dihydroxy-5-nitrophenyl)-1-butanone, 37
[134925-05-6]	1-(2,4-Dihydroxyphenyl)-2-methyl-1-octanone, 796
[135312-40-2]	5-(4-Hydroxyphenyl)-3,3-dimethyl-5-oxo-1-pentanoic acid, 585
[135649-79-5]	1-(4-Hydroxyphenyl)-1-heptadecanone, 1055
[135680-27-2]	1,4-Bis(4-methoxyphenyl)-2,3-bis(phenyl)-1,4-butanedione (racemic), 373
[136039-85-5]	3-Hexanoyl-4-hydroxybenzoic acid, 633
[136116-43-3]	1-(3-Methoxyphenyl)-1-octanone, 773
[136741-47-4]	1-(5-Chloro-2-hydroxy-4-methoxyphenyl)-3-methyl-1-butanone, 188
[136936-71-5]	1-(3-Fluoro-4-methoxyphenyl)-1-nonanone, 842
[136964-18-6]	1-(2-Fluoro-4-hydroxyphenyl)-1-octanone, 787
[137034-61-8]	1-(4-Hydroxyphenyl)-1-undecanone, 924
[137832-97-4]	1-(4-Hydroxy-2,3,5-trimethylphenyl)-1-octadecanone, 1080
[137832-98-5]	1-(4-Hydroxy-2,3,5-trimethylphenyl)-1-dodecanone, 969
[137832-99-6]	1-(4-hydroxy-3,5-dimethylphenyl)-1-octadecanone, 1078
[137833-00-2]	1-(4-Hydroxy-3,5-bis(1-methylethyl)phenyl)-1-octadecanone, 1084
[137833-01-3]	1-(4-Hydroxy-2,3,5-trimethylphenyl)-1-docosanone, 1108
[137833-02-4]	1-(4-Hydroxy-2,3-dimethyl-5-(1-methylethyl)phenyl)-1-octadecanone, 1083
[137833-03-5]	1-(4-Hydroxy-2,3,5-trimethylphenyl)-1-hexadecanone, 1047
[137866-03-6]	1-(3-Fluoro-4-methoxyphenyl)-1-octanone, 788

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[137937-40-7]	1-(2-Hydroxy-3-methylphenyl)-2-propyl-1-pentanone, 561
[137937-41-8]	1-(2-Hydroxy-4-methylphenyl)-2-propyl-1-pentanone, 561
[137937-44-1]	1-(4-Hydroxyphenyl)-2-propyl-1-pentanone, 556
[137937-46-3]	1-(4-Hydroxy-2-methylphenyl)-2-propyl-1-pentanone, 562
[137937-53-2]	1-(2-Methoxy-4-methylphenyl)-2-propyl-1-pentanone, 561
[137937-54-3]	1-(4-Methoxy-2-methylphenyl)-2-propyl-1-pentanone, 562
[138690-39-8]	1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-2-methyl-1-butanone, 138
[139409-36-2]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-2-methyl-1-butanone, 302
[140400-68-6]	1-[2,6-Dihydroxy-3-methyl-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone, 222
[140400-69-7]	1-[2,6-Diacetyloxy-3-methyl-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone, 223
[140400-70-0]	1-[2-Hydroxy-6-methoxy-3-methyl-4-[(3-methyl-2-butenyl)oxy]phenyl]-3-methyl-1-butanone, 224
[140466-94-0]	1-[5-(Dodecyloxy)-2-hydroxyphenyl]-1-hexanone, 694
[140943-07-3]	1-(2,5-Dihydroxyphenyl)-1-octanone (Oxime), 780
[140943-08-4]	1-(2,5-Dihydroxyphenyl)-1-tetradecanone (Oxime), 1006
[140943-12-0]	1-(2-Hydroxy-5-methoxyphenyl)-1-pentanone (Oxime), 497
[140943-13-1]	1-(2-Hydroxy-5-methoxyphenyl)-1-hexanone (Oxime), 643
[140943-14-2]	1-(2-Hydroxy-5-methoxyphenyl)-1-octanone (Oxime), 796
[140943-15-3]	1-(2-Hydroxy-5-methoxyphenyl)-1-dodecanone (Oxime), 962
[140943-16-4]	1-(2-Hydroxy-5-methoxyphenyl)-1-tetradecanone (Oxime), 1013
[140943-18-6]	1-(5-Ethoxy-2-hydroxyphenyl)-1-pentanone (Oxime), 501
[140943-19-7]	1-(5-Ethoxy-2-hydroxyphenyl)-1-hexanone (Oxime), 652
[140943-20-0]	1-(5-Ethoxy-2-hydroxyphenyl)-1-octanone (Oxime), 801
[140943-21-1]	1-(5-Ethoxy-2-hydroxyphenyl)-1-dodecanone (Oxime), 966
[140943-22-2]	1-(5-Ethoxy-2-hydroxyphenyl)-1-tetradecanone (Oxime), 1015
[140943-23-3]	1-(5-Butoxy-2-hydroxyphenyl)-1-hexanone (Oxime), 666
[140943-24-4]	1-(5-Butoxy-2-hydroxyphenyl)-1-octanone (Oxime), 808
[140943-25-5]	1-(5-Butoxy-2-hydroxyphenyl)-1-dodecanone (Oxime), 974
[140943-31-3]	1-(5-Ethoxy-2-hydroxyphenyl)-1-pentanone, 501
[140943-32-4]	1-(5-Ethoxy-2-hydroxyphenyl)-1-hexanone, 652
[140943-33-5]	1-(5-Ethoxy-2-hydroxyphenyl)-1-octanone, 801
[140943-34-6]	1-(5-Ethoxy-2-hydroxyphenyl)-1-decanone, 888
[140943-35-7]	1-(5-Ethoxy-2-hydroxyphenyl)-1-dodecanone, 966
[140943-36-8]	1-(5-Ethoxy-2-hydroxyphenyl)-1-tetradecanone, 1015
[140943-37-9]	1-(5-Butoxy-2-hydroxyphenyl)-1-hexanone, 666
[140943-38-0]	1-(5-Butoxy-2-hydroxyphenyl)-1-octanone, 808
[140943-39-1]	1-(5-Butoxy-2-hydroxyphenyl)-1-dodecanone, 974
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[141124-94-9]	1-(4-Hydroxy-3-nitrophenyl)-1-undecanone, 930
[141124-96-1]	1-(3-Amino-4-hydroxyphenyl)-1-undecanone, 930
[141681-77-8]	1-(4′-Methoxy[1,1′-biphenyl]-4-yl)-2-methyl-1-octanone (+), 817

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[142234-79-5]	1-(2,6-Dihydroxy-4-methoxyphenyl)-1-hexanone, 644
[142611-25-4]	1-(3,5-Dihydroxyphenyl)-2-nonadecanone, 1094
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[143286-57-1]	1-(2-Hydroxy-4-methoxyphenyl)-1-butanone (Oxime), 55
[143286-58-2]	1-(2-Hydroxy-4-methoxyphenyl)-1-heptanone (Oxime), 740
[143286-59-3]	1-[4-(Hexyloxy)-2-hydroxyphenyl]-1-heptanone (Oxime), 758
[143286-60-6]	1-(2-Hydroxy-4-methoxyphenyl)-1-octanone (Oxime), 796
[143286-61-7]	1-(4-Butoxy-2-hydroxyphenyl)-1-nonanone (Oxime), 849
[143286-62-8]	1-(4-Hexyloxy-2-hydroxyphenyl)-1-nonanone (Oxime), 856
[143286-63-9]	1-(2-Hydroxy-4-propoxyphenyl)-1-decanone (Oxime), 891
[143286-64-0]	1-[2-Hydroxy-4-(octyloxy)phenyl]-1-decanone (Oxime), 912
[143286-65-1]	1-(2-Hydroxy-4-methoxyphenyl)-1-dodecanone (Oxime), 962
[143286-66-2]	1-(4-Butoxy-2-hydroxyphenyl)-1-dodecanone (Oxime), 974
[143286-67-3]	1-(2-Hydroxy-4-pentyloxyphenyl)-1-dodecanone (Oxime), 976
[143286-68-4]	1-(2-Hydroxy-4-methoxyphenyl)-1-tetradecanone (Oxime), 1012
[143286-69-5]	1-(4-Butoxy-2-hydroxyphenyl)-1-tetradecanone (Oxime), 1019
[143286-81-1]	1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-hexanone (Oxime), 683
[143286-82-2]	1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-octanone (Oxime), 818
[143286-83-3]	1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-tetradecanone (Oxime), 1020
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[143286-89-9]	1-(2-Hydroxy-4-methoxyphenyl)-1-heptanone, 739
[143286-90-2]	1-[4-(Hexyloxy)-2-hydroxyphenyl]-1-heptanone, 758
[143286-91-3]	1-(2-Hydroxy-4-methoxyphenyl)-1-octanone, 795
[143286-92-4]	1-(4-Butoxy-2-hydroxyphenyl)-1-nonanone, 848
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[143286-94-6]	1-(2-Hydroxy-4-propoxyphenyl)-1-decanone, 891
[143286-95-7]	1-[2-Hydroxy-4-(octyloxy)phenyl]-1-decanone, 912
[143286-96-8]	1-(2-Hydroxy-4-methoxyphenyl)-1-dodecanone, 962
[143286-97-9]	1-(4-Butoxy-2-hydroxyphenyl)-1-dodecanone, 974
[143286-98-0]	1-(2-Hydroxy-4-pentyloxyphenyl)-1-dodecanone, 976
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[143287-00-7]	1-(2-Hydroxy-4-methoxyphenyl)-1-tetradecanone, 1012
[143287-01-8]	1-(4-Butoxy-2-hydroxyphenyl)-1-tetradecanone, 1019
[143287-04-1]	1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-hexanone, 683
[143287-05-2]	1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-octanone, 817
[143287-06-3]	1-[2-Hydroxy-4-(phenylmethoxy)phenyl]-1-tetradecanone, 1020
[143287-07-4]	1-(4-Butoxy-5-hexyl-2-hydroxyphenyl)-1-heptanone, 763
[143287-08-5]	1-(5-Hexyl-2-hydroxy-4-methoxyphenyl)-1-decanone, 906
[143287-09-6]	1-(4-Butoxy-5-hexyl-2-hydroxyphenyl)-1-decanone, 914
[143287-10-9]	1-(4-Butoxy-5-hexyl-2-hydroxyphenyl)-1-decanone (Oxime), 914
[143378-82-9]	1-(4-Hydroxy-3-methoxyphenyl)-1-nonanone, 845
[144292-57-9]	1-(2,3-Difluoro-4-benzyloxyphenyl)-1-decanone, 878
[144292-58-0]	1-(2,3-Difluoro-4-hydroxyphenyl)-1-decanone, 878
[144337-28-0]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-dodecanone, 987

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[144785-80-8]	3-Methyl-1-[2,4,6-trihydroxy-3-(3,7-dimethyl-2,6-octanediene)phenyl]-1-butanone, 232
[144785-81-9]	1-[4,6-(Diacetyloxy)-2-hydroxy-3-(3,7-dimethyl-2,6-octanediene)phenyl]-2-Methyl-1-butanone, 162
[144785-82-0]	1-[4,6-(Diacetyloxy)-2-hydroxy-3-(3,7-dimethyl-2,6-octanediene)phenyl]-3-methyl-1-butanone, 248
[144785-84-2]	3-Methyl-1-[2,4,6-tris(acetyloxy)-3-(3,7-dimethyl-2,6-octanediene)phenyl]-1-butanone, 233
[145747-19-9]	1-(2,4,5-Tris(acetyloxy)phenyl)-1-butanone, 17
[145747-22-4]	1-[2,5-Bis(acetyloxy)-4-hydroxyphenyl]-1-butanone, 89
[145747-23-5]	1-(2-Acetyloxy-4,5-dihydroxyphenyl)-1-butanone, 62
[145904-69-4]	1-[3-[(2*R*,4*S*)-3,4-Dihydro-7-hydroxy-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-4-yl]-2,4,6-trihydroxyphenyl]-1-dodecanone (+), 989
[145941-31-7]	1,1′-[Methylenebis(4,5,6-trihydroxy-3,1-phenylene)]bis-1-octanone, 827
[146923-05-9]	1-[2-Methoxy-4-(2-methyl-1-propenyl)phenyl]-1-pentanone, 506
[146923-06-0]	1-[3-Methoxy-4-(2-methyl-1-propenyl)phenyl]-1-pentanone, 507
[147862-99-5]	1-[2,4,6-Trihydroxyphenyl]-1-tetradecanone, 1008
[148516-07-8]	1-(4-Hydroxy-3,5-dimethylphenyl)-1-hexanone, 651
[148707-32-8]	1-[5-Acetyl-2-hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]-3-methyl-1-butanone *(E)*, 380
[149053-77-0]	3-Methyl-1-(2,4,6-trimethoxyphenyl)-1-butanone, 195
[149412-46-4]	5-Chloro-1-(4-fluoro-2-hydroxyphenyl)-1-pentanone, 571
[149454-86-4]	1-[4-(4-Heptanoylphenyloxy)phenyl]-1-heptanone, 724
[149696-17-3]	1-(2-Hydroxy-4,5-dimethylphenyl)-1-pentanone, 500
[150033-77-5]	1-(2-Hydroxy-5-methylphenyl)-1-pentanone, 493
[150396-49-4]	1-(3,4-Dimethoxyphenyl)-2-ethyl-1-hexanone, 618
[151029-60-6]	1-(3,4-Dihydroxyphenyl)-1-eicosanone, 1097
[152153-24-7]	1-(5-Chloro-2-hydroxy-4-methylphenyl)-1,3-butanedione, 316
[152269-19-7]	1-(4-Methoxyphenyl)-4,4-dimethyl-1-pentanone, 555
[152430-07-4]	1-(4-Acetyloxyphenyl)-2-methyl-1-decanone (*S*), 876
[152609-12-6]	1-[4′-Fluoro-4-hydroxy-6-methoxy[1,1′-biphenyl]-3-yl]-1-butanone, 263
[152609-14-8]	1-[4-(3-Chloropropoxy)-4′-fluoro-6-methoxy[1,1′-biphenyl]-3-yl]-1-butanone, 263
[153756-51-5]	1-(4-Ethyl-2,5-dimethoxyphenyl)-1-butanone, 69
[153756-53-7]	1-(4-Ethyl-2,5-dimethoxyphenyl)-3,3-dimethyl-1-butanone, 254
[154736-91-1]	1-[5-[[(2,5-Dihydroxyphenyl)methyl]amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone, 692
[154737-33-4]	1-(2-Hydroxyphenyl)-3,5,5-trimethyl-1-hexanone, 619
[154737-34-5]	1-(2-Hydroxy-5-nitrophenyl)-3,5,5-trimethyl-1-hexanone, 656
[154737-35-6]	1-(5-Amino-2-hydroxyphenyl)-3,5,5-trimethyl-1-hexanone, 660
[154737-36-7]	1-[5-[[(2,5-Dihydroxyphenyl)methylene]amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone, 691
[154921-40-1]	1-(2,4-Dihydroxy-6-methylphenyl)-1-butanone, 53
[154921-41-2]	1-(2,4-Dihydroxy-6-methylphenyl)-1-pentanone, 495
[155084-01-8]	1-(3,4,5-Trihydroxyphenyl)-1-tricosanone, 1111

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[156306-39-7]	1,1′-(6,6′-Dihydroxy-5,5′-dimethoxy[1,1′-biphenyl]-3,3′-diyl)bis-1-tridecanone, 1001
[157687-62-2]	1,1′-(6,6′-Dihydroxy-5,5′-dimethoxy[1,1′-biphenyl]-3,3′-diyl)bis-1-octanone, 827
[158869-45-5]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-8-bromo-1-octanone, 830
[158869-48-8]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-7-bromo-1-heptanone, 766
[158905-44-3]	1-(8-Hydroxy-5-quinolinyl)-1-tetradecanone, 1016
[159211-02-6]	1-(4-Benzyloxy-3-methoxyphenyl)-4-methyl-1-pentanone, 548
[159211-07-1]	1-(3-Benzyloxy-4-methoxyphenyl)-4-methyl-1-pentanone, 548
[159457-03-1]	1-(2,4-Dihydroxyphenyl)-3-methyl-1-butanone (Oxime), 177
[159768-89-5]	1-[2,4-Dihydroxy-3-(2-hydroxyethyl)-6-methoxyphenyl]-1-butanone, 85
[159847-59-3]	1-(2-Methoxy-4,5-dimethylphenyl)-1-pentanone, 500
[159977-39-6]	1-(5-Cyclohexyl-2,4-dihydroxyphenyl)-1-pentanone, 526
[161138-02-9]	1-(4-Butyloxy-2-hydroxyphenyl)-1-butanone (Oxime), 92
[161171-55-3]	1-(2-Hydroxy-4-propoxyphenyl)-1-pentanone (Oxime), 506
[161581-92-6]	1-(3-Fluoro-4-methoxyphenyl)-5-methyl-1-hexanone, 637
[161582-00-9]	1-(4-Hydroxyphenyl)-5-methyl-1-hexanone, 616
[162071-05-8]	Methyl 2,6-dihydroxy-3-isovaleryl-4-methoxybenzoate, 196
[162071-06-9]	Methyl 2,6-dihydroxy-3-isovaleryl-4-methoxy-5-(3-methyl-2-butenyl) benzoate, 224
[162071-07-0]	1-[4,6-Dihydroxy-2-methoxy-3-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone, 222
[163734-37-0]	1-(7-Hydroxy-5-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-3-methyl-1-butanone, 220
[163734-38-1]	1-(7-Hydroxy-5-methoxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-2-methyl-1-butanone, 144
[164396-78-5]	6-Bromo-1-(4-phenyloxyphenyl)-1-hexanone, 698
[165538-94-3]	1-(2-Chloro-4-hydroxyphenyl)-3-methyl-1-pentanone, 557
[165538-95-4]	1-(4-Hydroxy-2-methylphenyl)-3-methyl-1-pentanone, 559
[165740-62-5]	1-(2,5-Dihydroxyphenyl)-1-heptanone (Oxime), 726
[165740-65-8]	1-(2,4-Dihydroxyphenyl)-1-heptanone (Oxime), 726
[166816-20-2]	1-(4-Amino-5-chloro-2-methoxyphenyl)-5-chloro-1-pentanone, 572
[167159-65-1]	Ethyl 6-(3,4-dimethoxyphenyl)-6-oxo-1-hexanoate, 714
[168978-08-3]	1-(2-Hydroxy-4-propoxyphenyl)-1-butanone (Oxime), 84
[169553-39-3]	1-[4-Hydroxy-3-[[2-hydroxy-3-methyl-5-(1-oxooctadecyl)phenyl]methyl]-5-methylphenyl]-1-nonadecanone (Chemical Abstracts), 1096
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[169888-15-7]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-decanone (O-Methyloxime), 911
[169888-16-8]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-hexadecanone (O-Methyloxime), 1051
[170283-09-7]	Ethyl 4-(2,4-di(phenylmethoxy)phenyl)-2,4-dioxo-1-butanoate, 398
[170489-31-3]	1-(3,4,5-Trimethoxyphenyl)-1-butanone, 19

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[170489-32-4]	1-(3,4,5-Trimethoxyphenyl)-1-hexanone, 614
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[172264-98-1]	1-(3-Methoxyphenyl)-1-nonanone, 836
[172932-00-2]	1-(2,4-Dihydroxy-3-propylphenyl)-1-decanone, 891
[173054-85-8]	5-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-pentanone, 574
[173054-91-6]	5-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-pentanone, 576
[173054-96-1]	5-Bromo-1-(2-hydroxy-4-methoxyphenyl)-1-pentanone, 574
[173055-00-0]	5-Bromo-1-(2-hydroxy-5-methylphenyl)-1-pentanone, 573
[173055-06-6]	5-Bromo-1-(2-hydroxy-3,4-dimethoxyphenyl)-1-pentanone, 575
[173055-08-8]	5-Bromo-1-(2-hydroxy-3,4,6-trimethoxyphenyl)-1-pentanone, 576
[173055-10-2]	5-Bromo-1-(6-hydroxy-1,3-benzodioxol-5-yl)-1-pentanone, 573
[173055-13-5]	5-Bromo-1-(2-hydroxyphenyl)-1-pentanone, 564
[173055-16-8]	5-Bromo-1-(2-hydroxy-3-methoxyphenyl)-1-pentanone, 574
[173055-18-0]	4-Chloro-1-(2-hydroxy-5-methoxyphenyl)-1-butanone, 285
[173055-21-5]	6-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-hexanone, 706
[173055-23-7]	6-Bromo-1-(2-hydroxy-4-methoxyphenyl)-1-hexanone, 706
[173055-25-9]	6-Bromo-1-(5-fluoro-2-hydroxyphenyl)-1-hexanone, 704
[173055-27-1]	6-Bromo-1-(5-chloro-2-hydroxyphenyl)-1-hexanone, 703
[173055-29-3]	6-Bromo-1-(2-hydroxy-5-methylphenyl)-1-hexanone, 705
[173055-31-7]	6-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-hexanone, 707
[173055-33-9]	6-Bromo-1-(2-hydroxy-4,6-dimethoxyphenyl)-1-hexanone, 707
[173055-36-2]	7-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-heptanone, 765
[173055-38-4]	8-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-octanone, 829
[173055-40-8]	9-Bromo-1-(2-hydroxy-5-methoxyphenyl)-1-nonanone, 863
[173055-42-0]	7-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-heptanone, 765
[173055-44-2]	8-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-octanone, 829
[173055-46-4]	11-Bromo-1-(2-hydroxy-4,5-dimethoxyphenyl)-1-undecanone, 937
[173055-48-6]	7-Bromo-1-(2-hydroxy-4,6-dimethoxyphenyl)-1-heptanone, 765
[173380-47-7]	Difluoro[1-(2-hydroxy-4-methylphenyl)-1-butanonato-O,O′] boron, 47
[173469-67-5]	1-[4-Hydroxy-3-(1-oxopropyl)phenyl]-1-butanone, 385
[173469-74-4]	1-[3-Acetyl-4-hydroxyphenyl]-1-butanone, 376
[173469-75-5]	1-[4-Hydroxy-3-(1-oxo-3-phenyl-2-propenyl)phenyl]-1-butanone, 385
[173851-65-5]	1-(4-Methoxy-2-methylphenyl)-1-pentanone, 494
[173851-66-6]	1-(2-Hydroxy-4-methylphenyl)-1-pentanone, 492
[173851-67-7]	1-(4-Hydroxy-2-methylphenyl)-1-pentanone, 493
[173851-69-9]	1-(2-Methoxy-4-methylphenyl)-1-pentanone, 492
[173851-71-3]	1-[2-(Acetoxymethyl)-4-methoxyphenyl]-1-pentanone, 503
[173959-45-0]	1-(4-Ethoxy-2-hydroxyphenyl)-1-butanone (Oxime), 70
[173979-30-1]	2,2,3,3,4,4,5,5,6,6,6-Undecafluoro-1-(4-hydroxyphenyl)-1-hexanone, 696
[173979-31-2]	2,2,3,3,4,4,5,5,6,6,6-Undecafluoro-1-(2-hydroxyphenyl)-1-hexanone, 696
[174635-33-7]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-chloro-3-ethyl-1-pentanone, 577
[174635-34-8]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-fluoro-3-methyl-1-butanone, 295

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[174635-35-9]	1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-3-mercapto-3-methyl-1-butanone, 227
[175731-80-3]	1,5-Bis(2-hydroxyphenyl)-3-tert-butyl-1,5-pentanedione, 536
[175797-78-1]	1-[4′-(10-Undecenyl)[1,1′-biphenyl]-4-yl)-2-methyl-1-butanone (S), 262
[176043-79-1]	1-(2-Hydroxy-3-nitrophenyl)-3,5,5-trimethyl-1-hexanone, 656
[176043-97-3]	1-(3-Amino-2-hydroxyphenyl)-3,5,5-trimethyl-1-hexanone, 660
[176044-11-4]	1-[3-[[(2,5-Dihydroxyphenyl)methylene]amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone, 691
[176044-29-4]	1-[3-[[(2,5-Dihydroxyphenyl)methyl]amino]-2-hydroxyphenyl]-3,5,5-trimethyl-1-hexanone, 692
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[177426-78-7]	1-[2-Methoxy-4-(phenylmethoxy)phenyl]-1-hexanone, 684
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[179037-21-9]	1-(4-Methoxyphenyl)-2-methyl-1-nonanone, 840
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[198878-83-0]	3-Methyl-1-[2,4,5-trihydroxy-3,6-bis(3-methyl-2-butenyl)phenyl]-1-butanone, 231
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[213622-32-3]	3-[2-(4-Methylbenzoyl)acetyl]-2-hydroxy-5-methyl-1-butanone, 301
[213622-33-4]	3-[2-(4-Methoxybenzoyl)acetyl]-2-hydroxy-5-methyl-1-butanone, 301
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[216300-92-4]	1-(2,6-Dihydroxy-4-methylphenyl)-3-methyl-1-butanone, 192
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[217815-26-4]	1-(8-Hydroxy-2-methyl-7-quinolinyl)-1-decanone, 893
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[217815-29-7]	1-(8-Hydroxy-2-methyl-7-quinolinyl)-1-hexanone, 661
[218784-30-6]	11-Bromo-1-(2-hydroxy-4-methylphenyl)-1-undecanone, 935
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[224775-35-3]	8-Bromo-1-(4-methoxyphenyl)-1-octanone, 828
[227946-80-7]	1-(3-Chloro-2,4-dihydroxy-6-methoxyphenyl)-1-hexanone, 636
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[238074-77-6]	2-Bromo-1-(3,5-dibromo-2-hydroxyphenyl)-1-butanone, 268
[238074-78-7]	2-Bromo-1-(3,5-dibromo-2,4-dihydroxyphenyl)-1-hexanone, 702
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[251463-56-6]	1-[2-(Acetyloxy)-4-hydroxyphenyl]-1-dodecanone, 963
[251463-57-7]	1-[2-(Acetyloxy)-4-hydroxyphenyl]-1-hexadecanone, 1043
[251463-59-9]	1-[2-(Acetyloxy)-4-hydroxyphenyl]-3-methyl-1-butanone, 195
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[307000-33-5]	1-(2-Hydroxy-4-phenoxyphenyl)-3-methyl-1-butanone, 219
[307000-38-0]	1-(2-Hydroxy-4-phenoxyphenyl)-1-hexanone, 681
[307000-44-8]	1-(2-Hydroxy-4-phenoxyphenyl)-1-pentanone, 526
[307000-48-2]	1-(2-Hydroxy-4-phenoxyphenyl)-1-dodecanone, 979
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[342423-70-5]	1-(3-Methoxyphenyl)-1-hexanone, 600
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[344574-57-8]	1,6-Bis(2-hydroxy-5-methoxy-4-methylphenyl)-1,6-hexanedione, 690
[344578-29-6]	1,5-Bis(2-hydroxy-5-methoxy-4-methylphenyl)-1,5-pentanedione, 536
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[354585-22-1]	13-Methyl-1-(2,3,4-trihydroxyphenyl)-1-tetradecanone, 1023
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[357172-24-8]	1-[2,5-Dihydroxy-3,4-bis(methylthio)phenyl]-3-(2-phenylethyl)-1-undecanone, 934
[357172-26-0]	1-(2,5-dihydroxy-3,4,6-trimethylphenyl)-2-octyl-1-dodecanone, 985
[357172-28-2]	2-Butyl-1-(2,5-dihydroxy-4-methylphenyl)-1-octanone, 810
[357172-32-8]	2-Butyl-1-(2,5-dibenzyloxy-3,4,6-trimethylphenyl)-1-dodecanone, 981
[357172-44-2]	1-(2,5-Dimethoxy-3,6-diphenoxyphenyl)-2-(1,1-dimethylethyl)-1-octanone, 827
[357172-52-2]	1-[5-(Acetyloxy)-2-hydroxyphenyl]-2-hexyl-1-dodecanone, 982
[358369-06-9]	4-(3,4-Dimethoxyphenyl)-3-methyl-4-oxo-1-butanoic acid, 416
[358369-08-1]	4-(3,4-Dimethoxyphenyl)-2,3-dimethyl-4-oxo-1-butanoic acid, 419
[364039-57-6]	1-[7-Methoxy-2-(3,4,5-trimethoxy)-2*H*-1-benzopyran-3-yl]-1-butanone, 121
[371757-62-9]	1-(3-Fluoro-4-methoxyphenyl)-1-hexanone, 627
[371757-70-9]	1-(3-Chloro-5-fluoro-4-methoxyphenyl)-1-hexanone, 621
[372486-18-5]	1-(2-Hydroxy-4-methoxyphenyl)-1-pentanone, 496
[372486-19-6]	1-(2-Hydroxy-4-methoxyphenyl)-1-hexanone, 642
[374808-50-1]	Methyl 6-(2,5-dimethoxyphenyl)-6-oxo-1-hexanoate, 713
[374808-62-5]	11-Bromo-1-(2,5-dimethoxyphenyl)-1-undecanone, 935
[375172-14-6]	1-(2,5-Dihydroxyphenyl)-2-octyl-1-decanone, 877
[375172-48-6]	1-(2-Amino-3,6-dibutyloxy[1,1′-biphenyl]-4-yl)-2-hexyl-1-dodecanone, 986
[383383-01-5]	1-(3,4-Dihydroxy-2-nitrophenyl)-1-pentanone, 485

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[383383-10-6]	1-(4-Hydroxy-3-methoxy-2-nitrophenyl)-1-pentanone, 491
[390358-13-1]	1-(4′-Hydroxy[1,1′-biphenyl]-4-yl)-1-heptanone, 756
[392304-69-7]	4-(3,5-Dibromo-4-hydroxyphenyl)-4-oxo-1-butanoic acid, 419
[393519-46-5]	1-(2-Hydroxy-4-methoxyphenyl)-1-decanone, 884
[396100-57-5]	2-Bromo-1-(3-bromo-2-hydroxy-5-methylphenyl)-1-butanone, 272
[401935-06-6]	1-(5-Chloro-2-hydroxyphenyl)-1-hexanone (Oxime), 625
[404918-99-6]	1-(2-Amino-5-hydroxyphenyl)-3-methyl-1-butanone, 187
[404919-00-2]	1-(2-Amino-5-hydroxyphenyl)-1-hexanone, 628
[404919-01-3]	1-(2-Amino-5-hydroxyphenyl)-1-butanone, 38
[406174-64-9]	1-(2,4-Dihydroxyphenyl)-2-methyl-1-hexanone, 616
[406174-67-2]	1-(2,4-Diacetyloxyphenyl)-2-methyl-1-butanone (Racemic, 128
[406174-68-3]	1-(2,4-Diacetyloxyphenyl)-2-methyl-1-hexanone (Racemic), 616
[406174-71-8]	1-[2-(Acetyloxy)-4-hydroxyphenyl]-2-methyl-1-butanone (-), 134
[406174-72-9]	1-[2-(Acetyloxy)-4-hydroxyphenyl]-2-methyl-1-hexanone (-), 655
[406174-75-2]	1-(2,4-Diacetyloxyphenyl)-2-methyl-1-butanone dextrogyre (+), 128
[406174-76-3]	1-(2,4-Diacetyloxyphenyl)-2-methyl-1-hexanone (+), 617
[406174-79-6]	1-(2,4-Diacetyloxyphenyl)-2-methyl-1-butanone levogyre(-), 128
[406174-80-9]	1-(2,4-Diacetyloxyphenyl)-2-methyl-1-hexanone (-), 617
[406463-67-0]	1-[3-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-2,4,6-trihydroxy-5-(2-hydroxy-3-methyl-3-butenyl)phenyl]-1-pentanone, 538
[406463-68-1]	1-[6-[(3-Acetyl-2,4-dihydroxy-6-methoxy-5-methylphenyl)methyl]-3,4-dihydro-3,5,7-trihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-3-methyl-1-butanone, 344
[408309-74-0]	1-(5-Chloro-2-hydroxy-4-methylphenyl)-1-butanone, 45
[408310-63-4]	4-Cyclohexyl-1-(2,5-dihydroxyphenyl)-1-butanone, 256
[408336-52-7]	4-(6-Hydroxybiphenyl-3-yl)-4-oxo-1-butanoic acid, 452
[408336-68-5]	4-(6-Methoxybiphenyl-3-yl)-4-oxo-1-butanoic acid, 452
[412022-96-9]	4-(3-Cyclohexyl-4-methoxyphenyl)-4-oxo-1-butanoic acid, 453
[412033-83-1]	4-(5-Cyclohexyl-2-metoxyphenyl)-4-oxo-1-butanoic acid, 454
[412051-38-8]	2-Bromo-1-(4-hydroxyphenyl)-3-methyl-1-butanone, 293
[412340-39-7]	1,1′-(5-Ethyl-2-methoxy-1,3-phenylene)bis-2-bromo-3-methyl-1-butanone, 304
[416846-26-9]	1-(4-Ethyloxyphenyl)-1-hexadecanone, 1034
[423115-90-6]	1-(4-Methoxyphenyl)-1-butanone (Oxime), 7
[430425-41-5]	1-(2,5-Dimethoxyphenyl)-1-hexanone, 608
[430425-42-6]	1-(2,4-Dimethoxyphenyl)-1-decanone, 873
[434340-29-1]	1-(4-Chloro-2,5-dimethoxyphenyl)-1-decanone, 880
[434340-30-4]	2-Bromo-1-(4-chloro-2,5-dimethoxyphenyl)-1-decanone, 917
[438490-66-5]	1-(6-Hydroxy-3-(4-methoxyphenyl)-2-phenyl-5-benzofuranyl)-1-butanone, 125
[438490-69-8]	1-(6-Hydroxy-3-(4-methylphenyl)-2-phenyl-5-benzofuranyl)-1-butanone, 124
[439948-78-4]	1-(2-Hydroxyphenyl)-1-nonanone (Oxime), 835
[439948-79-5]	1-(2-Hydroxyphenyl)-1-decanone (Oxime), 868
[439948-80-8]	1-(2-Hydroxyphenyl)-1-undecanone (Oxime), 923

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[441353-19-1]	1-(2,4,6-Trimethoxyphenyl)-1-octanone, 784
[447439-58-9]	1-(4-Methoxy-2-iodophenyl)-1-pentanone, 484
[457926-60-2]	1-[(3*R*)-3-[(2*S*,4*S*)-3,4-Dihydro-7-hydroxy-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-4-yl]-2,4,6-trihydroxyphenyl]-1-dodecanone, 991
[457930-47-1]	1-[(3*R*)-3-[(2*R*,4*R*)-3,4-Dihydro-7-hydroxy-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-4-yl]-2,4,6-trihydroxyphenyl]-1-dodecanone, 990
[465526-56-1]	5-Butyl-1-(4-methoxyphenyl)-4-methylene-1-nonanone, 841
[467437-62-3]	1-[2-[(6-*O*-D-Apio-β-D-furanosyl-β-D-glucopyranosyl)oxy]-4,6-dihydroxyphenyl]-2-methyl-1-butanone (2*S*), 156
[473835-69-7]	1-(4-Methoxyphenyl)-2-methylene-1-hexanone, 615
[474668-86-5]	1-(3,4-Dihydroxyphenyl)-1-pentanone (O-Methyloxime), 473
[474668-95-6]	1-(3,4-Dihydroxyphenyl)-1-heptanone (O-Methyloxime), 727
[479580-83-1]	1-(2-Hydroxy-3-phenoxyphenyl)-1-butanone, 101
[484676-16-6]	1-(5-Bromo-3,4,5-trimethoxyphenyl)-1-pentanone, 567
[497934-63-1]	1-(5-Amino-2-hydroxyphenyl)-1-pentanone, 486
[500109-64-8]	1-[5,7-Dihydroxy-2,2-dimethyl-6-[[2,4,6-trihydroxy-3-methyl-5-(2-methyl-1-oxopropyl)phenyl]methyl]-2*H*-1-benzopyran-8-yl]-2-methyl-1-butanone, 166
[500109-65-9]	1-[6-[(3-Acetyl-2,4,6-trihydroxy-5-methylphenyl)methyl]-5,7-dihydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-2-methyl-1-butanone, 163
[500127-72-0]	1-[2-Chloro-4-(2-propynyl)phenyl]-1-butanone, 29
[500127-73-1]	1-(3-Chloro-4-hydroxyphenyl)-1-butanone, 29
[501083-60-9]	6-Chloro-1-(2-methoxyphenyl)-1-hexanone, 700
[501083-61-0]	5-Chloro-1-(2-hydroxyphenyl)-1-pentanone, 567
[501083-62-1]	6-Chloro-1-(2-hydroxyphenyl)-1-hexanone, 700
[501083-63-2]	5-Chloro-1-(3-hydroxyphenyl)-1-pentanone, 567
[501083-64-3]	6-Chloro-1-(3-hydroxyphenyl)-1-hexanone, 701
[501361-68-8]	1-(3,4-Dimethoxyphenyl)-1-octadecanone, 1067
[502139-81-3]	10-(2,5-Dihydroxyphenyl)-10-oxo-1-decanoic acid, 920
[505084-75-3]	1-(4-Hydroxy-2-methylphenyl)-2-methyl-1-butanone (2S), 133
[505084-77-5]	1-(2-Fluoro-4-hydroxyphenyl)-2-methyl-1-butanone (2S), 132
[508210-78-4]	1-[2-(Diphenylmethyl)-5-nitrophenyl]-1-butanone, 35
[526208-17-3]	1-(2-Hydroxyphenyl)-2-methyl-5-methylene-1-decanone, 876
[526208-18-4]	1-(2-Hydroxyphenyl)-6-methylene-1-undecanone, 929
[565203-85-2]	1-(6-Methoxy-3′-methoxy[1,1′-biphenyl]-3-yl)-1-pentanone, 529
[565203-88-5]	1-(6-Hydroxy-3′-methoxy[1,1′-biphenyl]-3-yl)-1-pentanone, 529
[568553-00-4]	4-(3,4-Dipropoxyphenyl)-4-oxo-1-butanoic acid, 409
[575487-37-5]	1-(4-Hydroxy-2,5-dimethylphenyl)-1-butanone, 68
[578716-69-5]	1-[3-Acetyl-2,6-dihydroxy-4-methoxy-5-(3-methyl-2-butenyl)phenyl]-3-methyl-1-butanone, 384
[596805-35-5]	1-[(2*R*)-2,3-Dihydro-6-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-3-methyl-1-butanone, 211
[596805-36-6]	1-[(2*S*)-2,3-Dihydro-6-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-3-methyl-1-butanone, 211
[596805-37-7]	1-[2,4-Dihydroxy-3-(2-hydroxy-3-methyl-3-butenyl)phenyl]-3-methyl-1-butanone, 213

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[596805-39-9]	1-[2,4-Dihydroxy-5-(2-hydroxy-3-methyl-3-butenyl)phenyl]-3-methyl-1-butanone, 214
[596805-40-2]	1-[2,4-Dihydroxy-5-(3-hydroxy-3-methyl-1-butenyl)phenyl]-3-methyl-1-butanone, 214
[596805-43-5]	1-[2,3-Dihydro-4-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-3-methyl-1-butanone (+), 211
[596805-44-6]	1-[2,3-Dihydro-4-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-3-methyl-1-butanone (-), 211
[645336-90-9]	1-(3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl)-1-heptadecanone, 1059
[647008-26-2]	1-(2,5-Dihydroxy-4-methoxy-3-methylphenyl)-1-hexanone, 653
[647008-30-8]	1-(2-Hydroxy-4-methoxy-3-methylphenyl)-1-hexanone, 652
[647008-31-9]	1-(2-Acetyloxy-4-methoxy-3-methylphenyl)-1-hexanone, 652
[654643-45-5]	3-Chloro-1-(4-methoxyphenyl)-1-butanone, 277
[658702-61-5]	1-[(2*R*,3*S*)-3,4-Dihydro-5,7-dihydroxy-2-methyl-3-(3-methyl-2-butenyl)-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran-8-yl]-2-methyl-1-butanone (-), 164
[658702-63-7]	1-[3,4-Dihydro-5,7-dihydroxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran-8-yl]-2-methyl-1-butanone (+), 151
[664376-65-2]	1-(2,4-Dihydroxy-3-methylphenyl)-3-methyl-1-butanone, 191
[664376-79-8]	1-(2,4-Dihydroxy-3-propylphenyl)-3-methyl-1-butanone, 206
[664376-82-8]	1-(3-Ethyl-2,4-dihydroxyphenyl)-3-methyl-1-butanone, 198
[664376-91-4]	1-(3-Bromo-2,4-dihydroxyphenyl)-3-methyl-1-butanone, 186
[666836-96-0]	1-[4-(2-Chloroethyloxy)phenyl]-1-decanone, 871
[666836-97-1]	1-[4-(N-Dimethylaminoethyloxy)phenyl]-1-decanone, 871
[666836-99-3]	1-(4-Chloro-2-hydroxyphenyl)-1-decanone, 879
[678184-56-0]	1-(4-Hydroxy-3-methyl-6-phenyl-2-benzofuranyl)-1-pentanone, 535
[678184-68-4]	1-[(4-Methoxymethyl)-3-methyl-6-phenyl-2-benzofuranyl)-1-butanone, 116
[678184-70-8]	1-(4-Methoxymethoxy-3-methyl-6-phenyl-2-benzofuranyl)-1-pentanone, 536
[695196-63-5]	1-(3-Fluoro-4-hydroxyphenyl)-1-hexanone, 626
[695196-65-7]	1-(4-Phenyloxyphenyl)-1-hexanone, 605
[702701-04-0]	4-(3-Cyclohexyl-4-hydroxyphenyl)-4-oxo-1-butanoic acid, 453
[709032-85-9]	4-Cyclohexyl-1-(2,4-dihydroxyphenyl)-1-butanone, 256
[717103-49-6]	1-[2-Hydroxy-5-methoxy-4-(3-methylbutyl)phenyl]-1-octanone, 816
[718608-83-4]	1-[2-(β-D-Glucopyranosyloxy)-4,6-dihydroxyphenyl]-3-methyl-1-butanone, 223
[718608-84-5]	1-[2,4-Bis(β-D-glucopyranosyloxy)-6-hydroxyphenyl]-3-methyl-1-butanone, 241
[719311-19-0]	2-Bromo-1-(4-trimethylsilyloxyphenyl)-4-methyl-1-pentanone, 574
[719315-63-6]	1-(2,5-Dimethoxyphenyl)-1-heptanone, 726
[719315-64-7]	1-[2-Hydroxy-5-(phenylmethoxy)phenyl]-1-heptanone, 759
[720675-30-9]	16-(2,4-Dihydroxyphenyl)-16-oxo-1-hexadecanoic acid, 1053
[720676-31-3]	Methyl 16-(2,4-dihydroxyphenyl)-16-oxo-1-hexadecanoate, 1053
[727687-84-5]	1-(3-Bromo-2-hydroxy-5-methylphenyl)-1-butanone, 44

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[727687-90-3]	2-Bromo-1-(3-bromo-2-hydroxyphenyl)-1-butanone, 269
[733016-52-9]	1-(4-Methoxyphenyl)-2-methyl-1-pentanone-*2-d*, 553
[749924-46-7]	2,2,3,3,4,4,4-Heptafluoro-1-(4-methoxyphenyl)-1-butanone (O-[(Trifluoromethyl)sulfonyl]oxime), 289
[749924-49-0]	2,2,3,3,4,4,4-Heptafluoro-1-(4-phenoxyphenyl)-1-butanone (O-[(Trifluoromethyl)sulfonyl]oxime), 289
[750646-76-5]	2-Bromo-1-(4-hydroxyphenyl)-1-pentanone, 565
[753013-71-7]	2,4-Dibromo-1-(2,6-dimethoxyphenyl)-1-butanone, 292
[757408-19-8]	3-Methyl-1-[2,3,4-trihydroxyphenyl]-1-butanone, 181
[758691-87-1]	1-(2-Hydroxy-5-nonylphenyl)-1-butanone (Oxime), 117
[760989-23-9]	1,1′-(4,6-Dihydroxy-1,3-phenylene)bis-1-octanone, 821
[778630-63-0]	1-(3-Hydroxyphenyl)-1-octanone, 773
[778637-79-9]	1-(2-Hydroxy-4,5-dimethylphenyl)-1-octanone, 799
[778641-04-6]	1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-octanone, 806
[791065-70-8]	1-(4-Hydroxyphenyl)-1-butanone (O-Ethyloxime), 5
[791137-06-9]	1-[4-(4-Hexanoylphenyloxy)phenyl]-1-hexanone, 605
[791615-78-6]	1-(4-Phenyloxy-2-methylphenyl)-1-hexanone, 641
[791615-79-7]	1-(4-Phenyloxy-2-methylphenyl)-1-octanone, 793
[791615-80-0]	1-(2-Methyl-4-phenyloxyphenyl)-1-dodecanone, 960
[791615-81-1]	1-(2-Methyl-4-phenoxyphenyl)-1-hexadecanone, 1042
[791615-82-2]	1-(4-Phenyloxy-2-methylphenyl)-1-octadecanone, 1076
[792705-86-3]	1-[1,1′-Biphenyl]-4-yl-2-hydroxy-1-hexanone, 679
[792706-16-2]	1-(1,1′-Biphenyl)-4-yl-3-hydroxy-1-pentanone, 524
[792708-48-6]	1-[1,1′-Biphenyl]-4-yl-2-hydroxy-1-hexanone (O-Methyloxime), 679
[792708-61-3]	1-[1,1′-Biphenyl]-4-yl-2-acetyloxy-1-hexanone, 679
[792708-75-9]	1-(4′-Fluoro[1,1′-biphenyl]-4-yl)-2-hydroxy-1-hexanone, 678
[792708-89-5]	1-(4′-Bromo[1,1′-biphenyl]-4-yl)-2-hydroxy-1-hexanone, 678
[792709-04-7]	1-(4′-Bromo-2′-fluoro[1,1′-biphenyl]-4-yl)-2-hydroxy-1-hexanone, 671
[798559-82-7]	1-[2,4-Dimethoxy-5-(2-methylpropyl)phenyl]-1-pentanone, 510
[798559-83-8]	1-[2,4-Dihydroxy-3-(hydroxymethyl)-5-(2-methylpropyl)phenyl]-1-pentanone, 514
[798559-84-9]	1-[2,4-Dimethoxy-3-(hydroxymethyl)-5-(2-methylpropyl)phenyl]-1-pentanone, 514
[798559-89-4]	1-[4-Hydroxy-3-(hydroxymethyl)-2-methoxy-5-(2-methylpropyl)phenyl]-1-pentanone, 527
[798559-92-9]	2,6-Dihydroxy-3-(2-methylpropyl)-5-(1-oxopentyl)benzaldehyde, 511
[798559-94-1]	1-[2,4-Dihydroxy-5-(2-methylpropyl)phenyl]-1-pentanone, 509
[808749-86-2]	1-(2,4,6-Trimethoxy-3-methylphenyl)-2-methyl-1-butanone, 139
[808751-11-3]	1-(2-Hydroxy-4,6-dimethoxy-3,5-dimethylphenyl)-2-methyl-1-butanone, 139
[808751-12-4]	1-(2-Hydroxy-4,6-dimethoxy-3,5-dimethylphenyl)-3-methyl-1-butanone, 210
[808751-13-5]	1-(6-Hydroxy-2,4-dimethoxy-3-methylphenyl)-2-methyl-1-butanone, 138
[810661-48-4]	1-(4-Methoxy-3-methylphenyl)-1-octanone, 794
[810661-49-5]	1-(3,4-Diethyloxyphenyl)-1-octanone, 781

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[811801-04-4]	1-[2-Hydroxy-3-methyl-4-(4-phenoxybutoxy)phenyl]-3-methyl-1-butanone, 235
[811801-06-6]	1-[4-[4-(2-Fluorophenoxy)butoxy]-2-hydroxy-3-methylphenyl]-3-methyl-1-butanone, 235
[811801-08-8]	1-[4-[4-(2,3-Difluorophenoxy)butoxy]-2-hydroxy-3-methylphenyl]-3-methyl-1-butanone, 235
[811801-17-9]	1-[3-Bromo-2-hydroxy-4-(4-phenoxybutoxy)phenyl]-3-methyl-1-butanone, 230
[811801-19-1]	1-[3-Bromo-4-[4-(2,3-difluorophenoxy)butoxy]-2-hydroxyphenyl]-3-methyl-1-butanone, 230
[817630-32-3]	5-Chloro-1-(3-chloro-4,5-dimethoxyphenyl)-1-pentanone, 572
[817630-35-6]	5-Chloro-1-(4-hydroxy-3-methoxy-5-nitrophenyl)-1-pentanone, 573
[817630-36-7]	5-Chloro-1-(4-benzyloxy-3-methoxyphenyl)-1-pentanone, 575
[817630-37-8]	5-Chloro-1-(4-hydroxy-3-methoxyphenyl)-1-pentanone, 575
[820215-94-9]	1-(3-Ethyl-2,4-dihydroxyphenyl)-2-methyl-1-hexanone, 659
[820968-19-2]	5-Chloro-1-(4-phenoxyphenyl)-1-pentanone, 568
[838822-54-1]	4-Chloro-1-(4-methoxy-2-methylphenyl)-1-butanone, 284
[848478-63-7]	3-Chloro-1-(4-hydroxyphenyl)-1-octanone, 829
[850352-39-5]	2-Bromo-1-(3,4-dimethoxyphenyl)-1-pentanone, 566
[850352-40-8]	2-Bromo-1-(2-bromo-4,5-dimethoxyphenyl)-1-pentanone, 570
[850816-19-2]	1-(2,4,6-Tribenzyloxyphenyl)-1-dodecanone, 952
[853913-75-4]	1-[2-(β-D-Glucopyranosyloxy)-4,6-dihydroxyphenyl]-1-pentanone, 527
[854460-42-7]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-2-methyl-1,3-butanedione, 330
[854465-70-6]	1-[3,4-Dihydro-7-methoxy-5-(phenylmethoxy)-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-3-methyl-1-butanone, 240
[854465-73-9]	1-[3,4-Dihydro-7-hydroxy-5-(phenylmethoxy)-2,2-dimethyl-2*H*-1-benzopyran-8-yl]-3-methyl-1-butanone, 240
[854659-09-9]	6-(4-Ethoxyphenyl)-6-oxo-1-hexanoic acid, 712
[854659-33-9]	1-(2,4-Dimethoxyphenyl)-1-pentanone, 471
[854659-36-2]	1-[1,1′-Biphenyl]-5-yl-2-methoxy-1-pentanone, 524
[854676-84-9]	4-(5-Bromo-2,4-dihydroxyphenyl)-4-oxo-1-butanoic acid, 421
[854677-51-3]	4-(2-Hydroxy-3-methylphenyl)-4-oxo-1-butanoic acid, 432
[854677-84-2]	4-(2-Amino-4,5-dimethoxyphenyl)-4-oxo-1-butanoic acid, 429
[854679-09-7]	4-(2,6-Dihydroxy-4-methylphenyl)-4-oxo-1-butanoic acid, 438
[854866-87-8]	4-Cyclohexyl-1-(2-hydroxy-4,6-dimethylphenyl)-1-butanone, 259
[854867-25-7]	1-[2-Hydroxy-5-(1,1-dimethylpropyl)phenyl]-1-butanone, 99
[854870-33-0]	1-[4-Methoxy-2-methyl-5-(1-methylethyl)phenyl]-1-butanone, 91
[854870-93-2]	1,1′-(2-Methoxy[1,1′-biphenyl]-5-yl)-1-butanone, 260
[854909-05-0]	Methyl 10-(2,4-dihydroxyphenyl)-10-oxo-1-decanoate, 919
[855153-59-2]	Methyl 5-(2,5-dimethoxyphenyl)-5-oxo-1-pentanoate, 581
[855159-27-2]	5-Hydroxy-4-methyl-6-(1-oxobutyl)-2*H*-1-benzopyran-2-one, 88
[855242-08-9]	1-(5-Chloro-2-hydroxy-4,6-dimethylphenyl)-1,3-butanedione, 321
[855605-97-9]	1-(2,5-Dimethoxyphenyl)-1-pentadecanone, 1027
[855620-89-2]	4-Cyclohexyl-1-(2-hydroxy-3,4-dimethylphenyl)-1-butanone, 258
[855875-24-0]	2,6-Dihydroxy-3-(1-oxobutyl)benzaldehyde, 386
[855890-69-6]	1-(2-Hydroxy-4-methoxy-6-methylphenyl)-1-heptadecanone, 1058

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[855890-85-6]	1-(2-Hydroxy-4-methoxy-3-methylphenyl)-1-heptadecanone, 1058
[855891-01-9]	1-(3,5-Dimethoxy-4-methylphenyl)-1-heptadecanone, 1057
[855892-35-2]	Ethyl 2-(3,5-dimethoxy-4-methylbenzoyl)heptadecanoate, 1059
[855899-90-0]	1-(2-Hydroxy-4,6-dimethylphenyl)-1-heptanone, 744
[855921-00-5]	1-(5-Chloro-3-hexyl-2-hydroxyphenyl)-1-heptanone, 758
[855954-88-0]	1-(2-Hydroxy-4-methoxy-3,6-dimethylphenyl)-1-heptadecanone, 1058
[855955-03-2]	1-(3,4,5-Trimethoxyphenyl)-1-heptadecanone, 1056
[855956-24-0]	1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-heptanone, 750
[855956-25-1]	1-(3,4-Dimethoxyphenyl)-1-hexadecanone, 1037
[856348-12-4]	1-(2-Hydroxy-4,5-dimethoxyphenyl)-1,3,5-hexanetrione, 645
[856349-95-6]	1-(2-Hydroxy-4,5-dimethylphenyl)-1-hexanone, 649
[856349-97-8]	1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-hexanone, 665
[856360-21-9]	1-(2,4-Dihydroxyphenyl)-1-docosanone, 1104
[856807-53-9]	4-(3,4-Dihexyloxyphenyl)-4-oxo-1-butanoic acid, 410
[856809-73-9]	4-(3,4-Dibutoxyphenyl)-4-oxo-1-butanoic acid, 410
[856809-86-4]	4-(2,5-Dimethoxy-4-methylphenyl)-4-oxo-1-butanoic acid, 437
[857165-59-4]	1-(3-Methoxyphenyl)-1-tridecanone, 995
[857165-80-1]	1-(3-Hydroxyphenyl)-1-tridecanone, 995
[857229-77-7]	4-(5-Chloro-2-methoxy-4-methylphenyl)-4-oxo-1-butanoic acid, 432
[857480-74-1]	6-(5-Chloro-2-hydroxyphenyl)-6-oxo-1-hexanoic acid, 714
[857803-59-9]	1-(2-Methoxyphenyl)-3-methyl-1-butanone, 174
[857973-71-8]	1-(4-Heptyl-2-hydroxy-5-methoxyphenyl)-4-methyl-1-pentanone, 552
[858189-64-7]	10-(2,4-Dihydroxyphenyl)-10-oxo-1-decanoic acid, 919
[858189-97-6]	Ethyl 10-(2,5-dihydroxyphenyl)-10-oxo-1-decanoate, 920
[858445-94-0]	Ethyl 4-(2,4-dimethoxyphenyl)-4-oxo-1-butanoate, 404
[859059-36-2]	4-(3,4-Diamyloxyphenyl)-4-oxo-1-butanoic acid, 410
[859080-81-2]	1-(2,4-Dimethoxyphenyl)-4-phenyl-1,3-butanedione, 354
[859310-32-0]	1-(4-Chloro-2-hydroxyphenyl)-1-dodecanone, 955
[859742-49-7]	1,10-Bis(3,4-dimethoxyphenyl)-1,10-decanedione, 903
[859786-47-3]	1-[2-Hydroxy-6-methyl-3-(1-methylethyl)phenyl]-1-pentanone, 508
[859939-56-3]	1-(2,4-Dihydroxy-5-ethylphenyl)-1-butanone, 69
[859947-01-6]	1-(4-Ethyloxyphenyl)-1-tetradecanone, 1005
[859968-25-5]	1-(3-Bromo-4-methoxyphenyl)-1-pentanone, 480
[859992-51-1]	1-(2-Hydroxy-5-methylphenyl)-1-octadecanone, 1075
[859994-77-7]	Ethyl 10-(2,4-dihydroxyphenyl)-10-oxo-1-decanoate, 919
[859995-51-0]	1-(3-Hydroxyphenyl)-1-nonanone, 836
[860189-36-2]	Ethyl 4-(2-hydroxy-4-(phenylmethoxy)phenyl)-2,4-dioxo-1-butanoate, 455
[860705-13-1]	1,4-Bis(2-hydroxy-3,4,6-trimethylphenyl)-1,4-butanedione, 372
[861310-96-5]	2-Bromo-1-(3-bromo-6-hydroxy-2,4-dimethylphenyl)-1-butanone, 273
[861349-33-9]	1-(5-Chloro-2-methoxyphenyl)-1,3-butanedione, 316
[861778-02-1]	1-(2-Hydroxy-4,6-dimethylphenyl)-1,3-butanedione, 322
[861889-69-2]	1-(3,5-Dichloro-2,4,6-trimethoxyphenyl)-1-hexanone, 622
[861889-70-5]	1-(3-Bromo-2,6-dihydroxy-4-methoxyphenyl)-1-hexanone, 635
[861889-71-6]	1-(2,6-Dihydroxy-3,5-diiodo-4-methoxyphenyl)-1-hexanone, 632

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[861889-72-7]	1-(2,6-Dihydroxy-3-iodo-4-methoxyphenyl)-1-hexanone, 638
[861889-73-8]	1-(3,5-Dichloro-2,6-dihydroxy-4-phenoxyphenyl)-1-hexanone, 672
[861889-74-9]	1-(3-Chloro-2,6-dihydroxy-4-phenoxyphenyl)-1-hexanone, 678
[861889-76-1]	1-(2,6-Dihydroxy-4-methoxyphenyl)-1-heptanone, 740
[861889-77-2]	1-(2,6-Dihydroxy-4-methoxyphenyl)-1-octanone, 797
[861889-78-3]	1-(2,6-Dihydroxy-4-methoxyphenyl)-3,3-dimethyl-1-butanone, 254
[861889-80-7]	1-(4-Ethoxy-2,6-dihydroxyphenyl)-1-hexanone, 653
[861889-81-8]	1-(4-Butoxy-2,6-dihydroxyphenyl)-1-hexanone, 666
[861889-82-9]	1-[4-(Cyclopentyloxy)-2,6-dihydroxyphenyl]-1-hexanone, 668
[861889-83-0]	1-(3,5-Dichloro-2,6-dihydroxy-4-methoxyphenyl)-3,3-dimethyl-1-butanone, 253
[861889-85-2]	1-(3,5-Dichloro-4-ethoxy-2,6-dihydroxyphenyl)-1-hexanone, 646
[861889-86-3]	1-(4-Butoxy-3,5-dichloro-2,6-dihydroxyphenyl)-1-hexanone, 662
[861889-87-4]	1-[3,5-Dichloro-4-(cyclopentyloxy)-2,6-dihydroxyphenyl]-1-hexanone, 667
[861889-88-5]	1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-1-butanone, 45
[861889-89-6]	1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-1-heptanone, 737
[861889-90-9]	1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-1-octanone, 790
[861889-91-0]	1-(3-Chloro-2,6-dihydroxy-4-methoxyphenyl)-3,3-dimethyl-1-butanone, 253
[861889-93-2]	1-(3-Chloro-4-ethoxy-2,6-dihydroxyphenyl)-1-hexanone, 648
[861889-94-3]	1-(4-Butoxy-3-chloro-2,6-dihydroxyphenyl)-1-hexanone, 664
[861889-95-4]	1-[3-Chloro-4-(cyclopentyloxy)-2,6-dihydroxyphenyl]-1-hexanone, 668
[862666-31-7]	1-(2,3-Dimethoxyphenyl)-1-nonanone, 838
[862666-32-8]	1-(2,3-Dimethoxyphenyl)-1-undecanone, 925
[862666-33-9]	1-(2,3-Dihydroxyphenyl)-1-pentanone, 470
[862666-34-0]	1-(2,3-Dihydroxyphenyl)-1-hexanone, 606
[862666-35-1]	1-(2,3-Dihydroxyphenyl)-1-heptanone, 725
[862666-36-2]	1-(2,3-Dihydroxyphenyl)-1-octanone, 778
[862666-37-3]	1-(2,3-Dihydroxyphenyl)-1-nonanone, 838
[862666-38-4]	1-(2,3-Dihydroxyphenyl)-1-undecanone, 925
[862666-39-5]	1-(2,3-Dihydroxyphenyl)-1-tridecanone, 996
[864072-49-1]	1-(4-Hydroxyphenyl)-1-pentanone (Oxime), 466
[867134-00-7]	6-(4-Ethoxy-3-nitrophenyl)-6-oxo-1-hexanoic acid, 715
[867213-74-9]	11-Bromo-1-(4-methoxyphenyl)-1-undecanone, 934
[868075-01-8]	1-(3-Chloro-4-methoxyphenyl)-1-butanone, 30
[868521-08-8]	6-Bromo-1-(4-hydroxy-3-methylphenyl)-1-hexanone, 706
[870084-45-0]	5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 160
[871882-61-0]	2-Chloro-1-(2-hydroxy-5-methylphenyl)-1-butanone, 276
[871882-79-0]	3-Chloro-1-(2-hydroxy-5-methylphenyl)-1-butanone, 277
[871886-71-4]	2-Chloro-1-(2-hydroxy-5-methylphenyl)-3-methyl-1-butanone, 294
[871901-16-5]	1-(3,4-Dimethoxyphenyl)-1-tetradecanone, 1008
[872178-00-2]	1-[2,4,6-Trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-dodecanone, 974
[873380-96-2]	1-(4-Hydroxy-3,5-dimethoxyphenyl)-3-methyl-1-butanone, 199
[873396-80-6]	4-(2-Ethoxy-5-methylphenyl)-4-oxo-1-butanoic acid, 435

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[873416-42-3]	1-(2-Hydroxy-5-methoxy-3-pentylphenyl)-1-octanone, 815
[873989-36-7]	1-(2-Hydroxy-3,5-dimethylphenyl)-1-butanone, 66
[874487-28-2]	4-(5-Cyclopentyl-2-methoxyphenyl)-4-oxo-1-butanoic acid, 451
[874507-02-5]	1-(2-Hydroxy-4,6-dimethylphenyl)-1-tetradecanone, 1014
[875850-72-9]	1-(2-Hydroxy-3,4,6-trimethoxyphenyl)-1,3-butanedione, 328
[875854-88-9]	1,1′-(2,6-Dihydroxy-4-methyl-1,3-phenylene)bis-1-butanone, 299
[876511-19-2]	1-(2-Hydroxy-5-methoxyphenyl)-3-methyl-1-butanone, 193
[877877-92-4]	1-[2,3,4-Trihydroxy-5-(1-methylethyl)phenyl]-1-undecanone, 931
[877877-96-8]	1-[2,3,4-Trihydroxy-5-(1-methylethyl)phenyl]-1-pentadecanone, 1029
[877877-98-0]	1-[2,3,4-Trihydroxy-5-(phenylmethyl)phenyl]-1-undecanone, 933
[877878-00-7]	1-[2,3,4-Trihydroxy-5-(1-phenylundecyl)phenyl]-1-undecanone, 934
[883566-08-3]	1-(2-Hydroxy-3,5-diiodo-4-methylphenyl)-1-butanone, 42
[883566-09-4]	1-(5-Chloro-2-hydroxy-3-iodophenyl)-1-butanone, 23
[883566-10-7]	1-(5-Bromo-2-hydroxy-3-iodophenyl)-1-butanone, 20
[883566-11-8]	1-(2-Hydroxy-5-iodo-3-methylphenyl)-1-butanone, 46
[883566-12-9]	1-(2-Hydroxy-3,5-diiodo-4,6-dimethylphenyl)-1-butanone, 61
[888026-39-9]	1-(2,4,6-Trimethoxyphenyl)-1-dodecanone, 952
[888489-66-5]	Myristinin A (+), 990
[903883-85-2]	1-[3,5-Bis(1,1-dimethylethyl)-4-acetyloxyphenyl]-1-pentanone, 535
[905590-12-7]	1-(4-Ethoxy-3-propylphenyl)-4-oxo-1-butanoic acid, 447
[909191-71-5]	1-(2-Hydroxy-4-methylphenyl)-1-octadecanone, 1075
[909255-15-8]	1-(3-Amino-2,4-dihydroxyphenyl)-3-methyl-1-butanone, 187
[909255-16-9]	1-(3-Amino-5-bromo-2,4-dihydroxyphenyl)-3-methyl-1-butanone, 187
[910457-86-2]	1-(3,5-Dichloro-2,6-dihydroxyphenyl)-1-octanone, 786
[916895-75-5]	1-(3-Chloro-2,4,6-trimethoxyphenyl)-1-hexanone, 626
[918814-59-2]	2,4-Dihydroxy-3-(3-methyl-1-oxobutyl)-6-(2-propen-1-yloxy) benzaldehyde, 392
[918814-60-5]	1,1′-[2,4-Dihydroxy-6-(2-propen-1-yloxy)-1,3-phenylene]bis-3-methyl-1-butanone, 305
[918814-63-8]	2,4-Dihydroxy-6-(3-methylbutoxy)-3-(3-methyl-1-oxobutyl)-1-butanone, 393
[918814-65-0]	1,1′-[2,4-Dihydroxy-6-(3-methylbutoxy)-1,3-phenylene]bis-3-methyl-1-butanone, 306
[918814-68-3]	1-[2,6-Dihydroxy-4-(2-propen-1-yloxy)phenyl]-3-methyl-1-butanone, 205
[918814-70-7]	1-[2,6-Dihydroxy-4-[(3-methylbutoxyl)]phenyl]-3-methyl-1-butanone, 216
[918896-70-5]	1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-2-methyl-1-butanone, 135
[919800-80-9]	1-(2-Decyl-4,5-dimethoxyphenyl)-1-decanone, 914
[919995-26-9]	1-[3-(3-Hydroxypropoxy)-4-methoxyphenyl]-3-methyl-1-butanone, 207
[919995-27-0]	1-[3-(3-Methoxypropoxy)-4-methoxyphenyl]-3-methyl-1-butanone, 207
[921758-91-0]	1-(2,6-Dihydroxyphenyl)-1-octadecanone, 1066
[921758-92-1]	1-(3-Chloro-2,6-dihydroxyphenyl)-1-octadecanone, 1072
[921758-93-2]	1-(3,5-Dichloro-2,6-dihydroxyphenyl)-1-octadecanone, 1070
[924889-46-3]	1-(3,4-Dihydro-5,7-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-1-butanone, 96
[924889-47-4]	1-(5,7-Dimethoxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-1-butanone, 95

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[924889-50-9]	5,7-Dimethoxy-2,2-dimethyl-2*H*-1-(benzopyran-8-yl)-3-methyl-1-pentanone, 562
[927911-85-1]	6-Chloro-1-(4-methoxy-3-methylphenyl)-1-hexanone, 706
[927911-86-2]	6-Chloro-1-(3-fluoro-4-methoxyphenyl)-1-hexanone, 704
[927911-89-5]	11-Bromo-1-(4-methoxy-3-methylphenyl)-1-undecanone, 936
[927911-90-8]	1-(4-Methoxy-3-methylphenyl)-3,3-dimethyl-1-butanone, 254
[927911-91-9]	1-(4-Methoxy-3-methylphenyl)-2-methyl-1-butanone, 133
[928769-73-7]	1-(4-Ethoxy-2-hydroxyphenyl)-1-pentanone (Oxime), 501
[930585-36-7]	1-(3,4-Dimethoxyphenyl)-1-tridecanone, 997
[930782-40-4]	1-(2-Dodecyl-4,5-dimethoxyphenyl)-1-dodecanone, 987
[933786-84-6]	1-[2,4-Dihydroxy-6-methoxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone, 107
[934302-22-4]	1-[5-Acetyl-2-(β-D-glucopyranosyloxy)phenyl]-3-methyl-1-butanone, 379
[934637-35-1]	2-Bromo-1-(2-methoxyphenyl)-1-pentanone, 565
[935277-48-8]	1-(2-Hydroxyphenyl)-4,4-dimethyl-1-pentanone, 555
[935277-51-3]	1-(2-Hydroxyphenyl)-2-methylene-1-hexanone, 615
[936642-87-4]	1-(2-Hydroxy-3,4-dipropylphenyl)-butanone, 109
[940307-82-4]	1-(3-Hydroxyphenyl)-3,3-dimethyl-1-butanone, 250
[942037-66-3]	1-(3-Fluoro-4-methoxyphenyl)-2-methylene-1-hexanone, 629
[944558-07-0]	3,5-Dimethoxy-2-(1-oxopentyl)benzoic acid, 490
[949902-14-1]	1-(3-Fluoro-2-hydroxyphenyl)-1-butanone, 32
[949902-16-3]	1-(3-Fluoro-2-methoxyphenyl)-1-butanone, 32
[952103-47-8]	1-(3-Bromo-2-methoxyphenyl)-1-heptanone, 733
[956239-90-0]	1-(2-Hydroxyphenyl)-1-octanone-*2,2-d2*, 772
[959137-60-1]	1-(2-Amino-5-methoxy-4-methylphenyl)-2-methyl-1-butanone, 137
[1000210-34-3]	1-[3-β-D-Glucopyranosyl-6-(β-D-glucopyranosyloxy)-2,4-dihydroxyphenyl]-3-methyl-1-butanone, 242
[1000210-35-4]	1-[4-[[6-O-(6-Deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-2,6-dihydroxy-phenyl]-3-methyl-1-butanone, 241
[1000598-85-5]	1-(2-Hydroxy-3-methylphenyl)-1-heptanone, 738
[1001024-93-6]	1-(2-Methoxyphenyl)-1,3-hexanedione, 597
[1001024-95-8]	2-Chloro-1-(2-methoxyphenyl)-1,3-butanedione, 309
[1001024-96-9]	2-Chloro-1-(2-methoxyphenyl)-1,3-hexanedione, 697
[1001441-59-3]	2-Bromo-1-(4-chloro-2-methoxyphenyl)-1-pentanone, 570
[1002158-21-5]	1-(2-Butyl-6-hydroxy-5-benzofuranyl)-1-hexanone, 681
[1006710-00-4]	1-(4-Hydroxyphenyl)-1-tridecanone, 996
[1023272-24-3]	4-Bromo-3,3-difluoro-1-(4-methoxyphenyl)-1-butanone, 292
[1023634-25-4]	4-Bromo-1-(4-methoxyphenyl)-1-butanone, 274
[1032174-10-9]	1-(4-Methoxy-3-nitrophenyl)-1-butanone, 36
[1032174-12-1]	1-(4-Methoxy-3-nitrophenyl)-1-pentanone, 485
[1033774-79-6]	2-Bromo-1-(4-methoxyphenyl)-1-heptanone, 764
[1039364-65-2]	5-Chloro-1-(2,5-dimethoxyphenyl)-2,2-difluoro-1-pentanone, 563
[1039364-66-3]	5-Chloro-1-(3,5-dimethoxyphenyl)-2,2-difluoro-1-pentanone, 564
[1049661-48-4]	5-Chloro-1-(2,6-dihydroxy-3,4-dimethoxyphenyl)-2,4,5-trimethyl-1-hexanone, 708

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[1067245-70-8]	1-[2-(β-D-Glucopyranosyloxy)-4,6-dihydroxyphenyl]-1-butanone, 108
[1080023-63-7]	1-[2,6-Dimethoxy-3,5-dimethyl-4-(phenyloxy)phenyl]-2-methyl-1-butanone, (2S), 146
[1080023-64-8]	1-(4-Hydroxy-2,6-dimethoxy-3,5-dimethylphenyl)-2-methyl-1-butanone (2S), 140
[1080023-65-9]	1-(4-Hydroxy-2,6-dimethoxy-3,5-dimethylphenyl)-2-methyl-1-butanone (2*R*), 140
[1080509-35-8]	5,7-Dihydroxy-4-(1-hydroxypropyl)-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one (1S), 239
[1080021-89-1]	4-Chloro-1-[4-hydroxy-3-(1-methylethyl)phenyl]-1-butanone, 287
[1080021-90-4]	4-Chloro-1-[3-(1,1-dimethylethyl)-4-hydroxyphenyl]-1-butanone, 288
[1092783-56-6]	1-(3-Dodecyl-2,4,6-trihydroxyphenyl)-1-dodecanone, 988
[1092783-58-8]	1,1′-(4,6-Dihydroxy-1,3-phenylene)bis-1-dodecanone, 986
[1092783-59-9]	1,1′-(2,4,6-Trihydroxy-5-methyl-1,3-phenylene)bis-1-dodecanone, 988
[1092783-61-3]	1-(3-Acetyl-2,4,6-trihydroxy-5-methylphenyl)-1-dodecanone, 969
[1092783-62-4]	1,1′-(2-Hydroxy-5-methyl-1,3-phenylene)bis-1-dodecanone, 988
[1093860-17-3]	1-[1,1′-Biphenyl]-2-yl-5-methoxy-1-pentanone, 523
[1096879-14-9]	1-(4-Methoxy-3-methylphenyl)-3-methyl-1-butanone, 191
[1103524-17-9]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-hexadecanone, 1052
[1103524-18-0]	1,1′-(2,4,6-Trihydroxy-1,3-phenylene)bis-1-octadecanone, 1087
[1103524-19-1]	1,1′-(4,6-Dibutoxy-2-hydroxy-1,3-phenylene)bis-3-methyl-1-butanone, 307
[1103524-20-4]	1,1′-(2,4-Dibutoxy-6-hydroxy-1,3-phenylene)bis-3-methyl-1-butanone, 307
[1103524-21-5]	1,1′-(4-Butoxy-2,6-dihydroxy-1,3-phenylene)bis-3-methyl-1-butanone, 305
[1103524-22-6]	1,1′-(5-Butyl-2,4,6-trihydroxy-1,3-phenylene)bis-3-methyl-1-butanone, 305
[1103524-25-9]	1,1′-[2,4-Dihydroxy-6-(2-hydroxyethoxy)-1,3-phenylene]bis-3-methyl-1-butanone, 304
[1104634-92-5]	2-Bromo-5-chloro-1-(4-methoxyphenyl)-1-pentanone, 564
[1108128-60-4]	2-Chloro-1-(4-hydroxyphenyl)-1-pentanone, 567
[1109229-46-0]	1-[2,4-Dihydroxy-3-[6-O-(3,4,5-trihydroxybenzoyl)-β-D-glucopyranosyl]-6-[[6-O-(3,4,5-trihydroxybenzoyl)-β-D-glucopyranosyl]oxy]phenyl]-3-methyl-1-butanone, 250
[1111287-73-0]	1-(4,5-Dimethoxy-2-octadecylphenyl)-1-octadecanone, 1088
[1111652-02-8]	5-Bromo-1-(2,6-dihydroxyphenyl)-1-pentanone, 566
[1111652-08-4]	6-Bromo-1-(2,6-dihydroxyphenyl)-1-hexanone, 699
[1142936-17-1]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-hexanone, 653
[1142936-18-2]	1-(2-Hydroxy-4,6-dimethoxyphenyl)-1-octanone, 802
[1142936-30-8]	1,1′-(4-Hydroxy-2,6-dimethoxy-1,3-phenylene)bis-1-octanone, 826
[1146443-98-2]	5-Chloro-1-(5-chloro-2-benzyloxyphenyl)-1-pentanone, 572
[1173986-37-2]	1,4-Bis(4-hydroxy-3-methoxyphenyl)-2,3-dimethyl-1,4-butanedione (-), 370
[1173986-38-3]	1,4-Bis(4-hydroxy-3-methoxyphenyl)-2,3-dimethyl-1,4-butanedione (+), 370
[1175530-97-8]	2-Methyl-1-[2,4,6-trimethoxy-3-(3-methyl-2-butenyl)phenyl]-1-butanone, 143
[1183770-52-6]	1-(3-Methoxyphenyl)-3-methyl-1-butanone, 174
[1186123-07-8]	1-(3,5-Dimethoxyphenyl)-1-heptadecanone, 1056
[1186304-76-6]	2-Bromo-1-(2-hydroxy-5-iodo-3-methylphenyl)-1-butanone, 272

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[1192824-04-6]	1-[(2-Phenylmethoxy)-4-nitrophenyl]-1-butanone, 35
[1196852-29-5]	1-(2-Methoxyphenyl)-2-methyl-1-butanone, 125
[1204225-56-8]	1,4-Bis(4-hydroxy-3-methoxyphenyl)-2,3-dimethyl-1,4-butanedione (Meso), 370
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[1204737-61-0]	1-(2,4-Dihydroxy-3-iodophenyl)-3-methyl-1-butanone, 186
[1204737-62-1]	1-(2,4-Dihydroxy-3-iodophenyl)-1-butanone, 34
[1204737-68-7]	1-(2,4-Diydroxy-3-iodophenyl)-3,3-dimethyl-1-butanone, 252
[1204738-04-4]	1-(3-Bromo-2,4-dihydroxyphenyl)-1-butanone, 27
[1208265-79-5]	4-(4-Chloro-3-fluoro-2-hydroxyphenyl)-4-oxo-1-butanoic acid, 420
[1237740-92-9]	1-(2-Hydroxyphenyl)-1,6-heptanedione, 733
[1245818-23-8]	1-(3-Chloro-2,4,6-trihydroxyphenyl)-1-butanone, 32
[1245904-83-9]	2-Bromo-1-(4-hydroxyphenyl)-1-hexanone, 697
[1250871-16-9]	1-(3,5-Dihydroxyphenyl)-1-dodecanone, 949
[1254222-60-0]	15-Hydroxy-3-methyl-1-(2,5-dihydroxyphenyl]-1-pentadecanone, 1028
[1254222-61-1]	13-Hydroxy-3-methyl-1-(2,5-dihydroxyphenyl)-1-tridecanone, 999
[1254222-62-2]	14-Hydroxy-3-methyl-1-(2,5-dihydroxyphenyl)-1-tetradecanone, 1009
[1254222-63-3]	16-Hydroxy-3-methyl-1-(2,5-dihydroxyphenyl]-1-hexadecanone, 1039
[1254222-72-4]	15-Hydroxy-3-methyl-1-(2,5-dihydroxyphenyl]-1-pentadecanone (Oxime), 1029
[1254222-75-7]	16-Hydroxy-3-methyl-1-(2,5-dihydroxyphenyl]-1-hexadecanone (Oxime), 1039
[1254222-90-6]	14-Hydroxy-1-(2,5-dihydroxyphenyl)-1-tetradecanone, 1009
[1257216-80-0]	1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-3-methyl-1-butanone, 198
[1257228-28-6]	1-(3,5-Dihydroxyphenyl)-1-octanone, 782
[1263095-96-0]	1-(4-Hydroxy-2-methylphenyl)-1-decanone, 884
[1263908-96-8]	4-[1-(Acetyloxy)propyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-2*H*-1-benzopyran-2-one, 158
[1344146-37-7]	6-(2,4-Dihydroxy-5-methylphenyl)-6-oxo-1-hexanoic acid, 717
[1346860-08-9]	1-(2,3-Dimethoxyphenyl)-1-pentadecanone, 1026
[1346860-11-4]	1-(2,3-Dihydroxyphenyl)-1-pentadecanone, 1026
[1393654-90-4]	1-(3,5-Dibromo-4-hydroxyphenyl)-1-dodecanone, 954
[1396756-55-0]	1-(2-Hydroxy-6-methylphenyl)-1-nonanone, 844
[1396756-56-1]	1-(5-Fluoro-2-hydroxyphenyl)-1-nonanone, 842
[1396756-57-2]	1-(5-Chloro-2-hydroxyphenyl)-1-nonanone, 842
[1396756-58-3]	1-(5-Iodo-2-hydroxyphenyl)-1-nonanone, 842
[1396756-63-0]	1-(2-Hydroxyphenyl)-5-phenyl-1-hexanone, 679

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