Roth Collection of Natural Products Data

Concise Descriptions and Spectra

Edited by
Lutz Roth and Gabriele Rupp

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Distribution:
VCH, P.O. Box 101161, D-69451 Weinheim, Federal Republic of Germany
Switzerland: VCH, P.O. Box, CH-4020 Basel, Switzerland
United Kingdom and Ireland: VCH, 8 Wellington Court, Cambridge CB1 1HZ, United Kingdom
USA and Canada: VCH, 220 East 23rd Street, New York, NY 10010-4606, USA
Japan: VCH, Eikow Building, 10-9 Hongo 1-chome, Bunkyo-ku, Tokyo 113, Japan

ISBN 3-527-28180-0

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Published jointly by
VCH Verlagsgesellschaft, Weinheim (Federal Republic of Germany)
VCH Publishers, New York, NY (USA)

Editorial Director: Dr. Hans-Joachim Kraus
Production Manager: Dipl.-Wirt.-Ing. (FH) Bernd Riedel

Titelbild: Chamomilla recutita (L.) Rauschert
von Kurt Kormann, Waldstr. 45, 75045 Walzbachtal

Library of Congress Card No. applied for

A catalogue record for this book is available from the British Library.

Die Deutsche Bibliothek – CIP-Einheitsaufnahme

Roth collection of natural products data : concise descriptions
and spectra / ed. by Lutz Roth and Gabriele Rupp. – Weinheim;
New York; Basel; Cambridge; Tokyo : VCH, 1995
ISBN 3-527-28180-0
NE: Roth, Lutz [Hrsg.]

Composition: Filmsatz Unger & Sommer GmbH, D-69469 Weinheim
Printing: Colordruck GmbH, D-69181 Leimen
Bookbinding: Wilh. Osswald + Co, D-67408 Neustadt

Printed in the Federal Republic of Germany

Preface

More and more attention is being paid to natural products chemistry. The number of recently discovered and described natural products is growing exponentially, while increased analytical possibilities are contributing considerably to the information we already possess on natural products.

Scientific journals cannot, on the one hand, process the increasing amounts of information offered to them; on the other hand, they cannot sufficiently meet the growing need for information. The space they have for publications is inadequate, and the data on substances can only be printed in an extremely abbreviated form. In stark contrast to this lack of space is the constantly growing abundance of detailed information. Today databases are a significant aid in searching for special data. They are, however, not suitable for people wanting to acquire an overview of this gigantic field.

It is the aim of the Roth Collection of Natural Products Data to bridge this gap. It strikes a happy medium between a concise encyclopedic presentation and an introduction to the large field of primary literature by offering data on selected natural products in a clearly structured fashion. It proposes to introduce and inform, to stimulate and inspire.

This collection comprises short monographs on 75 natural products of plant origins, clearly presented and detailed. Each monograph contains information on physical and chemical properties, toxicology and risk potential, followed by spectroscopic and chromatographic data with clearly indicated measurement conditions and peaks. In addition, structural formulas and illustrations of NMR, mass and IR spectra are provided. Selected and annotated references on each natural product facilitate the search for further information.

In view of the abundance of natural products known to us, a collection such as this one must of course restrict itself to a few representatives from important classes of substances. At any rate, for a comprehensive collection of as much information as possible on as many natural products as possible, databases with their search possibilities are more suitable. However, one must bear in mind that data is often missing for products which were described some time ago; this occurs, for example, because only the more recent publications have been included in databases.

This collection includes data both on recently discovered and long known natural products. Although their values, properties etc can be found described in the literature, they are most widely scattered. Thus it is theoretically possible for a terpene expert to be uncertain as to where to find the NMR data for such a common substance as limonene. Consequently it appeared to be a good idea to compile the data on such common natural products as limonene, camphene or apigenine. This was a most work-intensive process, especially because many spectra had to be remeasured in order to achieve a certain standardization.

This work is the starting point for a reliable collection of natural products that is as comprehensive as possible and that includes particularly important and typical representatives of all classes of substances. A goal such as this one cannot be realized through one single book but rather through a dedicated continuation. Seen in those terms, this collection is a beginning waiting to be continued.

Karlsruhe, October 1994

L. Roth
G. Rupp

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Cardanol, Monoene
Cardanol, saturated
Cardanol, Triene
Cardol, Diene
Cardol, Monoene
Cardol, saturated
Cardol, Triene
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Apometzgerin 6,8-di-C-arabinoside
Bryoflavone
5',3'''-Dihydroxyrobustaflavone
2,3-Dihydro-5'-hydroxyamentoflavone
2,3-Dihydro-5',3'''-dihydroxyamentoflavone
Tricin-6,8-di-C-arabinoside
Heterobryoflavone
Isofurcatain-7-0-β-D-glucoside
Saponarin
Lucenin-2
Tricetin-6-C-arabinoside-8-C-glucoside
Tricetin 6,8-di-C-glucoside

List of Compounds

In the following collection substances can be found in alphabetical order according to the names written in boldface type.

Synonyms and Systematic Names	Common Names
(-)-(3S,3aR,4S,9aS,9bS)-4-Acetoxy-2,3,3a,4,5,9,9a,9b-octanhydro-9-hydroxy-3,6,9-trimethyl-azuleno[4,5-b]-furan-2-one	**Matricine**
Alantolactone	
Anacardol	**Cardanol, saturated**
Apigenin	
Apigenin-7-glucoside	
Apigenin-7-β-D-glucoside	**Apigenin-7-glucoside**
Apigenol	**Apigenin**
Apigetrin	**Apigenin-7-glucoside**
Apometzgerin-6,8-di-C-α-arabinopyranoside	**Apometzgerin 6,8-di-C-arabinoside**
Apometzgerin-6,8-di-C-arabinoside	
6-Arabinopyranosyl-8-β-D-glucopyranosyl-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one	**Tricetin 6-C-arabinoside-8-C-glucoside**
6-C-α-L-Arabinopyranosyl-8-C-β-D-glucopyranosyl-tricetin	**Tricetin 6-C-arabinoside-8-C-glucoside**
Artecanin	
Aurantiogliocladin	
Austracamphene	**(+)-Camphene**
Axillin	**Deacetoxymatricarin**
5′,6″-Biluteolin	**5′,3‴-Dihydroxyrobustaflavone**
[1,1′-Biphenyl]-2,2′-diol, 5,5′-di-2-propenyl-	**Magnolol**
[1,1′-Biphenyl]-2,4′-diol, 3′,5-di-2-propenyl-	**Honokiol**
(-)-α-Bisabolol	
Bryoflavone	
Cajeputene	**(±)-Limonene**
Camphene	
Candelabrone	
Cardanol 15:0	**Cardanol, saturated**
Cardanol 15:1 (n-7)	**Cardanol, Monoene**
Cardanol 15:2 (n-4)	**Cardanol, Diene**
Cardanol 15:3 (n-1)	**Cardanol, Triene**
Cardanol, Diene	
Cardanol, Monoene	
Cardanol, saturated	
Cardanol, Triene	
Cardanol-diolefin	**Cardanol, Diene**
Cardanol-monoolefin	**Cardanol, Monoene**
Cardanol-triolefin	**Cardanol, Triene**
Cardol	**Cardol, saturated**

Synonyms and Systematic Names	Common Names
Cardol 15:0	**Cardol, saturated**
Cardol 15:1 (n-7)	**Cardol, Monoene**
Cardol 15:2 (n-4)	**Cardol, Diene**
Cardol 15:3 (n-1)	**Cardol, Triene**
Cardol, Diene	
Cardol, Monoene	
Cardol, Triene	
Cardol-diolefin	**Cardol, Diene**
Cardol-monoolefin	**Cardol, Monoene**
Cardol, saturated	
Cardol-triolefin	**Cardol, Triene**
Carvene	**(+)-Limonene**
5α,14α-Cevanine-3β,20β-dihydroxy-6-one	**Peiminine**
5α, 14α-Cevanine-3β,6α,20β-triol	**Peimine**
Chaetomidin	**Oosporein**
Chamazulene	
Chlorophyll a	
Chlorophyll b	
Cinene	**(±)-Limonene**
Citrene	**(+)-Limonene**
Clavacin	**Patulin**
Clavatin	**Patulin**
Claviformin	**Patulin**
Coriandrol	**S-Linalool**
Cosmetin	**Apigenin-7-glucoside**
Cosmosiin	**Apigenin-7-glucoside**
Cynene	**(±)-Limonene**
Daturine	**L-Hyoscyamine**
Deacetoxymatricarin	
Dehydrocorybulbine	
3-{[6-0-(6-Deoxy-α-L-mannopyranosyl)-≈β-D-glucopyranosyl]-oxy}-5,7-dihydroxy-2-≈(4-hydroxy-3-methoxyphenyl)-4*H*-1-benzopyran-4-one	**Narcissin**
6-(6-Deoxy-α-L-mannopyranosyl)-7-(β-D-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)4*H*-1-benzopyran-4-one	**Isofurcatain-7-O-β-D-glucoside**
6,8-Di-C-α-L-arabinopyranosylapometzgerin	**Apometzgerin-6,8-di-C-arabinoside**
6,8-Diarabinopyranosyl-5,7-dihydroxy-2-(3-hydroxy-4,5-dimethoxyphenyl)-4*H*-1-benzopyran-4-one	**Apometzgerin-6,8-di-C-arabinoside**
6,8-Diarabinopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-4*H*-1-benzopyran-4-one	**Tricin 6,8-di-C-arabinoside**
6,8-Di-C-α-L-arabinopyranosyl-3',4'-dimethoxytricetin	**Apometzgerin-6,8-di-C-arabinoside**
6,8-Di-C-α-L-arabinopyranosyltricin	**Tricin 6,8-di-C-arabinoside**
8-Dichloroacetyl-2,7-dimethyl-5-hydroxy-1,4-naphthoquinone	**Mollisin**
6,8-Di-β-D-glucopyranosyl-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one	**Tricetin 6,8-di-C-glucoside**

Synonyms and Systematic Names	Common Names
6,8-Di-C-β-D-glucopyranosyl-luteolin	**Lucenin-2**
6,8-Di-C-β-D-glucopyranosyl-tricetin	**Tricetin-6,8-di-C-glucoside**
II-2,3-Dihydroamentoflavone	
2,3-Dihydro-5′,3‴-dihydroxyamentoflavone	
(-)-3,4-Dihydro-6,8-dihydroxy-3-methyl-1*H*-2-benzopyran-1-one	**(-)-3,4-Dihydro-6,8-dihydroxy-3-methylisocoumarin**
(-)-3,4-Dihydro-6,8-dihydroxy-3-methylisocoumarin	
3,4-Dihydro-4,8-dihydroxy-1(2H)-naphthalenone	**Isosclerone**
8-[5-(2,3-Dihydro-5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-2-yl)-2,3-dihydroxy-phenyl]-5,7-dihydroxy-2-(3,4-dihydroxyphenyl)-4*H*-1-benzopyran-4-one	**2,3-Dihydro-5′,3‴-dihydroxyamentoflavone**
8-[5-(2,3-Dihydro-5,7-dihydroxy-4-oxo-4H-1-benzopyran-2-yl)-2,3-dihydroxyphenyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one	**2,3-Dihydro-5'-hydroxyamentoflavone**
2,3-Dihydro-5′-hydroxyamentoflavone	
3,4-Dihydro-8-hydroxy-3,5-dimethyl-1H-2-benzopyran-1-one	**Methylmellein**
(-)-2,5-Dihydro-5-hydroxy-4-[4′-hydroxyphenyl]-furan-2-one	**Hydroxybutenolide**
3,4-Dihydro-8-hydroxy-3-methyl-[1H]-2-benzopyran-1-one	**Mellein**
5,6-Dihydro-3-hydroxy-2,9,10-trimethoxy-13-methyl-dibenzo-[a,g]-quinolizinium	**Dehydrocorybulbine**
1,3-Dihydroxy-2-hydroxymethyl-9,10-anthraquinone	**Lucidin**
5,7-Dihydroxy-2(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one	**Apigenin**
8,12-Dihydroxy-4-methyl-11,16-dioxosenecionanium	**Senkirkine**
(-)-6,8-Dihydroxy-3-methylisochroman-1-one	**(-)-3,4-Dihydro-6,8-dihydroxy-3-methylisocoumarin**
8-[5-(5,7-Dihydroxy-4-oxo-4*H*-1-benzopyran-2-yl)-2,3-dihydroxyphenyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)4*H*-1-benzopyran-4-one	**5′-Hydroxyamentoflavone**
6-[5-(5,7-Dihydroxy-4-oxo-4*H*-1-benzopyran-3-yl)-2,3-dihydroxyphenyl]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one	**Bryoflavone**
6-[5-(5,7-Dihydroxy-4-oxo-4*H*-1-benzopyran-2-yl)-2,3-dihydroxyphenyl]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one	**5′,3‴-Dihydroxyrobustaflavone**
8-[5-(5,7-Dihydroxy-4-oxo-4*H*-1-benzopyran-3-yl)-2,3-dihydroxyphenyl]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one	**Heterobryoflavone**
8-[5-(5,7-Dihydroxy-4-oxo-4*H*-1-benzopyran-2-yl)-2-hydroxyphenyl]-2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one	**II-2,3-Dihydroamentoflavone**
2-(3,4-Dihydroxyphenyl)-6,8-di-β-D-glucopyranosyl-5,7-dihydroxy-4*H*-1-benzopyran-4-one	**Lucenin-2**
5′,3‴-Dihydroxyrobustaflavone	
4,8-Dihydroxy-1-tetralone	**Isosclerone**
Diisoprene	**(±)-Limonene**
2,3-Dimethoxy-5,6-dimethyl-1,4-benzoquinone	**Aurantiogliocladin**
Dimethulene	**Chamazulene**
2,2-Dimethyl-3-methylenebicyclo[1.2.2]heptane	**Camphene**
2,2-Dimethyl-3-methylenenorbornane	**Camphene**

Synonyms and Systematic Names	Common Names
3,7-Dimethyl-1,6-octadien-3-ol	**Linalool**
Dipentene	**(±)-Limonene**
Duboisine	**L-Hyoscyamine**
Epicorazine A	
(8S,9R,9aS,10aS)-9-Ethenyl-8-(β-D-glucopyranosyloxy)-2,3,9,9a,10,10a-hexahydro-5H,8H-pyrano[4,3-d]thiazolo-[3,2-a]pyridine-5-one	**Xylostosidine**
(1S,8S,9R,9aS,10aS)-9-Ethenyl-8-(β-D-glucopyranosyloxy)-2,3,9,9a,10,10a-hexahydro-5H,8H-pyrano[4,3-d]thiazolo-[3,2-a]pyridine-5-one-1-oxide	**Loxylostosidine A**
7-Ethyl-1,4-dimethylazulene	**Chamazulene**
Eudesma-4(14),11(13)-dien-12-oic acid,8β-hydroxy-, γ-lactone	**Isoalantolactone**
4αH-Eudesma-5,11(13)-dien-12-oic acid,8β-hydroxy-, γ-lactone	**Alantolactone**
Expansin	**Patulin**
Fabiatrin	
Fritillarine	**Peiminine**
6-C-β-D-Glucopyranosyl-apigenin-7-O-β-glucopyranoside	**Saponarin**
6-β-D-Glucopyranosyl-7-(β-D-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one	**Saponarin**
3-β-D-Glucopyranosyloxy-2-methoxy-6-hydroxy-benzoic acid-2′-β-D-glucopyranosyl-oxybenzylester	**Leiocarposide**
Helenin	**Alantolactone**
Hesperidene	**(+)-Limonene**
Heterobryoflavone	
3,3a,4,5,9a,9b-Hexahydro-3,6,9-trimethyl-azuleno-[4,5-b]-furan-2,7-dione	**Deacetoxymatricarin**
1a,2,12,12a,15a,18-Hexahydro-1a,12a,17-trimethyl-spiro[12,14-methano-3H,19H,20H-oxireno[8,9][1,6,12]trioxacyclooctadecino-[3,4-d]-[1]benzopyran-13(14H),2′-oxirane]-5,10,22,(22aH)-trione	**Verrucarin B**
Honokiol	
1-Hydroxy-6-acetoxyguaj-2,4-(10)-dien-8,12-olide	**Matricine**
5′-Hydroxyamentoflavone	
Hydroxybutenolide	
p-Hydroxy-β-[carboxymethyl]cinnamic acid	**Sphagnum acid**
1(S),6(S),9(R)-6-Hydroxy-8,8-dimethyl-4-(1-chloro-propenyl)-tricyclo-[4.4.0.0^{1,9}]-7-oxa-dec-3-ene-2,5-dione	**Mycorrhizin A**
4-Hydroxy-4H-furo-[3,2-c]pyran-2[6H]-one	**Patulin**
2-(4-Hydroxyphenyl)-5-hydroxy-7-β-D-glucosyl-4*H*-1-benzopyran-4-one	**Apigenin-7-glucoside**
3-[4-Hydroxy-phenyl]pentenedioic acid	**Sphagnum acid**
L-Hyoscyamine	
Isoalantolactone	
Isofurcatain-7-O-β-D-glucoside	
Isohelenin	**Isoalantolactone**

Synonyms and Systematic Names	Common Names
Iso-oosporein	**Oosporein**
4-Isopropenyl-1-methylcyclohexene	**Limonene**
Isosclerone	
Isoterebenthene	**(±)-Limonene**
Isovitexin-7-O-glucoside	**Saponarin**
Kautschine	**(±)-Limonene**
Kingiside	
Leiocarposide	
(+)-Leukodin	**Deacetoxymatricarin**
Levomenol	**(-)-α-Bisabolol**
l-Licareol	**R-Linalool**
Limonene	
Linalool	
Loganin	
Loganoside	**Loganin**
Loniceroside	**Secologanin**
Loxylostosidine A	
Lucenin-2	
Lucidin	
Luteolin-6,8-di-C-β-D-glucopyranoside	**Lucenin-2**
Luteolin-6,8-di-C-glucoside	**Lucenin-2**
Magnesium, 3-[(17S)-8-ethyl-13^{2}t-methoxycarbonyl-2,7,12,18t-tetramethyl-13^1-oxo-2-vinyl-13,13^2,17,18-tetrahydro-cyclopenta[at]-porphyrin-17r-yl]-propionato-[(7R,11R)-trans-phytylester]	**Chlorophyll a**
Magnesium, 3-[(17S)-7-formyl-8-ethyl-13^2-methoxycarbonyl-2,12,18t-trimethyl-13^1-oxo-3-vinyl-13^1,13^2,17,18-tetrahydro-cyclopenta[at]-porphyrin-17r-yl]-propionato-[(7R,11R)-trans-phytylester]	**Chlorophyll b**
Magnolol	
Matricine	
Melaleucol	**trans-Nerolidol**
Mellein	
p-Mentha-1,8-diene	**Limonene**
(13^{2}R)-13^2-Methoxycarbonyl-3^1,3^2-didehydro-phytochlorin-[7R,11R)-trans-phytylester]	**Chlorophyll a**
3-Methoxy-5-methyl-4-oxo-2,5-hexadiene	**Penicillic acid**
6-Methoxy-7-[(6-0-β-D-xylopyranosyl-β-D-glucopyranosyl)oxy]-2*H*-1-benzopyran-2-one	**Fabiatrin**
Methyl-(1S,5S,9R)-5-(formylmethyl)-1-(β-D-glucopyranosyloxy)-9-vinyl-5,9-dihydro-1H-pyran-4-carboxylate	**Secologanin**
Methyl-(1S,5S,8S,9S)-1-(β-D-glucopyranosyloxy)-1,5,6,7,8,9-hexahydro-8-methyl-7-one-4-pyrano[3,4-c]-pyran-4-carboxylate	**Kingiside**
Methyl-(1S,5S,7S,8R,9R)-1-(β-D-glucopyranosyloxy)-1,5,6,7,8,9-hexahydro-7-hydroxy-8-methylcylopenta(c)pyran-4-carboxylate	**Loganin**
Methylmellein	

Synonyms and Systematic Names	Common Names
(-)-(1'S,2S)-6-Methyl-2-(4'-methyl-3'-cyclohexen-1'-yl)-5-hepten-2-ol	**(-)-α-Bisabolol**
1-Methyl-4-(1-methylethenyl)-cyclohexene	**Limonene**
5-Methylochracin	**Methylmellein**
Mollisin	
Muconomycin A	**Verrucarin A**
Muconomycin B	**Verrucarin B**
Mycoin C_3	**Patulin**
Mycorrhizin A	
1,4-Naphthoquinone, 8-(dichloroacetyl)-5-hydroxy-2,7-dimethyl	**Mollisin**
Narcisoside	**Narcissin**
Narcissin	
trans-Nerolidol	
Ochracin	**Mellein**
9,12-Octadecadien-6-ynoic acid	
9,12,15-Octadecatrien-6-ynoic acid	
9-Octadecen-6-ynoic acid	
4,4a,7,7a,11,11a,14,14a-Octahydro-4,11-dihydroxy-[4S-(4α,4aα,6aβ,7aβ,11α,11a α,13aβ,14aβ)]-8H,13H-6a,13a-epidithio-1H,6H-pyrazino[1,2-a:4,5-a']-diindole-1,6,8,13-tetrone	**Epicorazine A**
Octahydro-6-hydroxy-6,8a-dimethyl-3-methylene-4H-bis-oxireno[1,8a:2,3]-azuleno[4,5-b]furan-2(3H)-one	**Artecanin**
4,5,6,7,16,16a,19a,22-Octahydro-4-hydroxy-5,16a,21-trimethyl-spiro[16,18-methano-1H,3H,23H-[1,6,12]trioxacyclooctadecino-[3,4-d]-[1]benzopyran-17(18H),2'-oxirane]-3,9,14-trione	**Verrucarin A**
Oosporein	
Patulin	
Peimine	
Peiminine	
Pelargidenon	**Apigenin**
Penicidin	**Patulin**
Penicillic acid	
(Z,Z)-5-n-(8,11-Pentadecadienyl)-1,3-benzenediol	**Cardol, Diene**
(Z,Z)-3-n-(8,11-Pentadecadienyl)-phenol	**Cardanol, Diene**
Pentadecadienylresorcinol	**Cardol, Diene**
(Z,Z)-5-n-(8,11,14-Pentadecatrienyl)-1,3-benzenediol	**Cardol, Triene**
(Z,Z)-3-n-(8,11,14-Pentadecatrienyl)-phenol	**Cardanol, Triene**
Pentadecatrienylresorcinol	**Cardol, Triene**
(Z)-5-n-(8-Pentadecenyl)-1,3-benzenediol	**Cardol, Monoene**
(Z)-3-n-(8-Pentadecenyl)-phenol	**Cardanol, Monoene**
Pentadecenylresorcinol	**Cardol, Monoene**
5-n-Pentadecyl-1-3-benzenediol	**Cardol, saturated**
3-n-Pentadecylphenol	**Cardanol, saturated**
Pentadecylresorcinol	**Cardol, saturated**

Synonyms and Systematic Names	Common Names
Renardine	**Senkirkine**
6-C-α-L-Rhamnopyranosyl-apigenin-7-O-β-gluco-pyranoside	**Isofurcatain-7-O-β-D-glucoside**
Saponarin	
Secologanin	
Senkirkine	
Sphagnum acid	
Squarrogenin 1	
Squarrogenin 2	
Terecamphene	**(-)-Camphene**
3a,8a,9,9a-Tetrahydro-5,8a-dimethyl-3-methylene-naphtho-[2,3-b]-furan-2,6(3H,4H)-dione	**Yomogin**
3,3′,6,6′-Tetrahydroxy-5,5′-dimethyl-2,2′-bi-p-benzoquinone	**Oosporein**
Tricetin-6-C-α-L-arabinopyranoside-8-C-β-D-gluco-pyranoside	**Tricetin 6-C-arabinoside-8-C-glucoside**
Tricetin 6-C-arabinoside-8-C-glucoside	
Tricetin 6,8-di-C-β-D-glucopyranoside	**Tricetin 6,8-di-C-glucoside**
Tricetin 6,8-di-C-glucoside	
Tricin 6,8-di-C-α-L-arabinopyranoside	**Tricin 6,8-di-C-arabinoside**
Tricin 6,8-di-C-arabinoside	
(+)-(5*R*,10*S*)-11,12,14-Trihydroxy-8,11,13-abietatriene-3,7-dione	**Candelabrone**
4′,5,7-Trihydroxyflavone	**Apigenin**
21(R),22(S),23(R),3β,22β,30-Trihydroxy-21-methoxy-21,23-epoxycycloart-24-ene	**Squarrogenin 1**
21(S),22(S),23(R),3β,22β,30-Trihydroxy-21-methoxy-21,23-epoxycycloart-24-ene	**Squarrogenin 2**
3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol	**trans-Nerolidol**
1αH,5αH-Tropan-3α-ol(-)-tropate	**L-Hyoscyamine**
3α-Tropanyl-S-(-)-tropate	**L-Hyoscyamine**
Verrucarin A	
Verrucarin B	
Versulin	**Apigenin**
Verticine	**Peimine**
Xylostosidine	
Yomogin	

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General Abbreviations

[α]	specific optical rotation: $[\alpha]_D^{24}$ at 24 °C for D (sodium) line Example: $[\alpha]_D^{20}$ + 220° (c = 1, MeOH), meaning 220 g of the substance dissolved in 100 ml methanol; when no solvent is given, the solvent is water.
AcOH	acetic acid
ADR	International regulations governing the transport of dangerous goods
alc	alcohol, ethanol
Ar	aryl
bp	boiling point (the pressure, if different from one atm, is indicated in brackets)
BRN	Beilstein registry number
c	concentration by volume (after optical rotations only)
CA	Chemical Abstracts
CAS	Chemical Abstracts Service
conc.	concentration
cor, corr.	corrected
d	density; specific gravity (d_4^{20} specific gravity at 20° referred to water at 4°)
dec, decomp.	decomposition
DMSO	dimethyl sulfoxide
e.g.	*exempli gratia*, example given, for example
EtOH	ethanol
GGVE/GGVS	Gefahrgutverordnung Eisenbahn/Straße (german regulations governing the transport of dangerous goods)
GLC	gas-liquid chromatography
HPLC	high performance (pressure, power) liquid chromatography
I	intensity
i.v.	intravenous
ID	Inhibition dose
INN	International Nonproprietary Name
IR	Infrared spectrometry
IUPAC	International Union of Pure and Applied Chemistry
J	coupling constant
k′	retention time
kg	kilogram
LD	Lethal Dose; LD_{50}, a dose which is lethal to 50% of the animals tested
M^+	molecular ion
m/e	mass to charge ratio
max	maximum
MeOH	methanol
min	minute(s)
mp	melting point
MS	Mass spectrometry
m/z	mass to charge ratio
n	index of refraction (n_D^{20} for 20° and sodium light)
NMR	nuclear magnetic resonance
no.	number
ORD	optical rotatory dispersion
PDM	Perdeuteromethylether
PM	Permethylether
ppm	parts per million
R	Nature of special risks attributed to dangerous substances
ref.	refer, reference
Rf	in paper chromatography ratio of movement of the band to the front of the solvent
RID	international regulations governing the transport of dangerous goods
RTECS	Registry of Toxic Effects of Chemical Substances
S	Safety advice concerning dangerous substances
s, sec	seconds

spp.	species (plural)
temp.	temperature
TLC	thin-layer chromatography
TMS	tetramethylsilane
UN	United Nations number, numbers assigned to many substances by a United Nations committee used for transport purposes
uncorr.	uncorrected
UV	ultraviolet spectrometry
v/v	% "volume in volume" expresses the number of milliliters of an active constituent in 100 milliliters of solution
ε	molar extinction coefficient (conc. in g-moles/l)
≈	approximately
*	There is no illustration for this spectrum

Hazard Labeling

C	corrosive
E	explosive
F	highly flammable
F+	extremely flammable
N	Dangerous for the environment
O	oxidizing
T	toxic
T+	very toxic
Xi	irritant
Xn	harmful

Abbreviations in IR and NMR Spectroscopy

vs	very strong
w	weak
m	medium
s	strong
vw	very weak
sh	shoulder
br	broad
s	singlet
d	doublet
dd	doublet of doublets
t	triplet
q, qu	quartet
quint	quintet
sext	sextet
sept	septet
m, mult	multiplet

Superscripts in the Data Form indicate the References at the end of each form.

CAS-Registry Numbers

78-70-6	**Linalool (racemic)**
79-92-5	**Camphene**
90-65-3	**Penicillic acid**
101-31-5	**L-Hyoscyamine**
126-90-9	**S-(+)-Linalool**
126-91-0	**R-(-)-Linalool**
149-29-1	**Patulin**
470-17-7	**Isoalantolactone**
475-54-7	**Oosporein**
478-08-0	**Lucidin**
479-61-8	**Chlorophyll a**
480-33-1	**R-Mellein**
483-54-5	**Aurantiogliocladin**
501-26-8	**Cardanol, Monoene**
501-24-6	**Cardanol, saturated**
519-62-0	**Chlorophyll b**
520-36-5	**Apigenin**
528-43-8	**Magnolol**
529-05-5	**Chamazulene**
546-43-0	**Alantolactone**
578-74-5	**Apigenin-7-glucoside**
604-80-8	**Narcissin**
667-92-5	**Mollisin**
1119-38-6	**S-(+)-trans-Nerolidol**
1200-93-7	**(±)-Mellein**
2290-11-1	**Verrucarin B**
2318-18-5	**Senkirkine**
3148-09-2	**Verrucarin A**
3158-56-3	**Cardol, saturated**
5794-03-6	**(+)-Camphene**
5794-04-7	**(-)-Camphene**
5989-27-5	**(+)-Limonene**
5989-54-8	**(-)-Limonene**
7705-14-8	**(±)-Limonene**
7734-92-1	**R-Methylmellein**
10067-18-2	**Yomogin**
17397-85-2	**Mellein**
17946-87-1	**Deacetoxymatricarin**
18059-10-4	**Peiminine**
18309-73-4	**Fabiatrin**
18524-94-2	**Loganin**
19314-92-2	**(-)-3,4-Dihydro-6,8-dihydroxy-3-methylisocoumarin**

19351-63-4 **Secologanin**
20310-89-8 **Saponarin**
22910-86-7 **Cardol, Monoene**

23089-26-1 **(-)-α-Bisabolol**
23496-41-5 **Peimine**
25406-67-1 **Kingiside**

29041-35-8 **Matricine**
29428-58-8 **Lucenin-2**
35354-74-6 **Honokiol**

40716-66-3 **trans-Nerolidol (racemic)**
51546-63-5 **Cardanol, Diene**
53766-42-0 **9,12,15-Octadecatrien-6-ynoic acid** (Z,Z,Z-isomer)

56795-52-9 **9,12-Octadecadien-6-ynoic acid** (Z,Z-isomer)
57100-28-4 **Sphagnum acid**
59870-72-3 **Dehydrocorybulbine**

59905-46-3 **Artecanin**
62256-05-7 **Epicorazine A**
62332-73-4 **Isosclerone**

62623-84-1 **S-Mellein**
64356-85-0 **Mycorrhizin A**
71953-77-0 **Leiocarposide**

74518-57-3 **Xylostosidine**
76491-13-9 **Apometzgerin 6,8-di-C-arabinoside**
76491-11-7 **Tricetin 6,8-di-C-glucoside**

77551-75-8 **R-(-)-trans-Nerolidol**
78119-20-7 **Loxylostosidine A**
79353-39-2 **Cardanol, Triene**

79473-25-9 **Cardol, Diene**
79473-24-8 **Cardol, Triene**
89886-37-3 **Apometzgerin 6,8-di-C-arabinoside**

86022-78-8 **Tricetin 6-C-arabinoside-8-C-glucoside**
89886-36-2 **Tricin 6,8-di-C-arabinoside**
83463-97-2 **Isofurcatain-7-O-β-D-glucoside**

104056-04-4 **5′,3‴-Dihydroxyrobustaflavone**
106577-42-8 **II-2,3-Dihydroamentoflavone**
111200-22-7 **Bryoflavone**

111200-23-8 **Heterobryoflavone**
113545-42-9 **Candelabrone**
114865-39-3 **5′-Hydroxyamentoflavone**

115374-25-9 **9-Octadecen-6-ynoic acid** (Z-isomer)
122475-58-5 **2,3-Dihydro-5′-hydroxyamentoflavone** (S-isomer)
122475-59-6 **2,3-Dihydro-5′,3‴-dihydroxyamentoflavone** (S-isomer)

123564-56-7 **Hydroxybutenolide**
125445-28-5 **Squarrogenin 1**
125445-29-6 **Squarrogenin 2**

Part I
Data Sheets

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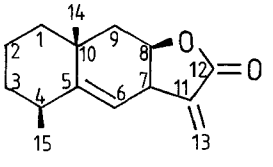
Alantolactone

H. Häberlein

1. Name of Compound

Common name **Alantolactone**		
Synonyms Helenin [1]		
Systematic name 4αH-Eudesma-5,11(13)-dien-12-oic acid,8β-hydroxy-,γ-lactone		
Substance Terpene	Subgroup Sesquiterpene lactone	
CAS registry number and other numbers [546-43-0]	Merck Index *11*, 198	BRN 13423

2. Formulas and Molecular Weight

Molecular formular $C_{15}H_{20}O_2$ Molecular weight 232.33	Structural formula 

3. Physical and Chemical Properties

State of matter crystalline solid	d_4^{20} not applicable	Iodine value not available
Melting Point mp 79 °C [2]	n_D^{20} not applicable	Acid value not applicable
Boiling point bp 275 °C [2]	$[\alpha]_D^{20}$: 220.0° (c = 1,MeOH) [3]	Saponification value not applicable
Flash point not applicable	Soluble in chloroform, dichloromethane, methanol, diethyl ether, acetone	
Color white	Odor indifferent	

4. Occurrence

Main constituent from Inula species [4]

5. Health Hazard Data

Toxicology Irritating substance In vitro cytotoxicity on human lung Carcinoma Cell Line	Hazard labeling Xn Harmful by inhalation, in contact with skin and if swallowed. May cause sensitization.
	ID_{50}: 4.6 µg/ml [5] (ID = inhibition dose)
Waste disposal procedures Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.	

6. Transportation and Storage Instructions

Storage temperature: 0–5 °C

7. Spectroscopic Data

MS			
Base peak	m/e 217	Molecular ion	m/e 232.32545
Ionization energy	70 eV	Ion source temp.	120 °C
Acceleration voltage	4000 V	Emission current	0.2 mA
Resolution	1000	Scan rate	2.6 s/decade
Spectrometer type and manufacturer		Vacuum Generators Micromass 7070 H	

IR			
Characteristic peaks 2960, 2940, 2900, 2830, 1725, 1640, 1450, 1380, 1250, 1240, 1155, 1120, 1050, 1030, 975, 920, 855, 850, 810 cm^{-1}			
Sample preparation	KBr	Resolution	–
Spectrometer type and manufacturer		IR Spectrometer 398, Perkin Elmer	

NMR		Nucleus	^1H
Chemical Shifts			
6.18 (d, 1H, *H*C-13); 5.60 (d, 1H, *H*C-13); 5.13 (d, 1H, *H*C-6); 4.80 (ddd, 1H, H_αC-8);	3.56 (m, 1H, H_αC-7); 2.43 (m, 1H, H_αC-4); 2.09 (dd, 1H, H_αC-9); 1.53 (dd, 1H, H_βC-9	1.17 (s, 3H, $H_{3\beta}$C-14) 1.07 (d, 3H, $H_{3\beta}$C-15) ppm	
Frequency	400 MHz	Solvent	$CDCl_3$
Standard	TMS	Sample temp.	23 °C
Spectrometer type and manufacturer		Bruker WH 400	

NMR *	^{1}H-decoupled	Nucleus	^{13}C
Chemical Shifts			
170.2 (s, C-12);	149.0 (s, C-5);	139.9 (s, C-11);	121.3 (t, C-13);
119.8 (d, C-6);	76.3 (d, C-8);	42.7 (t, C-9);	41.7 (t, C-3);
39.5 (d, C-7);	37.5 (d, C-4);	32.7 (t, C-1);	32.7 (s, C-10);
28.5 (qu, C-14);	22.5 (qu, C-15);	16.7 (t, C-2) ppm	
Frequency	100 MHz	Solvent	$CDCl_3$
Standard	TMS	Sample temp.	23 °C
Spectrometer type and manufacturer		Bruker WH 400	

UV	not applicable

8. Chromatographic Data

TLC			
Rf Value	0.30		
Solvent	acetone	Solvent system	toluene/ethyl acetate (97:3)
Saturated atmosphere	yes	Detection/Color	5% solution of $AlCl_3$ in ethanol, 10 min at 120 °C, brown under UV (366 nm)
Plate manufacturer	Riedel de Haën	Plate type/Product no.	DC-Mikrokarten Si F_{254nm} Art. 37341

GLC	For application of GLC for the separation of sesquiterpene lactones see ref. [6] and [7].

HPLC	see ref. [3]		
Retention time	k' = 6.33		
Column	4.0 mm × 250 mm	Stationary phase	silica gel (5 m)
Mobile phase	n-pentane/diethyl ether (90:10)	Flow rate	1 ml/min
Column temp.	room temperature	Pressure	150 bar
Detector	UV 210 nm	Sample solvent	n-pentane/diethyl ether (90:10)
Sample size	10 µl	Sample conc.	8.62×10^{-4} mol/l
Chromatograph type and manufacturer	Pump L-6200, UV-Detector 655A-23 Chromato-Integrator D-2500, Merck-Hitachi		

9. Remarks

Used in the chemotaxonomy of higher plants and in several methods of chromatography as reference substance.

10. References

[1] Karrer, W., *Konstitution und Vorkommen der organischen Pflanzenstoffe*, Birkhäuser Verlag, Basel 1958, No. 1900

[2] Glasby, J.S., *Encyclopaedia of the Terpenoids*, John Whiley & Sons (1982) pp. 124

[3] Häberlein, H., unpublished data

[4] Bohlmann, F., Mahanta, P.K., Jakupovic, J., Rastogi, R.C., Natu, A., *Phytochemistry 17* (1978) 1165-1172

[5] Woerdenbag, H.J., Meijer, C., Mulder, N.H., de Vries, E.G.E., Hendriks, H., Malingre, Th.M., *Planta Med. 2* (1986) 112-114

[6] Zinchenko, V.V., Khvorost, P.P., Bakai, S.I., Biryuk, V.A., Tarusin, A.D., Kravchina, T.S., *Rastit Resur. 19(4)*, (1983) 544-548

[7] Rosik, G.G., Zinchenko, V.V., Reznichenko, A.A., Koralev, I.P., *Khim.-Farm Zh. 21(5)*, (1987) 632-634

Additional analytical data are found in:

[8] Schmalle, H.W., *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* C42(6), (1986) 705-708 *(x-ray crystallography)*