

Dictionary of Natural Products

FIRST SUPPLEMENT

VOLUME 6 OF DICTIONARY OF NATURAL PRODUCTS

0054225

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CHAPMAN & HALL

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Dictionary of Natural Products

FIRST SUPPLEMENT

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First Supplement

1. Introduction

For detailed information about how to use the *Dictionary of Natural Products* (DNP) see the Introduction in Volume 1 of the Main Work.

1. Using DNP Supplements

As in the Main Work volumes, every Entry is numbered to assist ready location. The DNP Number consists of a letter of the alphabet followed by a five-digit number. In this First Supplement the first digit is invariably 1. Cross-references within the text to Entries having numbers beginning with zero refer to Main Work Entries.

Where a Supplement Entry contains additional or corrected information referring to an Entry in the Main Work the whole Entry is reprinted, with the accompanying statement "Updated Entry replacing ...". In such cases, the new Entry contains all of the information which appeared in the former Entry,

except for any which has been deliberately deleted. Therefore there is no necessity for the user to consult the Main Work or previous supplements.

2. Literature coverage

In compiling this Supplement the primary literature has been surveyed to the end of 1993. The printed supplement concentrates principally on important new natural products isolated during the period in question. A considerable number of amendments have been made during the review period to entries which have not been reprinted in the Supplement owing to space limitations. All of these can be accessed via the CD-ROM version.

3. Indexes

The indexes in the Supplement consist of Name, Molecular Formula and CAS Registry Number Index.

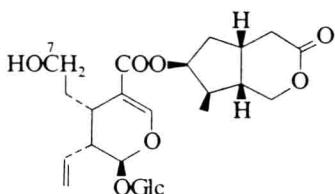
Contents

First Supplement Entries	<i>page 1</i>
Name Index	515
Molecular Formula Index	557
Chemical Abstracts Service Registry Number Index	609

A

Abelioside B

Updated Entry replacing A-00009
[99891-73-3]



$C_{25}H_{36}O_{12}$ M 528.552

Constit. of *Abelia grandiflora*.

Penta-Ac: Cryst. (EtOH). Mp 211-213°. $[\alpha]_D^{22} - 38^\circ$ (c, 0.5 in $CHCl_3$).

7-Aldehyde: [99891-69-7]. **Abelioside A. Laciniatoside II**

$C_{25}H_{34}O_{12}$ M 526.536

From *A. grandiflora* and *Dipsacus laciniatus*. Powder. $[\alpha]_D^{22} - 38^\circ$ (c, 1.3 in MeOH), $[\alpha]_D^{25} - 57^\circ$ (c, 0.98 in MeOH). Abelioside and Laciniatoside II assigned identical structs., not compared.

7-Aldehyde, Tetra-Ac: Cryst. (EtOH). Mp 170-172°. $[\alpha]_D^{22} - 41^\circ$ (c, 0.5 in $CHCl_3$).

Murai, F. et al, *Phytochemistry*, 1985, **24**, 2329.

Kocsis, A. et al, *J. Nat. Prod. (Lloydia)*, 1993, **56**, 1486 (*Laciniatoside II*)

24(23→22)-Abeo-16,23:18,20-diepoxycholesta-5,24-diene-3,18,23-triol

A-10001

$C_{20}H_{28}O_7$ M 380.437

($2\alpha,4\alpha,5\beta,7\beta,10\beta,13\alpha$)-form

2-Benzoyl, 4-Ac: [150621-50-4].

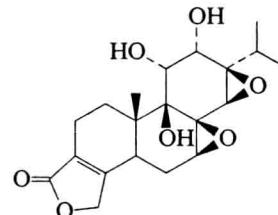
$C_{29}H_{34}O_9$ M 526.582

Constit. of *Taxus wallichiana*. Oil. $[\alpha]_D^{25} - 26^\circ$ (c, 1 in CH_2Cl_2).

Appendino, G. et al, *J. Chem. Soc., Perkin Trans. I*, 1993, 1563 (isol, pmr, cmr)

18(4→3)-Abeo-7,8:13,14-diepoxy-9,11,13-trihydroxy-4-abieten-18,19-olide

A-10004



$C_{20}H_{26}O_7$ M 378.421

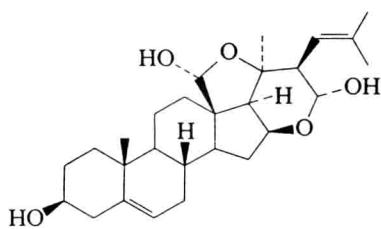
($7\beta,8\beta,9\beta,11\alpha,12\alpha,13\beta,14\beta$)-form [147809-20-9] **13,14-Epoxy-9,11,12-trihydroxytriptolide**

Constit. of *Tripterygium wilfordii*. Cryst. (Me_2CO). Mp 268-270°.

Zhang, C.P. et al, *Acta Pharm. Sin.*, 1993, **28**, 110 (isol, pmr, cmr)

24(23→22)-Abeo-16,23:18,20-diepoxycholesta-5,24-diene-3,18,23-triol

A-10002



$C_{28}H_{42}O_5$ M 458.637

($3\beta,16\beta,18R,20R,22R,23R$)-form

18-Me ether 3-O-[$\alpha-L$ -rhamnopyranosyl-(1→2)- $\beta-D$ -glucopyranosyl-(1→2)- $\beta-D$ -glucopyranoside]: [151392-07-3].

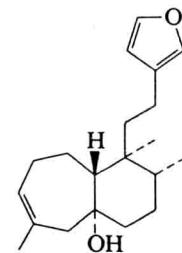
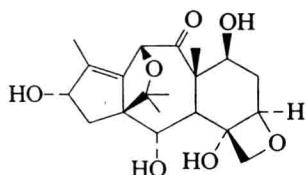
$C_{46}H_{72}O_{19}$ M 929.063

Constit. of *Ornithogalum saundersiae*. Amorph. powder. $[\alpha]_D - 78^\circ$ (MeOH).

Kuroda, M. et al, *Tetrahedron Lett.*, 1993, **34**, 6073 (isol, pmr, cmr)

11(15→1)-Abeo-5,20:10,5-diepoxy-2,4,7,13-tetrahydroxy-11-taxen-9-one

A-10003


5(4→19)-Abeo-15,16-epoxy-3,13(16),14-clerodatrien-5-ol

A-10006

$C_{20}H_{24}O_4$ M 328.407

Constit. of *Tripterygium wilfordii*. Cryst. Mp 179-182°. $[\alpha]_D + 296^\circ$ (c, 0.14 in $CHCl_3$).

Takaishi, Y. et al, *Tetrahedron Lett.*, 1992, **33**, 7177 (isol, pmr, cmr, cryst struct)

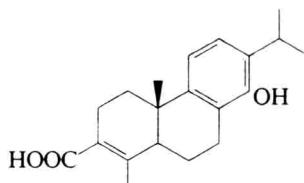
$C_{20}H_{30}O_2$ M 302.456
(ent-5β)-form

5,10-Dihydro-5α-hydroxy-10βH-printziane
Constit. of *Croton cortesianus*.

Kastner, U. et al. *Phytochemistry*, 1992, **31**, 4361 (isol, pmr, cmr)

18(4→3)-Abeo-14-hydroxy-3,8,11,13-abietatetraen-18-oic acid

A-10007



$C_{20}H_{26}O_3$ M 314.424

Me ether: 18(4→3)-Abeo-14-methoxy-3,8,11,13-abietatetraen-18-oic acid. *Triptoditerpenic acid B*

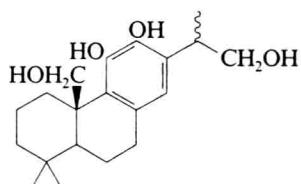
$C_{21}H_{28}O_3$ M 328.450
Constit. of *Tripterygium hypoglauicum*. Cryst. Mp 209–211°.

Zhang, L. et al. *Acta Pharm. Sin.*, 1993, **28**, 32 (isol, pmr, cmr)

8,11,13-Abietatriene-11,12,16,20-tetrol

A-10008

[150065-59-1]



$C_{20}H_{30}O_4$ M 334.455

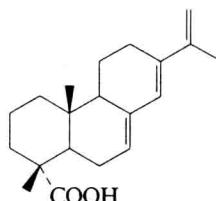
Constit. of *Salvia mellifera*. Amorph. solid.

Luis, J.G. et al. *Phytochemistry*, 1993, **33**, 635 (isol, pmr, cmr)

7,13,15-Abietatrien-18-oic acid

A-10009

[83905-82-2]



$C_{20}H_{28}O_2$ M 300.440

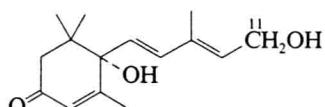
Constit. of *Pinus massonia*.

Cheung, H.T.A. et al. *Tetrahedron*, 1993, **49**, 7903 (isol, pmr, cmr)

Abscisic alcohol

A-10010

[113472-20-1]



$C_{15}H_{22}O_3$ M 250.337

Constit. of quince (*Cydonia oblonga*) fruit.

11-O-β-D-Glucopyranoside: [145153-00-0].

$C_{21}H_{32}O_8$ M 412.479
Constit. of quince (*C. oblonga*) fruit.

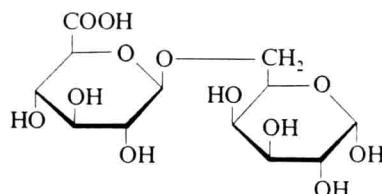
Lutz, A. et al. *J. Agric. Food Chem.*, 1992, **40**, 116 (isol, pmr, cmr)
Lutz, A. et al. *Phytochemistry*, 1993, **32**, 57 (isol, pmr, cmr, cd)

Acaciabiuronic acid

A-10011

Updated Entry replacing A-00104

6-O-β-D-Glucopyranuronosyl-D-galactose, 9CI, 8CI
[7264-19-9]



α-Pyranose-form

$C_{12}H_{20}O_{12}$ M 356.283

Probably the commonest aldobiouronic acid present as a structural unit in plant gums. Isol. from partial acid hydrolysates from the following plants; black wattle (*Acacia mollissima*), *A. senegal*, *A. pycnantha*, *A. karroo*, *A. cyanophylla*, egg plum (*Prunus domestica*), almond (*P. amygdalus*), peach (*P. persica*), *Anogeissus lattifolia* (gum ghatti), *Vigilia oroboides*, *Afraege pariculata*, *Ferula* and *Chorisia* spp. Also isol. from hydrolysates of maritime pine (*Pinus pinaster*) hemicellulose and wheat straw. Mp 118–119° (hydrate). $[\alpha]_D + 11.6^\circ \rightarrow -8.6^\circ$ (H₂O).

Ca salt: $[\alpha]_D + 2^\circ$ (H₂O).

Ba salt: $[\alpha]_D - 3^\circ$ to $+2^\circ$ (H₂O).

Me ester:

$C_{13}H_{22}O_{12}$ M 370.310
Mp 119°. $[\alpha]_D - 9^\circ$ (H₂O).

Hepta-Ac, Me ester:

$C_{27}H_{36}O_{19}$ M 664.570
Mp 202–203°. $[\alpha]_D - 17.5^\circ$ (CHCl₃).

z-Pyranose-form [52554-59-3]

$[\alpha]_D + 2^\circ$ (in H₂O).

1,2:3,4-Di-O-isopropylidene, 2',3',4'-tri-Ac, Me ester:
[35906-41-3].

$C_{25}H_{36}O_{15}$ M 576.550
Mp 114–115°. $[\alpha]_D - 65^\circ$ (c, 4.5 in CHCl₃).

Me glycoside, hexa-Me, Me ester:

$C_{29}H_{36}O_{12}$ M 468.497
 $[\alpha]_D + 42^\circ$ (CHCl₃).

β-Pyranose-form [52554-60-6]

Me glycoside, hexa-Me, Me ester: [22854-45-1].
Mp 86–90°. $[\alpha]_D - 35^\circ$ (CHCl₃).

Me glycoside, hexa-Ac, Me ester:

$C_{26}H_{36}O_{18}$ M 636.560
Mp 140°. $[\alpha]_D - 54^\circ$ (CHCl₃).

[1693-80-7]

Hotchkiss, R.D. et al. *J. Biol. Chem.*, 1936, **115**, 285 (deriv)
Goebel, W.F. et al. *J. Biol. Chem.*, 1938, **124**, 207 (isol)

Jackson, J. et al. *J. Chem. Soc.*, 1940, 74 (α Me gly)

Aspinall, G.O. et al. *J. Chem. Soc.*, 1955, 1160; 1961, 3461 (isol)

Mukherjee, S. et al. *J. Am. Chem. Soc.*, 1958, **80**, 2536 (isol)

Jones, J.K.N. et al. *Can. J. Chem.*, 1961, **39**, 162 (isol)

Bailey, R.W., *Oligosaccharides*, Pergamon Press, London, 1965, 4, 134 (occur)

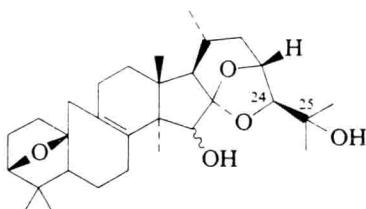
Dee, K.K. et al. *Carbohydr. Res.*, 1967, **4**, 177.

Peciar, C. et al. *Chem. Zvesti*, 1974, **28**, 83 (config, pmr)

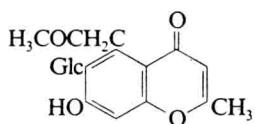
DiFabio, J.L. et al. *Carbohydr. Res.*, 1982, **99**, 41 (isol)

Acerinol

[19902-53-5]

 $C_{30}H_{46}O_5$ M 486.690Constit. of *Cimicifuga acerina*.25-Ac: [59665-60-0]. **25-Acetylacerinol** $C_{32}H_{48}O_6$ M 528.728Constit. of *C. acerina*.25-Me ether: [59665-58-6]. **25-Methylacerinol** $C_{31}H_{48}O_5$ M 500.717Constit. of *C. acerina*.24-Epimer: [151061-95-9]. **24-Epiacerinol** $C_{30}H_{46}O_5$ M 486.690Constit. of *C. heracleifolia*. Needles. Mp 230-231°. $[\alpha]_D +59.23^\circ$ (c, 0.27 in CHCl_3).Takemoto, T. et al. *CA*, 1969, **69**, 30278k (*isol*)Kusano, G. et al. *CA*, 1976, **85**, 5907r (*struct*)Li, J.X. et al. *Chem. Pharm. Bull.*, 1993, **41**, 832 (24-Epiacerinol)**5-Acetonyl-6-glucosyl-7-hydroxy-2-methyl-4H-1-benzopyran-4-one** A-10013

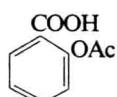
[84375-47-3]

 $C_{19}H_{22}O_9$ M 394.377Isol. from *Cassia multijuga* and *C. spectabilis*. Cryst. (EtOAc/pet. ether). Mp 190° dec.2"-O- β -D-Glucopyranoside: [94443-29-5]. $C_{25}H_{32}O_{14}$ M 556.519Isol. from the seeds of *C. spectabilis*. Mp 290°.Singh, J., *Phytochemistry*, 1982, **21**, 1177 (*isol*)Singh, M. et al. *Z. Naturforsch.*, B, 1984, **39**, 1425 (*isol, deriv*)**2-Acetoxybenzoic acid**

A-10014

2-Acetoxybenzoic acid, 9CI. *Salicylic acid acetate*, 8CI.Acetylsalicylic acid. *Aspirin, USAN*

[50-78-2]

 $C_9H_8O_4$ M 180.160Constit. of *Glycyrrhiza glabra* var. *typica* roots. Produced industrially by acetylation of 2-Hydroxybenzoic acid, H-01254. Analgesic, antipyretic and antiinflammatory agent. Used as soln. in 10% ammonia for photometric detn. of Mn (λ_{max} 385 nm; in the presence of H_2O_2). Cryst. Mp 135° (rapid heat), Fp 118°. pK_a 3.38 (25°, 1.0M KCl). Ca salt used in combination with urea as Carbaspirin calcium, USAN.

► Mod. toxic. Exp. teratogen. VO0700000.

Me ester: [580-02-9].

 $C_{10}H_{10}O_4$ M 194.187**A-10012**

Cryst. (pet. ether). Mp 49°.

Et ester: [529-68-0].

 $C_{11}H_{12}O_4$ M 208.213

Liq. Bp 289°. Bp 272°.

Propyl ester: [60310-03-4].

 $C_{12}H_{14}O_4$ M 222.240Light yellow liq. Bp 289°, Bp_{10} 162-164°.

Butyl ester: [52602-16-1].

 $C_{13}H_{16}O_4$ M 236.267

Liq. Bp 128-130°.

Ph ester: [134-55-4]. *Acetylsalol. Phennin. Spiroform. Vesipyrin* $C_{15}H_{12}O_4$ M 256.257Analgesic, antipyretic, and antibacterial agent. Cryst. (EtOH). Mp 97°. Bp_{11} 197-198°. [5749-67-7]Aldrich Library of Infrared Spectra, 3rd edn., **1**, 315D (*ir*)Ciusa, R. et al. *Chem. Zentralbl.*, 1943, **2**, 615 (*synth*)Henriques, H.P. et al. *Mikrochim. Acta*, 1971, 807 (*detn, Mn*)Scott, K., *J. Magn. Reson.*, 1972, **6**, 55 (*nmr*)Ali, S.L., *Pharm. Ztg.*, 1976, **121**, 621 (*esters, synth, ir, pmr*)Florey, K., *Anal. Profiles Drug Subst.*, 1979, **8**, 1 (*rev*)Mitscher, L.A. et al. *J. Nat. Prod. (Lloydia)*, 1980, **43**, 259 (*occur*)Barnett, H.J.M. et al. *Acetylsalicylic Acid*, Raven Press, N.Y., 1982 (*book*)Martindale, *The Extra Pharmacopoeia*, 28th/29th Ed.,

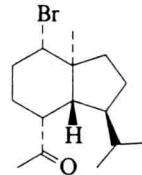
Pharmaceutical Press, London, 1982/1989, 2601.

Rainsford, K.D., *Aspirin and the Salicylates*, Butterworths, London, 1984 (*book*)Collier, H.O.J. et al. *Discoveries Pharmacol.*, 1984, **2**, 555 (*rev, pharmacol*)Hallam, J. et al. *Int. Congr. Symp. Ser. R. Soc. Med.*, 1984 (*rev*)Kim, Y. et al. *Chem. Pharm. Bull.*, 1985, **33**, 2641 (*cryst struct*)Chang, C.J. et al. *Magn. Reson. Chem.*, 1986, **24**, 768 (*cmr*)Pelz, J., *Pharmazie*, 1986, **41**, 733 (*history*)Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th Ed., Akademie-Verlag, Berlin, 1987, 1120 (*synonyms*)Bundgaard, H. et al. *J. Med. Chem.*, 1989, **32**, 727 (*esters, synth, props*)Vane, J.R. et al. *Aspirin and the Salicylates*, Ed., Chapman and Hall, 1992 (*book*)Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th Ed., Van Nostrand-Reinhold, 1992, ADA725.**7-Acetyl-4-bromo-1-isopropyl-3a-methylindane**

A-10015

1-(7-Bromo-7a-methyl-3-(1-methylethyl)octahydro-1H-inden-4-yl)ethanone

[149492-40-0]

 $C_{15}H_{25}BrO$ M 301.266Constit. of *Laurencia marianensis*. Cryst. Mp 49-53°. $[\alpha]_D -13.0^\circ$ (c, 0.1 in CHCl_3).de Nys, R. et al. *Aust. J. Chem.*, 1993, **46**, 933 (*isol, pmr, cmr*)

A-10014

2-Acetoxybenzoic acid, 9CI. *Salicylic acid acetate*, 8CI.Acetylsalicylic acid. *Aspirin, USAN*

[50-78-2]

 $C_9H_8O_4$ M 180.160Constit. of *Glycyrrhiza glabra* var. *typica* roots. Produced industrially by acetylation of 2-Hydroxybenzoic acid, H-01254. Analgesic, antipyretic and antiinflammatory agent. Used as soln. in 10% ammonia for photometric detn. of Mn (λ_{max} 385 nm; in the presence of H_2O_2). Cryst. Mp 135° (rapid heat), Fp 118°. pK_a 3.38 (25°, 1.0M KCl). Ca salt used in combination with urea as Carbaspirin calcium, USAN.

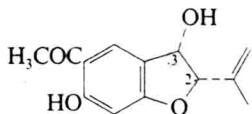
► Mod. toxic. Exp. teratogen. VO0700000.

Me ester: [580-02-9].

 $C_{10}H_{10}O_4$ M 194.187

5-Acetyl-2,3-dihydro-3,6-dihydroxy-2-isopropenylbenzofuran

1-[2,3-Dihydro-3,6-dihydroxy-2-(1-methylethenyl)-5-benzofuranyl]ethanone, 9Cl



$C_{13}H_{14}O_4$ M 248.235

(2S,3S)-form [143381-65-1]

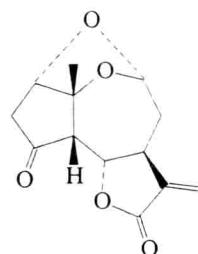
Constit. of *Senecio desfontainei*.

Hussein, N.S. et al. *Pharmazie*, 1992, **47**, 468 (*isol.*)

A-10016

Achilleppolide

A-10019



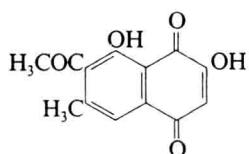
$C_{13}H_{14}O_5$ M 250.251

Constit. of *Achillea pseudoaleppica*. Oil. $[\alpha]_D^{25} + 2^\circ$ (c. 0.3 in MeOH).

Appendino, G. et al. *Phytochemistry*, 1993, **34**, 1171 (*isol., pmr, cmr*)

7-Acetyl-2,8-dihydroxy-6-methyl-1,4-naphthoquinone

[80597-54-2]



$C_{13}H_{10}O_5$ M 246.219

Yellow solid. Mp 206-209° dec.

2-Me ether: [64756-97-4]. 7-Acetyl-8-hydroxy-2-methoxy-6-methyl-1,4-naphthoquinone. *Orientalone*

$C_{14}H_{12}O_5$ M 260.246

Constit. of *Prunus cerasoides*, *Rumex nepalensis* and *R. orientalis*. Yellow-orange cryst. (C_6H_6 /petrol). Mp 191-192°.

8-Me ether: [95455-42-8]. 7-Acetyl-2-hydroxy-8-methoxy-6-methyl-1,4-naphthoquinone

$C_{14}H_{12}O_5$ M 260.246

Yellow solid. Mp 173-177° dec.

Di-Me ether: [80597-53-1]. 7-Acetyl-2,8-dimethoxy-6-methyl-1,4-naphthoquinone

$C_{15}H_{14}O_5$ M 274.273

Yellow solid. Mp 182-184°.

Sharma, M. et al. *Indian J. Chem., Sect. B*, 1977, **15**, 544; 1978, **16**, 289 (*Orientalone*)

Jung, M.E. et al. *Tetrahedron*, 1984, **40**, 4751 (*synth., pmr, cmr*)

Garg, M. et al. *Proc. Natl. Acad. Sci., India, Sect. A*, 1985, **55**, 95 (*Orientalone*)

A-10017

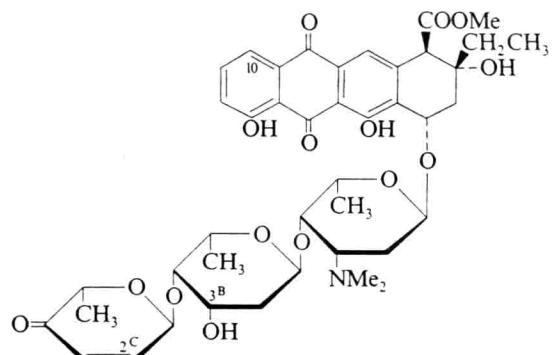
Aclacinomycin Y

A-10020

Updated Entry replacing A-00297

MA 144Y. Antibiotic MA 144Y

[66789-14-8]



$C_{42}H_{51}NO_{15}$ M 809.863

Anthracycline antibiotic. Isol. from *Streptomyces galilaeus*.

Antitumour antibiotic. Mp 153-155°. $[\alpha]_D^{22} + 66^\circ$ (c. 1 in CHCl₃).

► PI9279700.

10-Hydroxy: [88477-80-9]. *Pyrraculomycin*. 10-Hydroxyaclacinomycin Y. *Cinerubin Y†*

$C_{42}H_{51}NO_{16}$ M 825.862

Isol. from *S. sp. JA 6705*. Active against gram-positive bacteria and mycobacteria. Dark red cryst. (C_6H_6 /MeOH). Mp 160-167°.

10-Hydroxy, 3^B-deoxy: *Cinerubin R*

$C_{42}H_{51}NO_{15}$ M 809.863

Prod. by *Streptomyces eurythermus*. Active against gram-positive bacteria. Mp 158-162°.

10-Hydroxy, 2^C,3^C-dihydro: *Spartanamicin B*

$C_{42}H_{53}NO_{16}$ M 827.878

Prod. by a *Micromonospora* sp. Antifungal agent. Orange-red solid.

Yoshimoto, A. et al. *J. Antibiot.*, 1979, **32**, 472 (*isol.*)

Oki, T. et al. *J. Antibiot.*, 1979, **32**, 791, 801 (*isol., uv, ir, pmr, cmr*)

Hoshino, T. et al. *J. Antibiot.*, 1983, **36**, 1458 (*synth*)

Tresselt, D. et al. *Z. Chem.*, 1987, **27**, 444 (*deriv*)

Nakata, M. et al. *J. Antibiot.*, 1992, **45**, 1599 (*Cinerubin R*)

Nair, M.G. et al. *J. Antibiot.*, 1992, **45**, 1738 (*Spartanamicin B*)

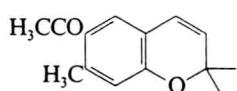
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th Ed., Van Nostrand-Reinhold, 1992, ADG425.

6-Acetyl-2,2,7-trimethyl-2H-1-benzopyran

A-10018

1-(2,2,7-Trimethyl-2H-1-benzopyran-6-yl)ethanone, 9Cl. *Gleucolin*

[76470-14-9]



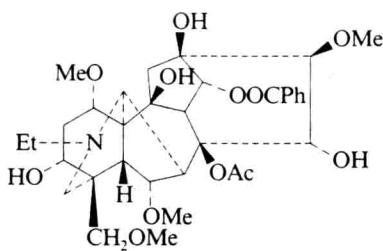
$C_{14}H_{16}O_2$ M 216.279

Constit. of the stems and leaves of *Eupatorium glechonophyllum*.

Becerra, J. et al. *Rev. Latinoam. Quim.*, 1980, **11**, 148 (*isol.*)

Aconifine

Updated Entry replacing A-00302
Nagarine[†]
[41849-35-8]



C₃₄H₄₇NO₁₂ M 661.745

Alkaloid from tubers of *Aconitum karakolicum* and roots of *A. nagarum* var. *lasiandrum* (Ranunculaceae). Mp 198–200°. [α]_D¹⁹ + 30.6° (c, 1.10 in CHCl₃).

B,HBr: Mp 209°.

Tetra-Ac: Mp 227°.

N-De-Et, N-Me: [76918-93-9]. *Beiwutine*

C₃₃H₄₅NO₁₂ M 647.718

Alkaloid from *A. kusnezoffii* (Ranunculaceae). Mp 196–198°.

N-De-Et, N-Me, O³-Ac: *3-O-Acetylbeiwutine*

C₃₅H₄₇NO₁₃ M 689.755

Alkaloid from roots of *A. liaotungense* (Ranunculaceae). Cryst. Mp 187°. [α]_D + 25.8° (c, 0.95 in EtOH).

Sultankhodzhaev, M.N. et al. *Khim. Prir. Soedin.*, 1973, **9**, 127; 1980, **16**, 665; *Chem. Nat. Compd. (Engl. Transl.)*, 129, 481 (Aconifine)

Wang, Y.-G. et al. *Yaoxue Xuebao*, 1980, **15**, 526; *CA*, **94**, 117772k (Beiwutine)

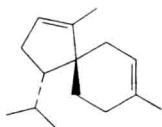
Wang, H. et al. *Huaxue Xuebao*, 1981, **39**, 869; *CA*, **97**, 107080f (Aconifine)

Zhu, Y. et al. *Heterocycles*, 1982, **17**, 607 (struct, rev)

Zhu, D.-Y. et al. *Phytochemistry*, 1993, **32**, 767 (3-O-Acetylbeiwutine)

3,9-Acoradiene

[55781-50-5]



C₁₅H₂₄ M 204.355

Constit. of Vetiver oil (*Vetivera zizanoides*). Oil.

[35944-18-4, 38229-83-3, 59573-57-8]

Demole, E. et al. *Helv. Chim. Acta*, 1971, **54**, 1845 (synth)

Kaiser, R. et al. *Tetrahedron Lett.*, 1972, 2009, 2013 (isol, struct)

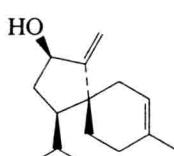
Zalkow, L.H. et al. *Tetrahedron Lett.*, 1975, 75 (abs config)

Chen, Y.-J. et al. *Tetrahedron*, 1993, **49**, 10263 (synth)

3,10(14)-Acoradien-9-ol

Rosaacorenol

[138867-22-8]



C₁₅H₂₄O M 220.354

A-10021

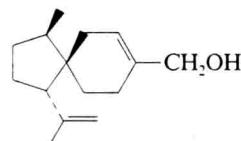
Constit. of *Rosa rugosa*. Syrup.

Hashidoko, Y. et al. *Phytochemistry*, 1991, **30**, 3729; 1993, **32**, 387 (isol, synth, pmr, cmr)

3,11-Acoradien-15-ol

β-Acoradienol

[149496-35-5]



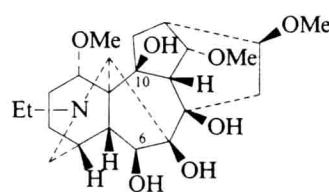
C₁₅H₂₄O M 220.354

Constit. of *Neocallitropsis pancheri*. Oil. [α]_D²⁵ + 3° (c, 0.37 in CHCl₃).

Raharivelomanana, P. et al. *Phytochemistry*, 1993, **33**, 235 (isol, pmr, cmr)

Acoseprine

[146028-66-2]

A-10025

C₂₃H₃₇NO₇ M 439.548

Alkaloid from roots of *Aconitum septentrionale* (Ranunculaceae). Cryst. (Me₂CO/hexane). Mp 105–107°. [α]_D + 19.6° (c, 0.245 in CHCl₃).

10-Deoxy: [144049-71-8]. *Acosepticine*

C₂₃H₃₇NO₆ M 423.548

Alkaloid from roots of *A. septentrionale* (Ranunculaceae). Amorph. solid. [α]_D + 23.4° (c, 0.385 in CHCl₃).

10-Deoxy, O⁶-Ac: [144074-85-1]. *6-O-Acetylacosepticine*

C₂₅H₃₉NO₇ M 465.586

Alkaloid from roots of *A. septentrionale* (Ranunculaceae). Cryst. (Et₂O). Mp 168.5–170.5°. [α]_D – 1.2° (c, 0.2 in CHCl₃).

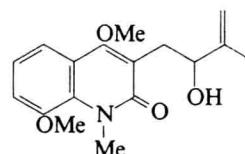
Sayed, H.M. et al. *J. Nat. Prod. (Lloydia)*, 1992, **55**, 1595 (isol, ir, pmr, cmr, ms, struct)

Ross, S.A. et al. *Tetrahedron*, 1992, **48**, 1183 (6-O-Acetylacosepticine)

Acutifolin

[145237-07-6]

A-10026



C₁₇H₂₁NO₄ M 303.357

Alkaloid from the leaves of *Zanthoxylum acutifolium* (Rutaceae). Viscous oil. [α]_D + 40° (c, 0.00025 in CHCl₃).

O-Hexadecanoyl: [145204-98-4]. *Acutifolin palmitate*

C₃₃H₅₁NO₅ M 541.770

Alkaloid from leaves of *Z. acutifolium* (Rutaceae). Viscous oil. [α]_D + 15° (c, 0.00066 in CHCl₃).

N-De-Me: [145237-08-7]. *Acutifolidin*

A-10023**A-10023****A-10026**

$C_{16}H_{19}NO_4$ M 289.330

Alkaloid from leaves of *Z. acutifolium* (Rutaceae).
Amorph. solid. Mp 121-123°. $[\alpha]_D + 18.6^\circ$ (c, 0.00053 in $CHCl_3$).

Me ether: [145204-97-3]. **O-Methylacutifolin**

 $C_{18}H_{23}NO_4$ M 317.384

Alkaloid from leaves of *Z. acutifolium* (Rutaceae).
Viscous oil. $[\alpha]_D - 6.4^\circ$ (c, 0.00156 in $CHCl_3$).

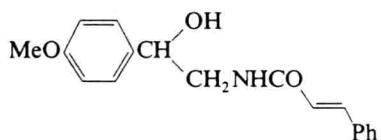
Arruda, M.S.P. et al, *Phytochemistry*, 1992, **31**, 3617 (*isol, uv, ir, pmr, cmr, ms, struct*)

Aegeline

A-10027

Updated Entry replacing A-00488

N-[2-Hydroxy-2-(4-methoxyphenyl)ethyl]-3-phenyl-2-propenamide, 9C1. **Egeline**, 8C1. N- β -Hydroxy- β -p-methoxyphenethylcinnamamide. N-Cinnamoyl-2-hydroxy-2-(4-methoxyphenyl)ethylamine. Cinnamic acid 2-hydroxy-2-(p-methoxyphenyl)ethylamide
[456-12-2]

 $C_{18}H_{19}NO_3$ M 297.353Originally assigned the formula $C_{18}H_{18}O_4$.**(+)-form** [15298-36-9]

Synthetic. Cryst. ($EtOH$). Mp 196-197°. $[\alpha]_D^{22} + 36.0^\circ$ (c, 0.4 in $CHCl_3$), $[\alpha]_D^{21} - 48.1^\circ$ (c, 0.5 in $EtOH$).

(-)-form [15298-37-0]

Synthetic. Cryst. ($EtOH$). Mp 196-197°. $[\alpha]_D - 35.1^\circ$ ($CHCl_3$), $[\alpha]_D + 47.5^\circ$ (c, 0.5 in $EtOH$).

(\pm)-form [37791-13-2]

Alkaloid from the leaves of *Aegle marmelos*, *Zanthoxylum coriaceum* and *Z. ocumarense* (Rutaceae). Cryst. ($EtOH/EtOAc$). Mp 176° (173-175°).

Ac: Plates ($EtOAc$). Mp 124°.*Dihydro*: Plates ($EtOH/EtOAc$). Mp 140°.*Me ether*: [70546-93-9]. N-[2-Methoxy-2-(4-methoxyphenyl)ethyl]cinnamide. *Aegle marmelos Alkaloid D* $C_{19}H_{21}NO_3$ M 311.380

Isol. from *A. marmelos*. Cryst. (C_6H_6 /hexane). Mp 135°. Artifact.

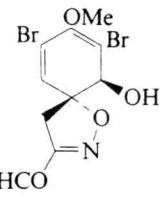
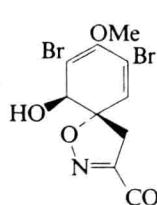
Et ether: [70546-94-0]. N-[2-Ethoxy-2-(4-methoxyphenyl)ethyl]cinnamide. *Aegle marmelos Alkaloid B* $C_{20}H_{23}NO_3$ M 325.407

Isol. from *A. marmelos*. Cryst. (C_6H_6 /hexane). Mp 99-100°. Artifact.

Chatterjee, A. et al, *J. Indian Chem. Soc.*, 1952, **29**, 425 (*isol*)Chakravarti, R.N. et al, *Chem. Ind. (London)*, 1955, 1632 (*struct*)Chatterjee, A. et al, *J. Org. Chem.*, 1959, **24**, 687 (*isol, uv, ir, struct, synth*)Albónico, S.M. et al, *J. Chem. Soc. C*, 1967, 1327 (*synth*)Della Casa de Marcano, D. et al, *Phytochemistry*, 1972, **11**, 1531 (*isol*)Manandhar, M.D. et al, *Phytochemistry*, 1978, **17**, 1814 (*derivs*)Patra, A. et al, *Indian J. Chem., Sect. B*, 1979, **17**, 385 (*isol, uv, ir*)Swinehart, J. et al, *Phytochemistry*, 1980, **19**, 1219 (*isol*)Patra, A. et al, *Org. Magn. Reson.*, 1981, **16**, 65 (*cmr*)Sharma, B.R. et al, *Phytochemistry*, 1981, **20**, 2606 (*isol*)Somanathan, R. et al, *Synth. Commun.*, 1983, **13**, 273 (*synth, ir, ms, pmr, cmr*)**Aerothionin**

A-10028

Updated Entry replacing A-00501
[28714-26-3]

 $C_{24}H_{26}Br_4N_4O_8$ M 818.107

Metab. from the sponges *Aplysina aerophoba* (*Verongia aerophoba*), *A. fistularis* and *A. thiona*. Plates (Me_2CO/C_6H_6). Mp 134-137° dec. $[\alpha]_D + 252^\circ$ (Me_2CO). *Di-Ac*: Needles (Me_2CO). Mp 206-208°. $[\alpha]_D + 236^\circ$ ($CHCl_3$).

2"-Hydroxy: **11-Hydroxyaerothionin** $C_{24}H_{26}Br_4N_4O_9$ M 834.107

Metab. from the verongid sponge *Pseudoceratina durissima*. Glass. $[\alpha]_D + 189^\circ$ (c, 0.15 in $MeOH$).

2",3"-Dihydroxy: [122759-72-2]. **Dihydroxyaerothionin** $C_{24}H_{26}Br_4N_4O_{10}$ M 850.106

Metab. of *Verongula rigida*. Powder. Mp 162-164°. $[\alpha]_D^{25} - 64.2^\circ$ (c, 0.1 in $MeOH$).

2"-Oxo: **11-Oxaerothionin** $C_{24}H_{24}Br_4N_4O_9$ M 832.091

Metab. from the Caribbean sponge *Aplysina lacunosa*. Exhibits pronounced and selective antitumour activity against human colon (HCT116) cell line. Powder. Mp 174.6-176.6° dec. $[\alpha]_D^{25} + 181.15^\circ$ (c, 2.17 in $DMSO$).

Homologue: [34232-66-1]. **Homoaerothionin** $C_{25}H_{28}Br_4N_4O_8$ M 832.134

Constit. of the sponge *A. aerophoba*. Amorph. solid. Has a C_5 bridging chain instead of C_4 .

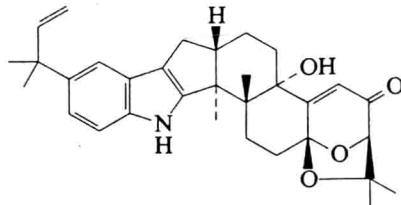
Homologue, di-Ac: [35036-48-7].

Mp 166-167°. $[\alpha]_D + 191.5^\circ$ ($CHCl_3$).

Fattorusso, E. et al, *J. Chem. Soc., Chem. Commun.*, 1970, 752 (*uv, ir, pmr, struct*)Fattorusso, E. et al, *Gazz. Chim. Ital.*, 1971, **101**, 61 (*Homoaerothionin*)Moody, K. et al, *J. Chem. Soc., Perkin Trans. 1*, 1972, **18** (*isol, uv, ir, pmr, struct*)Forrester, A.R. et al, *Justus Liebigs Ann. Chem.*, 1978, **66** (*synth*)McMillan, J.A. et al, *Tetrahedron Lett.*, 1981, **22**, 39 (*cryst struct, uv, pmr, cd, abs config*)Nishiyama, S. et al, *Bull. Chem. Soc. Jpn.*, 1985, **58**, 3453 (*synth*)Gunasekera, M. et al, *J. Nat. Prod. (Lloydia)*, 1989, **52**, 753 (*Dihydroxyaerothionin*)Kernan, M.R. et al, *J. Nat. Prod. (Lloydia)*, 1990, **53**, 615 (*11-Hydroxyaerothionin*)Acosta, A.L. et al, *J. Nat. Prod. (Lloydia)*, 1992, **55**, 1007 (*11-Oxaerothionin*) **β -Aflatrem**

A-10029

[144446-23-1]

 $C_{32}H_{39}NO_4$ M 501.664

Metab. from the sclerotia of *Aspergillus flavus*. Also present in extracts of *A. parasiticus* and *A. subolivaceus*. Exhibits anti-insect acitivity. Yellow cryst. Mp 188-190°. $[\alpha]_D + 77.9^\circ$ (c. 0.011 in CHCl_3).

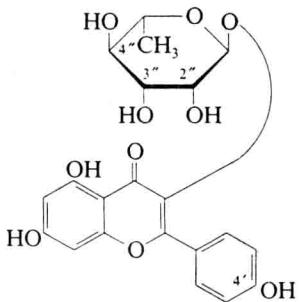
TePaske, M.R. et al. *J. Nat. Prod. (Lloydia)*, 1992, **55**, 1080 (*isol. uv, pmr, cmr, ms, struct*)

Afzelin**A-10030**

Updated Entry replacing A-00540

$3\text{-O-}\alpha\text{-L-Rhamnopyranosyloxy-4',5,7-trihydroxyflavone}$.

Kaempferol 3- α -L-rhamnoside. Afzeloside. Kaempferin [482-39-3]



$\text{C}_{21}\text{H}_{20}\text{O}_{10}$ M 432.383

Isol. from *Afzelia* sp. heartwood and many other plant spp. Yellow prisms + $\frac{1}{2}\text{H}_2\text{O}$ (EtOH aq.). Mp 172-174°.

$4''\text{-O-}\beta\text{-D-Glucopyranoside}$: [52657-01-9]. **Multiflorin B**

$\text{C}_{27}\text{H}_{30}\text{O}_{15}$ M 594.525

Isol. from *Rosa multiflora*, *Prunus persica* and *P. japonica*.

$2''$ or $3''\text{-O-Ac, 4''-O-}\beta\text{-D-glucopyranoside}$: [61358-52-9]. **Multiflorin A**

$\text{C}_{29}\text{H}_{32}\text{O}_{16}$ M 636.562

Isol. from *R. multiflora* and *P. persica*.

$O''\text{-}\beta\text{-D-Xylopyranoside}$:

$\text{C}_{26}\text{H}_{28}\text{O}_{14}$ M 564.499

Isol. from *Woodsia polystictoides*.

$7\text{-O-}\alpha\text{-L-Rhamnopyranoside}$: [482-38-2]. **Kaempferitrin**.

Kaempferol 3,7-dirhamnoside. Lespedelin

$\text{C}_{27}\text{H}_{30}\text{O}_{14}$ M 578.526

Isol. from *Indigofera arrecta*, *Lespedeza cyrtobotrya* and many other plant spp. Needles + $4\text{H}_2\text{O}$. Mp 202-203° (185-186°).

► DJ2977500.

$O''\text{-Sulfate}$: [62794-01-8].

$\text{C}_{21}\text{H}_{20}\text{O}_{13}\text{S}$ M 512.447

Isol. from *Davidsonia pruriens*.

$7\text{-O-}\alpha\text{-L-Arabinopyranoside}$: [71801-95-1].

$\text{C}_{26}\text{H}_{28}\text{O}_{14}$ M 564.499

Isol. from *Asplenium trichomanes*.

$2''\text{-Ac}$: [135618-15-4]. $2''\text{-O-Acetylafzelin}$

$\text{C}_{23}\text{H}_{22}\text{O}_{11}$ M 474.420

Constit. of *Zingiber zerumbet*. Yellow amorph. solid. $[\alpha]_D^{20} - 93^\circ$ (c, 1 in Me_2CO).

$3''\text{-Ac}$: [135618-16-5]. $3''\text{-O-Acetylafzelin}$

$\text{C}_{23}\text{H}_{22}\text{O}_{11}$ M 474.420

Constit. of *Z. zerumbet*. Yellow powder. Mp 117°. $[\alpha]_D^{20} - 126.0^\circ$ (c, 1 in Me_2CO).

$4''\text{-Ac}$: [135618-17-6]. $4''\text{-O-Acetylafzelin}$

$\text{C}_{23}\text{H}_{22}\text{O}_{11}$ M 474.420

Constit. of *Z. zerumbet*. Yellow powder. Mp 199-201°. $[\alpha]_D^{14} - 119.0^\circ$ (c, 1 in MeOH).

$2'',4''\text{-Di-Ac}$: [133882-73-2]. $2'',4''\text{-Diacetylafzelin}$

$\text{C}_{25}\text{H}_{24}\text{O}_{12}$ M 516.457

Isol. from *Z. zerumbet*. Pale yellow amorph. solid. Mp 111°. $[\alpha]_D^{18} - 95.0^\circ$ (c, 1.0 in Me_2CO).

$3'',4''\text{-Di-Ac}$: [77307-50-7]. $3'',4''\text{-Diacetylafzelin}$

$\text{C}_{25}\text{H}_{24}\text{O}_{12}$ M 516.457

Isol. from *Z. zerumbet*. Pale yellow amorph. solid. Mp 154°. $[\alpha]_D^{18} - 125.4^\circ$ (c, 0.7 in Me_2CO).

King, F.E. et al. *J. Chem. Soc.*, 1950, 168 (*isol*)

Vermes, B. et al. *Phytochemistry*, 1976, **15**, 1320 (*synth*)

Takagi, S. et al. *Yakugaku Zasshi*, 1976, **96**, 1217; 1977, **97**, 109; 1979, **99**, 439 (*Multiflorin*)

Wilkins, C.K. et al. *Phytochemistry*, 1977, **16**, 144 (*sulfate*)

Yamasaki, K. et al. *Tetrahedron Lett.*, 1977, 1231 (*cmr*)

Multiflorin)

Hiraoka, A. et al. *Biochem. Syst. Ecol.*, 1978, **6**, 171 (*O''-xyloside*)

Imperato, F. *Experientia*, 1979, **35**, 1134 (*7-arabinoside*)

Itokawa, H. et al. *Chem. Lett.*, 1982, 49 (*ms*)

Zapesochnaya, G.G., Khim. Prir. Soedin., 1982, **18**, 695; *Chem. Nat. Compd. (Engl. Transl.)*, 1983, 658 (*pmr*)

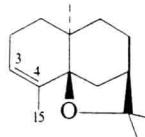
Nakatani, N. et al. *Agric. Biol. Chem.*, 1991, **55**, 455 (*diacetates*)

Masuda, T. et al. *Phytochemistry*, 1991, **30**, 2391 (*acetates*)

 α -Agarofuran**A-10031**

Updated Entry replacing A-00544

[5956-12-7]



$\text{C}_{15}\text{H}_{24}\text{O}$ M 220.354

Constit. of Agar wood oil (from fungus infected *Aquilaria agallocha*). Oil. Bp₈ 134°. $[\alpha]_D + 37.1^\circ$ (c, 6.1 in CHCl_3).

$3\alpha,4\alpha\text{-Epoxide}$: [73465-83-5].

$\text{C}_{15}\text{H}_{24}\text{O}_2$ M 236.353

Constit. of *Alpinia japonica*. Oil. $[\alpha]_D^{25} - 20.8^\circ$ (c, 0.4 in EtOH).

$3\beta,4\beta\text{-Epoxide}$: [60064-95-1].

$\text{C}_{15}\text{H}_{24}\text{O}_2$ M 236.353

Constit. of *A. japonica*. Needles. Mp 90-91°. $[\alpha]_D - 48.2^\circ$ (c, 0.36 in CHCl_3).

$3,4\beta\text{-Dihydro}$: [5956-09-2]. **Dihydroagarofuran**

$\text{C}_{15}\text{H}_{26}\text{O}$ M 222.370

Constit. of *A. japonica* and *Ferula* spp. Oil. Bp_{0.8} 82°. $[\alpha]_D - 79.4^\circ$ (c, 0.75 in CHCl_3).

$3,4\text{-Dihydro, } 4\alpha\text{-hydroxy}$: [15052-76-3]. 4α -Hydroxydihydroagarofuran

$\text{C}_{15}\text{H}_{26}\text{O}_2$ M 238.369

Constit. of *A. japonica*. Needles (hexane). Mp 128-129.5°. $[\alpha]_D - 71.6^\circ$ (c, 0.16 in EtOH).

$\Delta^{4,15}\text{-Isomer}$: [6040-08-0]. **β -Agarofuran**

$\text{C}_{15}\text{H}_{24}\text{O}$ M 220.354

Constit. of Agar wood oil (*A. agallocha*). Oil. Bp₈ 130°. $[\alpha]_D^{20} - 127.1^\circ$ (c, 8.3 in CHCl_3). $n_D^{28} 1.4973$.

$3,4\beta\text{-Dihydro, } 10\text{-epimer: cis-Dihydroagarofuran}$

$\text{C}_{15}\text{H}_{26}\text{O}$ M 222.370

Constit. of a *Prostanthera* sp. Waxy solid. Mp 20-22°. $[\alpha]_D^{25} - 87.6^\circ$ (neat).

[20053-66-1]

Maheshwari, M.L. et al. *Tetrahedron*, 1963, **19**, 1077 (*isol*)

Barrett, H.C. et al. *J. Am. Chem. Soc.*, 1967, **89**, 5665 (*struct*)

Marshall, J.A. et al. *J. Org. Chem.*, 1968, **33**, 435 (*synth*)

Huffmann, J.W. et al. *J. Org. Chem.*, 1976, **41**, 3705 (*synth*)

Thomas, A.F. *Tetrahedron Lett.*, 1976, 1717 (*isol*)

Büchi, G. et al. *J. Org. Chem.*, 1979, **44**, 54 (*synth*)

Itokawa, H. et al. *Chem. Pharm. Bull.*, 1980, **28**, 681; 1985, **33**, 1148 (*isol, derivs, cryst struct*)

Huffman, J.W. et al. *J. Org. Chem.*, 1982, **47**, 3254 (*synth*)

Southwell, I.A. et al. *Phytochemistry*, 1993, **33**, 857 (*cis-Dihydroagarofuran*)

ω-Agatoxin

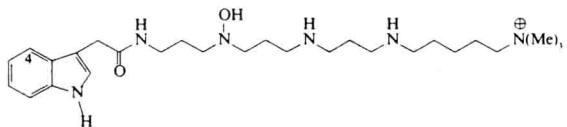
A series of peptides. ω -Agatoxin IA is a 66-aminoacid polypeptide. Isol. from the venom of the funnel-web spider *Agelenopsis aperta*. Calcium channel antagonists. [121889-77-8, 124758-89-0, 124860-33-9, 124860-34-0, 137094-79-2, 137094-80-5, 137094-81-6, 137094-82-7]

Adams, M.E. et al, *J. Biol. Chem.*, 1990, **265**, 861 (*isol*)

 α -Agatoxin AG 488

Agel 489a

[129724-53-4]



$C_{27}H_{49}N_6O_2$ M 489.723

Struct. revised in 1992. Isol. from the venom of the funnel-web spider *Agelenopsis aperta*.

4-Hydroxy: [129724-54-5]. α -Agatoxin AG 504. *Agel 505a* $C_{27}H_{49}N_6O_3$ M 505.722

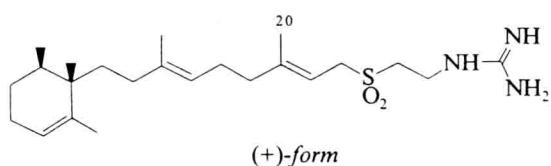
Isol. from the venom of *A. aperta*.

Quistad, G.B. et al, *Biochem. Biophys. Res. Commun.*, 1990, **169**, 51 (*isol*)

Jasys, V.J. et al, *J. Org. Chem.*, 1992, **57**, 1814 (*isol. synth*)

Agelasidine C

Updated Entry replacing A-00556



(+)-form

$C_{23}H_{41}N_3O_2S$ M 423.662

(+)-form [96617-52-6]

Isol. from the Okinawan sea sponge *Agelas nakamurai*. Shows antispasmodic and antibacterial activity.

B,HCl: Syrup. $[\alpha]_D^{25} + 8.5^\circ$ (c, 2.0 in MeOH).

(-)-form

Isol. from *A. clathrodes*. Oil. $[\alpha]_D^{29} - 5.6^\circ$ (c, 7.2 in MeOH).

20-Hydroxy: *Agelasidine D*

$C_{23}H_{41}N_3O_3S$ M 439.661

Isol. from *A. clathrodes*. Oil. $[\alpha]_D^{29} - 3.6^\circ$ (c, 2.75 in MeOH).

[96617-52-6]

Nakamura, H. et al, *J. Org. Chem.*, 1985, **50**, 2494 (*isol, uv, ir, pmr, cmr, struct*)

Asao, K. et al, *Chem. Lett.*, 1989, 1813 (*synth*)

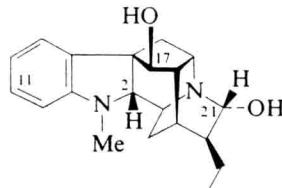
Morales, J.J. et al, *J. Nat. Prod. (Lloydia)*, 1992, **55**, 389 (*isol*)

A-10033**Ajmaline, BAN**

Updated Entry replacing A-00610

Ajmalan-17,21-diol, 9CI. Raugalline. Rauwolfine. Gilurytmal. Tachmalin

[4360-12-7]



$C_{20}H_{26}N_2O_2$ M 326.438

Alkaloid from *Rauwolfia serpentina* and most *R. spp.*

Melodinus balansae and *Tonduzia longifolia*

(Apocynaceae). Antiarrhythmic drug which functions by inhibition of glucose uptake by heart tissue mitochondria. Mp 158-160° (MeOH solvate), Mp 205-207° (anhyd.).

▷ AX8050000.

B,HCl: [4410-48-4].

Amber prisms + 2H₂O. Mp 133-134°, Mp 253-255° (anhyd.).

▷ AX8100000.

B,2HCl: Plates. Mp 305-306° dec.

O¹⁷-Ac: [19918-92-4].

Rods (Et₂O), cryst. (EtOH). Mp 150° (rods), Mp 214-215° (cryst.).

O²¹-Ac: Needles (EtOAc). Mp 190-192°.

Di-Ac: [19775-56-5].

Needles (metastable) or rods. Mp 132°, Mp 187-189° (double Mp).

Picrate: Plates (EtOH). Mp 126-127°, Mp 223° (anhyd.).

B,Mel: Mp 229° dec.

N-Propyl hydrogen tartrate: [2589-47-1]. *Prajmalium bitartrate, BAN, INN. GT 1012. NPAB*

$C_{27}H_{38}N_2O_8$ M 518.606

Cardiac antiarrhythmic drug. Cryst. (EtOH/Et₂O). Mp 149-152°.

▷ AX7750000.

O¹⁷-Chloroacetyl: [47562-08-3]. *Lorajmine, INN*

$C_{22}H_{27}ClN_2O_3$ M 402.920

Cardiac depressant, antiarrhythmic. Cryst. Mp 232-235°. $[\alpha]_D + 27.5^\circ$ (CHCl₃).

O¹⁷-Chloroacetyl, B,HCl: [40819-93-0]. *Lorajmine hydrochloride, USAN. Nevergor. Ritmos. Ritmosel. Viaductor. Win 11831*

Cryst. Mp 230-235°. $[\alpha]_D + 40^\circ$ (CHCl₃).

N-De-Me: [23944-24-3]. *Norajmaline*

$C_{19}H_{24}N_2O_2$ M 312.411

Alkaloid from *R. macrophylla*, *R. obscura* and *R. suaveolens* (Apocynaceae). Yellow-grey amorph. powder. $[\alpha]_D + 36^\circ$ (c, 0.67 in CHCl₃).

11-Hydroxy: [73012-74-5]. *Ajmalinol. Ajmalan-11,17-21-triol, 9CI*

$C_{20}H_{26}N_2O_3$ M 342.437

Alkaloid from *R. vomitoria* (Apocynaceae).

2-Epimer: [51019-46-6].

Noncryst. $[\alpha]_D + 55^\circ$ (c, 1 in CHCl₃).

17-Epimer: [509-37-5]. *Sandwicine. Epiajmaline*

$C_{20}H_{26}N_2O_2$ M 326.438

Alkaloid from *R. sandwicensis*, *R. mauiensis* and *R. vomitoria* (Apocynaceae). Antiarrhythmic agent.

Amorph. (MeOH aq. or Me₂CO/hexane). $[\alpha]_D^{20} + 174^\circ$ (c, 1 in MeOH).

17-Epimer; *B,2HCl*: Cryst. (Me₂CO). Mp 210-213°. $[\alpha]_D + 129^\circ$ (MeOH).

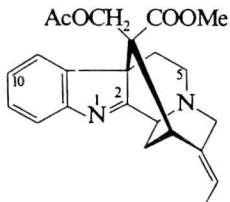
17-Epimer; *B,2H1*: Cryst. (Me_2CO). Mp 238–240°. $[\alpha]_D^{20} + 84^\circ$ (CHCl_3).
 17-Epimer, O¹⁷-Ac: Cryst. (MeOH). $[\alpha]_D^{20} + 188.5^\circ$ (c. 1 in CHCl_3).
 17-Epimer, di-O-Ac: Cryst. (pet. ether). Mp 105–108°. $[\alpha]_D^{20} + 104^\circ$ (c. 1 in CHCl_3).
 20,21-Diepimer: see Isoajmaline, I-00272
 17-O-(3,4,5-Trimethoxybenzoyl): [59846-31-0]. **Willicourtine**
 $\text{C}_{30}\text{H}_{36}\text{N}_2\text{O}_6$ M 520.624
 Alkaloid from *R. obscura* and *R. vomitoria* (Apocynaceae).
 21-O-(3,4,5-Trimethoxybenzoyl): [110941-51-0]. **Ajmalimine**
 $\text{C}_{30}\text{H}_{36}\text{N}_2\text{O}_6$ M 520.624
 Alkaloid from the roots of *R. serpentina* (Apocynaceae).
 Needles (MeOH/EtOAc). Mp 188–189°. $[\alpha]_D^{20} + 105^\circ$.
 [31081-68-2, 35080-11-6, 110906-81-5]

Anet, F.A.L. et al, *J. Chem. Soc.*, 1954, 1242 (*isol. uv. struct*)
 Woodward, R.B., *Angew. Chem.*, 1956, **68**, 13 (*rev. struct*)
 Gorman, M. et al, *Tetrahedron*, 1957, **1**, 328 (*Sandwicine*)
 Bartlett, M.F. et al, *J. Am. Chem. Soc.*, 1962, **84**, 622 (*abs config*)
 Bonati, A. et al, *Farmaco, Ed. Sci.*, 1963, **18**, 851 (*Prajmalium*)
 Keck, J., *Z. Naturforsch. B*, 1963, **18**, 177 (*Prajmalium*)
 Biemann, K. et al, *J. Am. Chem. Soc.*, 1964, **86**, 4624 (*ms*)
 Masamune, S. et al, *J. Am. Chem. Soc.*, 1967, **89**, 2506 (*synth*)
 Ronchetti, F. et al, *Phytochemistry*, 1971, **10**, 1385 (*Sandwicine*)
 Koch, M. et al, *Arzneim.-Forsch.*, 1972, **22**, 2079, 2085; 1973, **23**, 642 (*Prajmalium*)
 Ahmad, V. et al, *Pak. J. Sci. Ind. Res.*, 1972, **15**, 249 (*synth*)
 Majumdar, S.P. et al, *Phytochemistry*, 1973, **12**, 1167 (*Norajmaline*)
 Petter, A. et al, *Arzneim.-Forsch.*, 1974, **24**, 873, 874, 876 (*rev. pharmacol. props*)
 Timmins, P. et al, *Phytochemistry*, 1974, **13**, 281 (*Norajmaline*)
 Hubert-Briere, Y. et al, *Tetrahedron*, 1975, **31**, 3049 (*synth. epimer*)
 Kuhnert-Brandstaetter, M. et al, *Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 699 (*polymorphs*)
 van Tamelen, E.E. et al, *Bioorg. Chem.*, 1976, **5**, 309 (*synth*)
 Timmins, P. et al, *Planta Med.*, 1976, **29**, 283 (*Willicourtine*)
 Prewo, R. et al, *Acta Crystallogr., Sect. B*, 1978, **34**, 454 (*cryst. struct*)
 Chatterjee, A. et al, *Tetrahedron Lett.*, 1978, 3879 (*cmr*)
 Siddiqui, S. et al, *J. Chem. Soc. Pak.*, 1979, **1**, 1; *CA*, **92**, 111204p (*Ajmalinol*)
 Capra, C. et al, *Farmaco, Ed. Prat.*, 1980, **35**, 49 (*Lorajmine*)
 Iwu, M.M., *Planta Med.*, Suppl. 1980, 13 (*Willicourtine*)
 Martindale, *The Extra Pharmacopoeia*, 28th/29th Ed., Pharmaceutical Press, London, 1982/1989, 7777–78, 7787–88.
 Danielli, B. et al, *Tetrahedron*, 1984, **40**, 5255 (*cmr*)
 Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th Ed., Akademie-Verlag, Berlin, 1987, 5833, 6564, 6995 (*synonyms*)
 Siddiqui, S. et al, *Planta Med.*, 1987, **53**, 288 (*Ajmalimine*)
 Johnston, M.D. et al, *J. Heterocycl. Chem.*, 1988, **25**, 1803 (*cmr*)
 Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th Ed., Van Nostrand-Reinhold, 1992, AFH250, AFH280, DNB000, PNC875.

Akuammiline**A-10036**

Updated Entry replacing A-00634

Methyl 17-(acetoxy)akuammilan-16-carboxylate, 10CI.
 Methyl 16-[(acetoxy)methyl]akuammilan-17-oate, 9CI
 [1897-26-3]



$\text{C}_{23}\text{H}_{26}\text{N}_2\text{O}_4$ M 394.469

Alkaloid from *Picralima nitida*, *Conopharyngia durissima*, *Vinca minor*, *Rauwolfia oreogitton* and *R. vomitoria* (Apocynaceae). Cryst. (Et_2O). Mp 157–161°. $[\alpha]_D^{24} + 83^\circ$ (c. 0.5 in CHCl_3).

B,HCl: Cryst. + $1\text{H}_2\text{O}$ (H_2O or EtOH). Mp 196°. $[\alpha]_D^{20} - 29.6^\circ$ (c. 3.84 in H_2O).

B,HI: Needles (EtOH aq.). Mp 210°.

B,HNO₃: Prisms (H_2O). Mp 204°.

B,MeI: Needles (H_2O). Mp 233°. $[\alpha]_D^{20} - 83^\circ$ (c. 1.36 in EtOH).

O-De-Ac: [1897-30-9]. **Rhazimol**, *Deacetylakuammiline*, *Ercinamine*
 $\text{C}_{21}\text{H}_{24}\text{N}_2\text{O}_3$ M 352.432

Alkaloid from *V. minor*, *P. nitida*, *R. vomitoria*, *R. oreogitton* and *Rhazya stricta* (Apocynaceae). Pale-yellow amorph. powder. $[\alpha]_D^{21} + 19.7^\circ$ (MeOH).

1,2β-Dihydro: [77485-26-8]. **1,2β-Dihydroakuammiline**
 $\text{C}_{23}\text{H}_{28}\text{N}_2\text{O}_4$ M 396.485

Alkaloid from the leaves of *Rauwolfia oreogitton* (Apocynaceae). Off-white amorph. powder. $[\alpha]_D^{21} - 9.4^\circ$ (MeOH).

1,2β-Dihydro, *O-de-Ac*: [77485-27-9]. **Deacetyl-1,2β-dihydroakuammiline**
 $\text{C}_{21}\text{H}_{26}\text{N}_2\text{O}_3$ M 354.448

Alkaloid from the leaves of *R. oreogitton* (Apocynaceae). Mp 228–230°. $[\alpha]_D^{21} + 99^\circ$ (MeOH).

10-Methoxy: [38734-62-2]. **Raufloricine**

$\text{C}_{24}\text{H}_{28}\text{N}_2\text{O}_5$ M 424.496

Alkaloid from *V. minor* and from the root bark of *R. confertiflora* (Apocynaceae). Cryst. ($\text{Me}_2\text{CO}/\text{hexane}$ or EtOAc). Mp 190–193°. $[\alpha]_D^{20} + 129^\circ$ (c. 1.5 in CHCl_3).

10-Hydroxy, *O-de-Ac*: [85783-98-8]. **Ercinamine**, *10-Hydroxydeacetylakuammiline*

$\text{C}_{21}\text{H}_{24}\text{N}_2\text{O}_4$ M 368.432

Alkaloid from *Catharanthus roseus* and *V. erecta*. Mp 238–240°. $[\alpha]_D + 53^\circ$.

10-Methoxy, *O-de-Ac*: [38734-63-3]. **Nervobscurine**, *10-Methoxydeacetylakuammiline*

$\text{C}_{22}\text{H}_{26}\text{N}_2\text{O}_4$ M 382.458

Alkaloid from *V. minor*. Amorph. $[\alpha]_D^{25} + 83^\circ$ (c. 0.72 in EtOH).

5β-Hydroxymethyl: [77485-24-6]. **5β-Hydroxymethylakuammiline**

$\text{C}_{24}\text{H}_{28}\text{N}_2\text{O}_5$ M 424.496

Alkaloid from the leaves of *R. oreogitton* (Apocynaceae). Off-white amorph. powder. $[\alpha]_D^{21} - 141^\circ$ (MeOH).

Henry, T.A., *J. Chem. Soc.*, 1932, 2759 (*isol*)

Dugan, J.J. et al, *Helv. Chim. Acta*, 1969, **52**, 701 (*isol. uv. ir. pmr. ms*)

Savaşkan, S. et al, *Helv. Chim. Acta*, 1972, **55**, 2861 (*Akuammiline, Raufloricine, Nervobscurine*)

de Maindreville, M.D. et al, *C. R. Hebd. Séances Acad. Sci. Ser. C*, 1975, **280**, 131 (*config*)

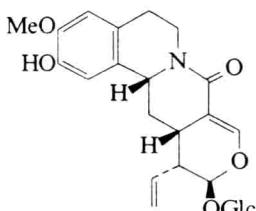
Akinloye, B.A. et al, *Phytochemistry*, 1980, **19**, 2741 (*Dihydroakuammiline, Rhazimol, Deacetyldihydroakuammiline*)

Gueritte, F. et al, *J. Nat. Prod. (Lloydia)*, 1983, **46**, 144 (*Ercinamine*)

Yagudaev, M.R. et al, *Khim. Prir. Soedin.*, 1983, **19**, 483; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, 454 (*Ercinamine, Ercinaminine*)

Alangiside

Updated Entry replacing A-00650
[34482-51-4]



$C_{25}H_{31}NO_{10}$ M 505.521

Alkaloid from the roots, leaves and fruit of *Alangium lamarckii* (best source unripe fruit) (Alangiaceae). Amorph. powder + 2.5 H₂O. Mp 187° dec. (shrinks at 164°). $[\alpha]_D^{26} - 105^\circ$ (c. 1.0 in MeOH).

Tetra-Ac: Amorph. powder. $[\alpha]_D^{21} - 50.4^\circ$ (c. 1.81 in CHCl₃).

Me ether: Needles + 1.5 H₂O (EtOAc). Mp 236°.

O-De-Me: [47763-23-5]. **Demethylalangiside**

$C_{24}H_{29}NO_{10}$ M 491.494

Alkaloid from the roots of *Cephaelis ipecacuanha* (Rubiaceae) and leaves of *Alangium platanifolium* var. *trilobum* (Alangiaceae). Needles (MeOH aq.). Mp 180–182°. $[\alpha]_D^{24} - 73^\circ$ (c. 0.2 in MeOH).

O-De-Me, 6'-(4-hydroxy-3-methoxycinnamoyl): 6'-O-Feruloyldemethylalangiside

$C_{34}H_{37}NO_{13}$ M 667.665

Alkaloid from leaves of *A. platanifolium* var. *trilobum* (Alangiaceae). Powder. Isol. as a mixt. of *cis*- and *trans*-forms.

O-De-Me, 6'-(4-hydroxy-3,5-dimethoxycinnamoyl): 6'-Sinapoyldemethylalangiside

$C_{35}H_{39}NO_{14}$ M 697.691

Alkaloid from leaves of *A. platanifolium* var. *trilobum* (Alangiaceae). Powder. Isol. as mixt. of *cis*- and *trans*-isomers.

Kapil, R.S. et al. *J. Chem. Soc., Chem. Commun.*, 1971, 904 (ir, pmr, struct, abs config)

Shoeb, A. et al. *J. Chem. Soc., Perkin Trans. 1*, 1975, 1245 (isol, uv, ir, pmr, ms, struct)

Nagakura, N. et al. *J. Chem. Soc., Chem. Commun.*, 1978, 896 (cmr)

Höfle, G. et al. *Chem. Ber.*, 1980, **113**, 566 (synth, uv, ir, pmr, cmr, ms)

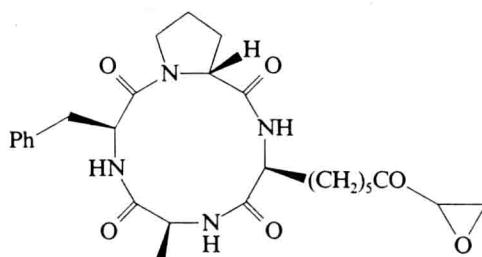
Itoh, A. et al. *Phytochemistry*, 1991, **30**, 3117; 1992, **31**, 1037 (Demethylalangiside, 6'-O-Feruloyldemethylalangiside, 6'-O-Sinapoyldemethylalangiside)

1-Alaninechlamydocin

A-10038

Cyclo(L-alanyl-D-phenylalanyl-D-prolyl- η -oxo-L- α -aminooxiranocanoyl), 9CI

[141446-96-0]



$C_{27}H_{36}N_4O_6$ M 512.605

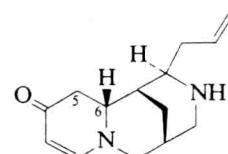
Cyclic peptide antibiotic. Metab. of *Diheterospora chlamydosporia*. Antitumour agent. Alanine analog. of Chlamydocin, C-00930.

Kim, S.D. et al. *C.A.* 1992, **116**, 231433 (isol)

Albine

A-10039

Updated Entry replacing A-00676
Dehydroalbine
[53915-26-7]



Absolute configuration

$C_{14}H_{20}N_2O$ M 232.325

Alkaloid from *Lupinus albus* and *L. termis* seeds (Leguminosae). Mp 50°. $[\alpha]_D^{25} - 103^\circ$. The N-Methyl deriv. was formerly reported erroneously (see Alkaloid LC2, A-10048).

B.HClO₄: Mp 253°. $[\alpha]_D^{25} - 76^\circ$ (H₂O).

N-Formyl: **N-Formylalbine**

$C_{15}H_{20}N_2O_2$ M 260.335

Trace alkaloid in seeds and leaves of *L. albescens* (Leguminosae). Provisional identification.

5,6-Didehydro: **Δ^5 -Dehydroalbine**

$C_{14}H_{18}N_2O$ M 230.309

Alkaloid from seeds of *L. termis* (Leguminosae). Oil. $[\alpha]_D^{25} - 44.6^\circ$ (c. 0.02 in MeOH).

Wiewiórowski, M. et al. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1964, **12**, 213, 217 (isol, ir)

Chekhlov, A.N. et al. *J. Struct. Chem. (Engl. Transl.)*, 1974, **15**, 848 (cryst struct)

Wolinska-Mocylarz, J. et al. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1976, **24**, 613 (ir, struct)

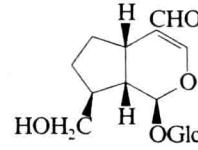
Mohamed, M.H. et al. *Phytochemistry*, 1991, **30**, 3111 (Δ^5 -Dehydroalbine)

Planchuelo-Ravelo, A.M. et al. *Z. Naturforsch., C*, 1993, **48**, 414 (N-Formylalbine)

Aldoxoside

A-10040

[142905-20-2]



$C_{16}H_{24}O_9$ M 360.360

Constit. of *Cordylanthus tenuis* and *C. kingii*. Gum. $[\alpha]_D - 47^\circ$ (c. 0.07 in MeOH).

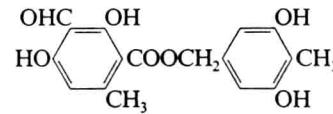
Justice, M.R. et al. *Phytochemistry*, 1992, **31**, 2021.

Alectorialin

A-10041

Decarboxyalectorialic acid

[55483-02-8]



$C_{17}H_{16}O_7$ M 332.309