

Mathew, K.K. et al., Indian J. Chem., Sect. B, 1981, 20, 340, (合成法)  
Williams, P.J. et al., Phytochemistry, 1982, 21, 2013, (6-arabinosylglucosides, rutinosides)  
Free, J.B. et al., Bee World, 1984, 65, 175  
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Ackermann, I.E. et al., Annalen, 1989, 79, (合成法, 配糖体)  
Lewis, R.J., Food Additives Handbook, Van Nostrand Reinhold International, New York, 1989, DTD000; DTD200; DTD800  
Voirin, S.G. et al., Carbohydr. Res., 1990, 207, 39, (synth glycosides, H-NMR, C13-NMR)  
Voirin, S.G. et al., J. Agric. Food Chem., 1990, 38, 1373, (Acuminoside)  
Howell, A.R. et al., J.C.S. Perkin 1, 1990, 2715, (合成法)  
Ahmad, A.A., Pharmazie, 1991, 46, 362, (6,7-Epoxygeranyl acetate)  
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1355; 1372  
Guo, W. et al., Phytochemistry, 1993, 33, 1373, (xylopyranosylglucopyranoside)  
Yoshikawa, K. et al., Phytochemistry, 1993, 34, 1431, (Kenposide A)  
Fukuda, T. et al., Chem. Pharm. Bull., 1996, 44, 2173, (Kudingoside A)  
Tian, J. et al., Chin. Chem. Lett., 1996, 7, 341; 1997, 8, 125, (Ligurobustosides)  
Yoshikawa, M. et al., Chem. Pharm. Bull., 1997, 45, 1498, (Sacranoside B)  
Oka, N. et al., Nat. Prod. Lett., 1997, 10, 187, (Rosa damascena glycosides)  
Eisenreich, W. et al., Tet. Lett., 1997, 38, 3889, (生合成)  
Sy, L.-K. et al., J. Nat. Prod., 1998, 61, 907, (Geranyl benzoate)  
Tian, J. et al., Phytochemistry, 1998, 48, 1013, (Ligurobostosides)  
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, DTD000; GCY000; DTD200; DTD800

\*\*\* RTECS (化学物質毒性データ) \*\*\*

生体影響物質 : 天然物. 一時刺激物質.

\*\*\* 健康障害に関するデータ \*\*\*

\*\*\* 皮膚/眼の刺激に関するデータ \*\*\*

<< 試験方法 >> 標準ドライズ試験.

曝露経路 : 皮膚への塗布

被験動物 : げっ歯類-ウサギ.

投与量・期間 : 500 mg/24 時間

反応の症度 : 軽度

参照文献

FCTXAV Food and Cosmetics Toxicology. (London, UK) V.1-19, 1963-81. For publisher information, see FCTOD7. [Vol., 頁, 年 (19-)] 14,623,1976

\*\*\* 急性毒性に関するデータ \*\*\*

<< 試験方法 >> LD50 試験(50%致死量試験).

曝露経路 : 経口投与.

被験動物 : げっ歯類-ラット.

投与量・期間 : 4500 mg/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

FCTXAV Food and Cosmetics Toxicology. (London, UK) V.1-19, 1963-81. For publisher information, see FCTOD7. [Vol., 頁, 年 (19-)] 14,623,1976

<< 試験方法 >> LD50 試験(50%致死量試験).

曝露経路 : 筋肉内投与.

被験動物 : げっ歯類-マウス

投与量・期間 : 3 gm/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

JSICAZ Journal of Scientific and Industrial Research, Section C: Biological Sciences. (New Delhi, India) V.14-21, 1955-62. For publisher information, see IJEBA6. [Vol., 頁, 年 (19-)] 21,342,1962

<< 試験方法 >> LD50 試験(50%致死量試験).

曝露経路 : 皮膚への塗布

被験動物 : げっ歯類-ウサギ.

投与量・期間 : >5 gm/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参考文献

FCTXAV Food and Cosmetics Toxicology. (London, UK) V.1-19, 1963-81. For publisher information, see FCTOD7. [Vol., 頁, 年(19-)] 14, 623, 1976

\*\*\*米国N I O S H基準の発展とサーベランス\*\*\*

米国N I O S H職業暴露調査データ

全米職業曝露調査(NOES)-米国全国職業ばく露調査(1983)

全米職業曝露調査(NOES) Hazard Code - X9625

No. of Facilities: 1991 (評価)

No. of Industries: 4

No. of Occupations: 9

No. of Employees: 13881 (評価)

No. of Female Employees: 7957 (評価)

\*\*\*米国に於ける状況\*\*\*

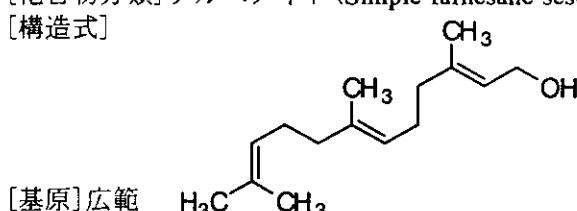
#### EPA TSCA Section 8(b) CHEMICAL INVENTORY

##### S 2,6,10-Farnesatrien-1-ol; (2E,6E)-form

[CAS No.] 106-28-5

[化合物分類] テルペノイド (Simple farnesane sesquiterpenoids)

[構造式]



[基原] 広範

farnesol

圃に分布. The main farnesol isomer, e.g. >90% of the component of the oil of *Hibiscus abelmoschus*. Nasonov pheromone of the 蜂蜜 *Apis mellifera*; constit. of temporal gland secretions of the African elephant (*Loxodonta africana*)

[沸点] Bp<sub>1</sub> 137 °C

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Aldrich Library of FT-IR Spectra, 1st edn., 1985, 1, 149B, (IR)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, 1, 226B; 226C, (NMR)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, 3, 219D; 220A, (IR)

Bates, R.B. et al., J.O.C., 1963, 28, 1086, (分離, 構造決定)

Burrell, J.W.K. et al., J.C.S.(C), 1966, 2144, (合成法)

Corey, E.J. et al., J.A.C.S., 1967, 89, 4245, (合成法)

Hill, H.C. et al., J.C.S.(C), 1968, 93, (Mass)

Richards, J.B. et al., Biochem. J., 1972, 128, 1345, (生合成)

Jacob, G. et al., Phytochemistry, 1972, 11, 1683, (生合成)

Evans, R.H. et al., Chem. Comm., 1973, 465, (生合成)

Nilles, G. et al., J. Agric. Food Chem., 1973, 21, 342, (合成法)

Morris, W.W., J. Assoc. Off. Anal. Chem., 1973, 56, 1037, (IR)

Tengo, J. et al., J. Chem. Ecol., 1975, 1, 253, (hexanoyl, 分離)

Crombie, L. et al., J.C.S. Perkin 1, 1975, 913, (C13-NMR)

Cardillo, C.R. et al., Chem. Comm., 1976, 190, (合成法)

Pauling, H. et al., Helv. Chim. Acta, 1976, 59, 1233, (合成法)

Org. Synth., 1977, 56, 112, (合成法, IR)

Pickett, J.A. et al., J. Chem. Ecol., 1980, 6, 425, (分離)

Van Tamelen, E.E. et al., Bioorg. Chem., 1982, 11, 133, (合成法)

Wheller, J.W. et al., J. Chem. Ecol., 1982, 8, 821, (分離)

Bohlmann, F. et al., Phytochemistry, 1982, 21, 2537, (angelate)

Amin, C et al., Helv. Chim. Acta, 1984, 67, 1540, (合成法, IR, H-NMR, Mass)

Yamagisawa, A. et al., Chem. Lett., 1988, 1899, (合成法)

Andersen, J.F. et al., J. Chem. Ecol., 1988, 14, 1153, (分離)

Yoshioka, T. et al., Phytochemistry, 1990, 29, 3469, (生合成)  
Christensen, D.J. et al., Bioorg. Med. Chem., 1994, 2, 631, (合成法)  
Inoue, H. et al., Phytochemistry, 1994, 36, 1203, (分離, 生合成)  
Leyes, A.E. et al., Org. Lett., 1999, 1, 1071, (生合成)  
Adesanya, S.A. et al., Phytochemistry, 1999, 51, 1039, (Rubiginoside)  
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992,  
FAB800

### § 8-Hydroxyoctanoic acid

[CAS No.] 764-89-6

[化合物分類] 脂肪族化合物 (Saturated unbranched carboxylic acids and lactones)

[構造式] HOCH<sub>2</sub>(CH<sub>2</sub>)<sub>6</sub>COOH

[分子式] C<sub>8</sub>H<sub>16</sub>O<sub>3</sub>

[分子量] 160.213

[正確な分子量] 160.109945

[基原] 次の植物から分離: *Apis mellifera* のロイヤルゼリー

[融点] Mp 62-63 °C (58 °C)

[溶解性] 水に可溶, 石油エーテルに難溶

#### 文献

Chuit, P. et al., Helv. Chim. Acta, 1929, 12, 463, (合成法)  
Palomaa, M.H., Ber., 1941, 74, 294, (Me ether)  
Friess, S.L. et al., J.A.C.S., 1952, 74, 2679, (hydrazide)  
Bulock, J.D. et al., Chem. Ind. (London), 1954, 990, (amide)  
Huisgen, R. et al., Tetrahedron, 1959, 6, 253, (lactone)  
Bestmann, H.J. et al., Annalen, 1966, 699, 33, (合成法)  
Weaver, N. et al., Lipids, 1968, 3, 535, (分離)  
Mukaiyama, T. et al., Chem. Lett., 1976, 49, (lactone)  
Anol, R.A. et al., Lipids, 1982, 17, 414, (合成法)  
Goodman, M.M. et al., J. Med. Chem., 1985, 28, 807, (誘導体, 合成法, H-NMR, Mass)  
Hagen, J.P. et al., J.O.C., 1993, 58, 506, (合成法, IR, H-NMR, lactone)  
Menger, F.M. et al., J.O.C., 1996, 61, 7382, (Me ether, 合成法, H-NMR, C13-NMR)

### § Hymenoptaecin

[CAS No.] 149022-34-4

[化合物分類] アミノ酸とペプチド (Linear polypeptides)

[構造式] 不明

[基原] *Apis mellifera* のリンパ液

[用途] 抗菌作用

[その他のデータ] 物理化学的性質に関する報告はない

#### 文献

Casteels, P. et al., J. Biol. Chem., 1993, 268, 7044

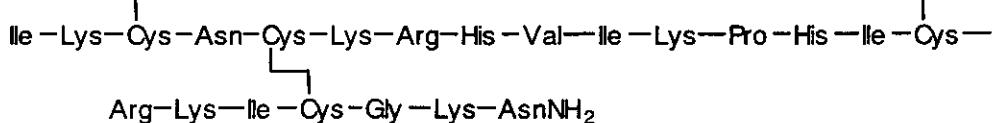
### § *Apis mellifera* Mast cell degranulating peptide (CAS名)

[化学名・別名] Peptide 401. MCD Peptide

[CAS No.] 32908-73-9

[化合物分類] アミノ酸とペプチド (Linear polypeptides)

[構造式]



[分子式]

$\text{H}_{192}\text{N}_{40}\text{O}_{24}\text{S}_4$

[分子量] 2587.244

[正確な分子量] 2585.3916

[基原] 次の動物から分離: *Apis mellifera* の毒液(ヨーロッパミツバチ)

[用途]強い抗炎症薬

[その他のデータ]強い塩基性

-----文献-----

Hider, R.C. et al., Biochim. Biophys. Acta, 1981, 667, 197, (conformn)

Dempsey, C.E., J.C.S. Perkin 1, 1982, 2625, (合成法, 成書)

Dotimas, E.M. et al., Biochim. Biophys. Acta, 1987, 911, 285, (分離, HPLC)

Buku, A. et al., Int. J. Pept. Protein Res., 1989, 33, 86, (合成法)

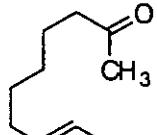
§ 9-Oxo-2-decanoic acid; (E)-form

[化学名・別名] Queen substance. Queen bee pheromone

[CAS No.] 334-20-3

[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones)

[構造式]



[基原] Queen substance of 蜜蜂 *Apis mellifera*. 薬効があるといわれている

[性状] 結晶 (MeOH 溶液 or Me<sub>2</sub>CO)

[融点] Mp 54-55.5 °C

[沸点] Bp<sub>0.01</sub> 37-39 °C

[溶解性] BERDY SOL: メタノール, ヘキサンに可溶; 水に難溶

[UV]: [neutral]  $\lambda_{\text{max}}$  362 nm (MeOH)

-----文献-----

Van der Plas, H.C. et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.), 1964, 83, 701, (合成法, 成書)

Cromer, D.T. et al., Acta Cryst. B, 1972, 28, 2128, (結晶構造)

Boch, R. et al., J. Chem. Ecol., 1975, 1, 133, (field trials)

Trost, B.M. et al., J.O.C., 1975, 40, 148, (合成法)

Tsuji, J. et al., Tet. Lett., 1977, 2267, (合成法)

Subramaniam, C.S. et al., Indian J. Chem., Sect. B, 1978, 16, 318, (合成法, IR, H-NMR)

Lombardi, L. et al., Synthesis, 1978, 131

Hase, T.A. et al., Synth. Commun., 1979, 9, 63, (合成法)

Tamaru, Y. et al., Tetrahedron, 1979, 35, 329, (合成法, IR, H-NMR)

Villemin, D., Chem. Ind. (London), 1986, 69, (合成法)

Dhokte, V.P. et al., Synth. Commun., 1987, 17, 355, (合成法)

Bestmann, H.J. et al., Synthesis, 1988, 49, (合成法, IR, H-NMR, Mass)

Ebert, G.W., Synth. Commun., 1991, 21, 1527, (合成法)

§ Procamine

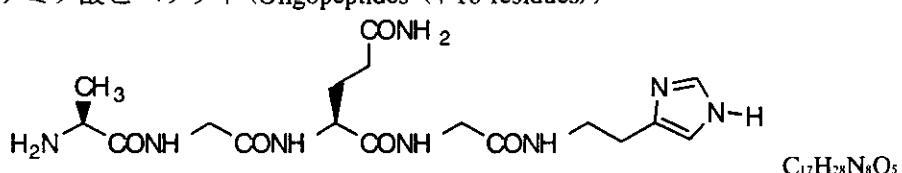
[化学名・別名] Alanylglycylglutaminyl-N-[2-(1H-imidazol-4-yl)ethyl] glycinamide (CAS名)

[CAS No.] 51943-80-7

[その他の CA No.] 83310-28-5

[化合物分類] アミノ酸とペプチド (Oligopeptides (4-10 residues))

[構造式]



[分子式]

[分子量] 424.459

[正確な分子量] 424.218267

[基原] 蜂蜜 (*Apis mellifera*) の毒液

-----文献-----

Peck, M.L. et al., J. Agric. Food Chem., 1974, 22, 51

Szokan, G. et al., J. Liq. Chromatogr., 1994, 17, 3333, (分離)

§ Royalisin

[CAS No.] 128906-89-8

[関連 CAS No.] 128906-90-1

[化合物分類] アミノ酸とペプチド (Linear polypeptides)

[構造式] 不明

[基原] 次の植物から分離: 蜂蜜 *Apis mellifera* のロイヤルゼリー

[用途] グラム陽性菌に対して強い抗菌性を示す

-----文献-----

Fujiwara, S. et al., J. Biol. Chem., 1990, 265, 11333, (分離, 構造決定)

§ § ミツバチ科トウヨウミツバチ (*Apis indica* Radoszkowski) がその巣に集めたハチミツ。

該当物質なし

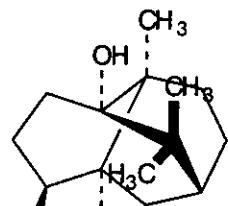
\*\*\*\*\*パチュリー (Patchouli) \*\*\*\*\*

§ § シソ科パチョリ (*Pogostemon cablin* Benth.) の茎

§ 5(1 → 10)-Abeo-1,12-patchoulane diol

[化合物分類] テルペノイド (Rearranged patchoulane sesquiterpenoids)

[構造式]



[分子式]

$\text{HOH}_2\text{C}$

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

[分子量]

238.369

[正確な分子量] 238.19238

[基原] *Pogostemon cablin* and prod. of biological oxidation of 5(1 → 10)-Abeo-1-patchoulanol

[性状] 結晶 (hexane/C<sub>6</sub>H<sub>6</sub>)

[融点] Mp 132.5-133 °C

-----文献-----

Trifilieff, E., Phytochemistry, 1980, 19, 2467, (分離, 構造決定)

Niwa, H. et al., Tet. Lett., 1984, 25, 2797, (合成法)

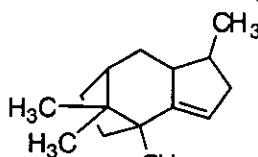
§ 11(1 → 10)-Abeo-1(5)-patchoulene;  $\Delta^{12}$ -Isomer

[化学名・別名] 11(1 → 10)-Abeo-1-patchoulene,  $\delta$ -Patchoulene

[CAS No.] 53823-16-8

[化合物分類] テルペノイド (Rearranged patchoulane sesquiterpenoids)

[構造式]



[分子式]

$\text{C}_{15}\text{H}_{24}$

[分子量]

204.355

[正確な分子量] 204.1878

[基原] *Pogostemon cablin*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{25} -61.7$  (EtOH)

-----文献-----

Büchi, G. et al., J.A.C.S., 1961, 83, 927, (分離, 構造決定)

Bates, R.B. et al., J.A.C.S., 1962, 84, 1307, (合成法)

Narayanan, C.S. et al., Tetrahedron, 1964, 20, 963, (分離)

Mookherjee, B.D. et al., J. Agric. Food Chem., 1974, 22, 771, ( $\delta$ -Patchoulene)  
Akhita, A. et al., Phytochemistry, 1987, 26, 2705, (合成)

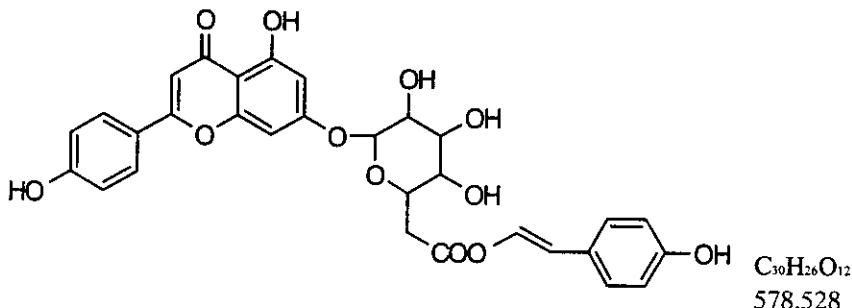
**§ Cosmosiin; 6"-O-(4-Hydroxycinnamoyl)**

[化学名・別名] Terniflorin, Echinacin

[CAS No.] 61237-19-2

[化合物分類] フラボノイド (Flavones; 3 × O-置換基)

[構造式]



[基原] 次の植物から分離: *Pogostemon cablin*, *Clematis terniflora*, *Echinops echinatus*

[性状] 結晶

[融点] Mp 261-263 °C

[その他のデータ] 同定されたサンプルは明らかではない。融点は Echinacin のものである。

文献

- Nakaoki, T., Yakugaku Zasshi, 1935, 55, 967; CA, 30, 725, (分離)  
Teoule, R. et al., Bull. Soc. Chim. Fr., 1960, 2116, (Glycosides, 合成法)  
Aritomi, M., Chem. Pharm. Bull., 1963, 11, 1225, (Terniflorin)  
Batterham, T.J. et al., Aust. J. Chem., 1964, 17, 428, (H-NMR)  
Coussio, J.D. et al., An. Asoc. Quim. Argent., 1965, 53, 257, (Rhoifolin)  
Petrenko, V.V., Khim. Prir. Soedin., 1965, 1, 414; Chem. Nat. Compd. (Engl. Transl.), 1965, 1, 326, (Quinqueloside)  
Gella, E.V. et al., Farm. Zh. (Kiev), 1966, 21, 58; 1967, 22, 80; CA, 65, 13810; 68, 49985, (Menthoside, Piperitoside)  
Nordby, H.E. et al., Phytochemistry, 1968, 7, 1653, (Isonhoifoliu)  
Wagner, H. et al., Chem. Ber., 1969, 102, 2083, (Isorhoifolin)  
Bandyukova, V.A. et al., Khim. Prir. Soedin., 1969, 5, 595; Chem. Nat. Compd. (Engl. Transl.), 1969, 5, 512, (2"-xyloside)  
Subramanian, S.S. et al., Phytochemistry, 1970, 9, 2581, (Apigenin 4',7-diglucoside)  
Kreuzaler, F. et al., Phytochemistry, 1973, 12, 1149, (malonate)  
Harborne, J.B. et al., Phytochemistry, 1974, 13, 1557, (sulfate)  
Karl, C. et al., Phytochemistry, 1976, 15, 1084, (4"-4-hydroxycinnamoyl)  
Markham, K.R. et al., Tetrahedron, 1978, 34, 1389, (C13-NMR)  
Kunde, R. et al., Planta Med., 1979, 37, 124, (6"-acetate)  
Redaelli, C. et al., Phytochemistry, 1980, 19, 985; 1982, 21, 1828, (acetates)  
Ishikura, N., Agric. Biol. Chem., 1981, 45, 1855, (誘導体)  
Itokawa, H. et al., Chem. Pharm. Bull., 1981, 29, 254, (6"-4-hydroxycinnamoyl)  
Itokawa, H. et al., Chem. Lett., 1982, 49, (Mass)  
Rao, L.J.M. et al., Phytochemistry, 1983, 22, 1058, (di-4-hydroxycinnamoyl)  
Stein, W. et al., Z. Naturforsch., C, 1985, 40, 469, (6"-Malonylcemosiin)  
Singh, K.N. et al., Chem. Ind. (London), 1986, 713, (Echinatin, Echinacin)  
Chaudhuri, P.K. et al., Phytochemistry, 1986, 25, 1770, (4"-*Z*-4-Hydroxycinnamoylcemosiin)  
Becker, R. et al., Z. Naturforsch., C, 1986, 41, 507, (2",4"-dirhamnoside)  
Markham, K.R. et al., J. Nat. Prod., 1987, 50, 660, (6"-arabinosides)  
Tomas-Barberan, F.A. et al., Phytochemistry, 1988, 27, 165, (2"-alloside)  
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988  
Yuldashev, M.P. et al., Khim. Prir. Soedin., 1989, 25, 352; Chem. Nat. Compd. (Engl. Transl.), 1989, 25, 303, (6"-Crotonylcosmosiin)

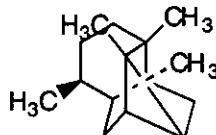
- Gabreli, C. et al., Phytochemistry, 1990, 29, 681, (4'-(E)-4-Hydroxycinnamoylcosmosiin)  
 Takeda, K. et al., Phytochemistry, 1993, 34, 421, (H-NMR, C13-NMR)  
 Kaneko, T. et al., Phytochemistry, 1995, 39, 115, (6"-apiofuranoside)  
 El-Ansari, M.A. et al., Phytochemistry, 1995, 40, 1543, (3-Coumaroylcosmosiin)  
 Roth, L. et al., Roth Collection of Natural Product Data, VCH, Weinheim, 1955  
 Kikuchi, M. et al., J. Nat. Prod., 1996, 59, 314, (Apigenin 2<sup>6</sup>-rhamnosylgentiobioside)  
 Tschan, G.M. et al., Phytochemistry, 1996, 41, 643, (Chamaemeloside)  
 Harraz, F.M. et al., Phytochemistry, 1996, 43, 521, (6"-coumaroyl-3"-Ac)  
 Ram, S.N. et al., Planta Med., 1996, 62, 187, (Echitin)  
 Gudej, J. et al., Acta Pol. Pharm., 1997, 54, 233, (6"-Caffeoylcosmosiin)  
 Veitch, N.C. et al., Phytochemistry, 1998, 48, 389, (Apigenin 7-cellulosides)  
 Brinkmeier, E. et al., Z. Naturforsch., C, 1998, 53, 1, (7-sophorotrioside)

### § Cycloseychellene

[CAS No.] 52617-34-2

[化合物分類] テルペノイド (Tetracyclic sesquiterpenoids)

[構造式]



[分子式]

[分子量] 204.355

[正確な分子量] 204.1878

[基原] *Pogostemon cablin*

[性状] オイル

### 文献

- Terhune, S.J. et al., Tet. Lett., 1973, 4705, (分離)  
 Welsh, S.C. et al., J.O.C., 1981, 46, 4819; 1985, 50, 2676, (構造決定, 合成法)  
 Niwa, H. et al., Tet. Lett., 1983, 24, 937, (合成法)  
 Akhila, A. et al., Phytochemistry, 1988, 27, 2105, (生合成)

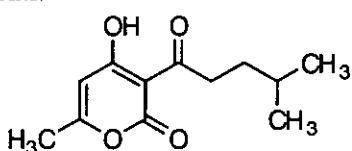
### § Dhelwangin

[化学名・別名] 4-Hydroxy-6-methyl-3-(4-methyl-1-oxopentyl)-2H-pyran-2-one (CAS名). Pogosone

[CAS No.] 23800-56-8

[化合物分類] 含酸素複素環式化合物 (2-Pyrones), 薬物: 抗菌性剤 (Antibacterial agents), 薬物: 抗カビ薬 (Antifungal agents)

[構造式]



[分子式]

[分子量] 224.256

[正確な分子量] 224.10486

[基原] 次の植物の葉から分離: *Pogostemon patchouli*, *Pogostemon cablin*

[用途] 抗菌, 抗カビ薬

[性状] 結晶

[融点] Mp 41-41.6 °C

[溶解性] BERDY SOL: クロロホルム, 塩基に可溶; ベンゼンに易溶; 水に難溶

[Log P 計算値] Log P 2.98 (計算値)

[UV]: [neutral]  $\lambda_{max}$  225 ( $\epsilon$  10300); 310 ( $\epsilon$  12630) (EtOH)

### 文献

Klein, E. et al., Tet. Lett., 1969, 2279, (合成法)

Anon, CA, 1977, 87, 172771, (分離, 構造決定)

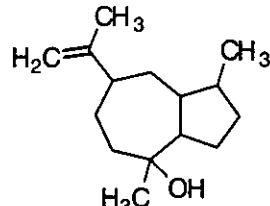
### § 11-Guaien-10-ol; (1 $\beta$ ,4 $\beta$ ,5 $\alpha$ ,10 $\alpha$ )-form

[化学名・別名] Pogostol

[CAS No.] 21698-41-9

[化合物分類] テルペノイド (Simple guaiane sesquiterpenoids)

[構造式]



[基原]

[性状] オイ

[比旋光度]:  $[\alpha]_D -20.2$  (*c*, 8.7 in CHCl<sub>3</sub>)

*Pogostemon cablin* から得られるパチョリオイル

文献

Hikino, H. et al., Chem. Pharm. Bull., 1968, 16, 1608, (分離)

Brunn, K., Parfum. Kosmet., 1978, 59, 109, (分離)

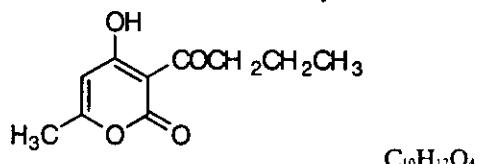
Fleischer, T.C. et al., J. Nat. Prod., 1997, 60, 1054, (Me ether)

#### § 4-Hydroxy-6-methyl-3-(1-oxobutyl)-2H-pyran-2-one (CAS名)

[CAS No.] 22073-85-4

[化合物分類] 含酸素複素環式化合物 (2-Pyrones)

[構造式]



[分子式]

[分子量] 196.202

[正確な分子量] 196.07356

[基原] *Holothrips hagai*, *Holothrips japonicus*, *Pogostemon cablin*

[性状] 結晶 (MeOH)

[融点] Mp 57-59 °C

C<sub>10</sub>H<sub>12</sub>O<sub>4</sub>

文献

Marcus, E. et al., J. Het. Chem., 1969, 6, 13, (合成法)

Caputo, O. et al., Gazz. Chim. Ital., 1977, 107, 455, (合成法)

De Rijke, D. et al., Phytochemistry, 1978, 17, 1664, (分離)

Suzuki, T. et al., Appl. Entomol. Zool., 1993, 28, 108, (分離)

#### § § シソ科ジャワパチュリー (*Pogostemon heyneanus* Benth.) の茎葉。

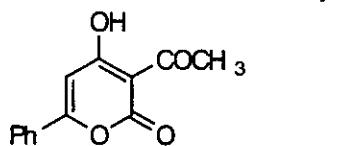
##### § 3-Acetyl-4-hydroxy-6-phenyl-2H-pyran-2-one (CAS名)

[化学名・別名] Pogopyrone B

[CAS No.] 17313-50-7

[化合物分類] 含酸素複素環式化合物 (2-Pyrones), 单環芳香族 (Miscellaneous aryl derivatives)

[構造式]



C<sub>13</sub>H<sub>10</sub>O<sub>4</sub>

[分子式]

[分子量] 230.22

[正確な分子量] 230.05791

[基原] *Pogostemon heyneanus*

[性状] 結晶 (Me<sub>2</sub>CO)

[融点] Mp 170 °C

文献

Marcus, E. et al., J. Het. Chem., 1969, 6, 13, (合成法)

Purushothaman, K.K. et al., Indian J. Chem., Sect. B, 1984, 23, 611

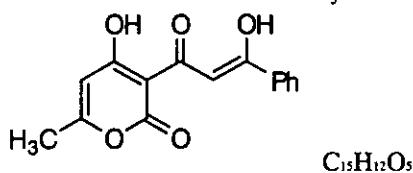
Thailambal, V.G. et al., Acta Cryst. C, 1985, 41, 802, (結晶構造)

§ Pogopyrone A

[CAS No.] 93066-92-3

[化合物分類] 单環芳香族 (Miscellaneous aryl derivatives), 含酸素複素環式化合物 (2-Pyrone)

[構造式]



[分子式]

[分子量] 272.257

[正確な分子量] 272.068475

[基原] *Pogostemon heyneanus*

[性状] 結晶 (EtOAc)

[融点] Mp 148 °C

-----文献-----

Purushothaman, K.K. et al., Indian J. Chem., Sect. B, 1984, 23, 611

\*\*\*\*\*ハッカ (Corn-mint, Japanese mint) \*\*\*\*\*

§ § シソ科ハッカ (*Mentha arvensis* var. *piperascens* Malinv. (*M. haplocalyx* Briquet var. *piperascens* (Malinvaud) Wu et Li)) の茎葉または全草。

該当物質なし

\*\*\*\*\*バックビーン (Buckbean) \*\*\*\*\*

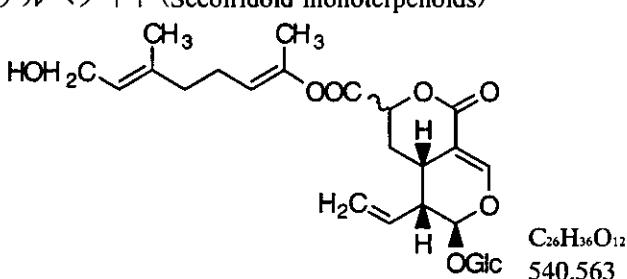
§ § ミツガシワ科ミツガシワ (*Menyanthes trifoliata* L.) の茎葉。

§ Foliamenthin

[CAS No.] 21848-66-8

[化合物分類] テルペノイド (Secoiridoid monoterpenoids)

[構造式]



[分子式]

[分子量]

[正確な分子量] 540.22068

[基原] *Menyanthes trifoliata*

[性状] 結晶

[融点] Mp 194-196 °C

[比旋光度]: [α]<sub>D</sub> -63 (MeOH)

-----文献-----

Loew, P. et al., Chem. Comm., 1968, 1276, (構造決定, 生合成)

Battersby, A.R. et al., Chem. Comm., 1968, 1277, (誘導体)

Junior, P., Planta Med., 1991, 57, 181, (Exaltoside, Epiexaltoside)

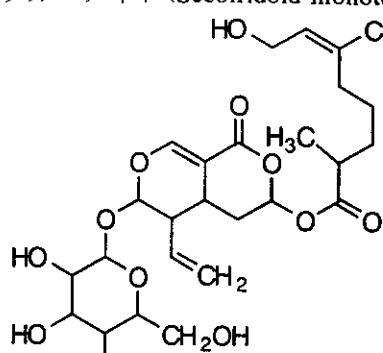
§ Foliamenthin; 2',3'-Dihydro (R-)

[化学名・別名] Dihydrofoliamenthin

[CAS No.] 22314-48-3

[化合物分類] テルペノイド (Secoiridoid monoterpenoids)

[構造式]



[分子式]

C<sub>26</sub>H<sub>38</sub>O<sub>12</sub>

[分子量]

542.579

[正確な分子量] 542.23633

[基原] *Menyanthes trifoliata*

[性状] 無定型

[比旋光度]: [α]<sub>D</sub> -65 (MeOH)

文献

Loew, P. et al., Chem. Comm., 1968, 1276, (構造決定, 生合成)

Battersby, A.R. et al., Chem. Comm., 1968, 1277, (誘導体)

Junior, P., Planta Med., 1991, 57, 181, (Exaltoside, Epiexaltoside)

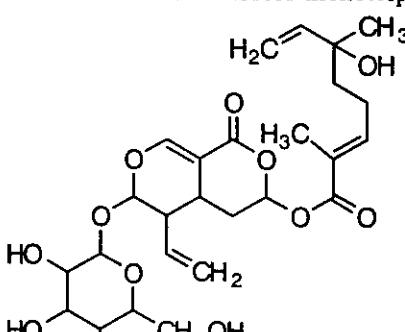
§ Foliamenthin; 8'-Deoxy, Δ<sup>7</sup>-isomer, 6'-hydroxy

[化学名・別名] Menthiafolin

[CAS No.] 19351-64-5

[化合物分類] テルペノイド (Secoiridoid monoterpenoids)

[構造式]



[分子式]

C<sub>26</sub>H<sub>36</sub>O<sub>12</sub>

[分子量]

540.563

[正確な分子量] 540.22068

[基原] *Menyanthes trifoliata*

[性状] 結晶

[融点] Mp 186 °C

[比旋光度]: [α]<sub>D</sub> -68 (MeOH)

文献

Loew, P. et al., Chem. Comm., 1968, 1276, (構造決定, 生合成)

Battersby, A.R. et al., Chem. Comm., 1968, 1277, (誘導体)

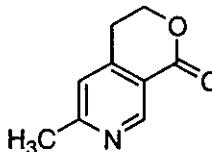
Junior, P., Planta Med., 1991, 57, 181, (Exaltoside, Epiexaltoside)

§ Gentianidine

[CAS No.] 2202-12-2

[化合物分類] 薬物: 筋肉骨格弛緩剤 (Muscle relaxants-skeletal), 薬物: 抗炎症薬 (Antiinflammatory agents), 薬物: 抗高血圧薬 (Antihypertensive agents), アルカロイド化合物 (Secologanin-derived monoterpenoid alkaloids)

[構造式]



[分子式]

C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>

[分子量] 163.176

[正確な分子量] 163.063329

[基原] 次の植物から得られるアルカロイド: *Gentiana asclepiadea*, *Gentiana macrophylla*, *Erythraea centaurium*, *Menyanthes trifoliata*, *Centaurium spicatum* (リンドウ科, ミツガシワ科)

[用途] Hypothermic, 抗高血圧, 抗炎症薬, 筋肉骨格弛緩剤. 低毒性

[融点] Mp 131-132 °C

[Log P 計算値] Log P 1.25 (計算値)

文献

Liang, H.-T. et al., Yaoxue Xuebao, 1964, 11, 412; CA, 62, 5309g, (分離, IR, UV, H-NMR, 合成法)

Popov, S. et al., Dokl. Bolg. Akad. Nauk, 1968, 21, 435; CA, 69, 52368v, (Mass)

Marekov, N.L. et al., Tetrahedron, 1968, 24, 1323, (合成法)

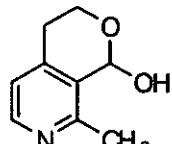
§ Gentiatibetine

[化学名・別名] Gentiotibetine

[CAS No.] 26005-36-7

[化合物分類] アルカロイド化合物 (Secologanin-derived monoterpenoid alkaloids)

[構造式]



[分子式]

C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>

[分子量] 165.191

[正確な分子量] 165.078979

[基原] 次の植物から得られるアルカロイド: *Gentiana asclepiadea*, *Gentiana lutea*, *Gentiana olivieri*, *Gentiana punctata*, *Gentiana purpurea*, *Gentiana tibetica*, *Menyanthes trifoliata* (リンドウ科, ミツガシワ科)

[融点] Mp 161.5 °C

文献

Rulko, F. et al., Pol. J. Chem. (Roczn. Chem.), 1967, 41, 567, (UV, IR, H-NMR, Mass, 構造決定)

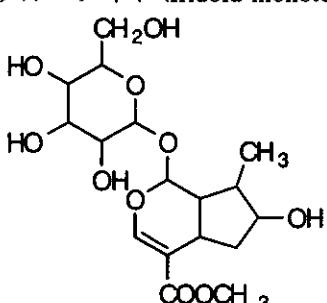
§ Loganic acid; Me ester

[化学名・別名] Loganin. Meliatin. Loganoside

[CAS No.] 18524-94-2

[化合物分類] テルペノイド (Iridoid monoterpenoids)

[構造式]



[分子式]

C<sub>17</sub>H<sub>26</sub>O<sub>10</sub>

[分子量]

390.386

[正確な分子量] 390.1526

[基原] *Strychnos nux-vomica*, *Menyanthes trifoliata*, その他の属

[用途] 多くのアルカロイドの生合成中間物質

[性状] 結晶 (EtOH)

[融点] Mp 223 °C

[比旋光度]: [α]<sub>D</sub> -83 (H<sub>2</sub>O)

[溶解性] BERDY SOL: 水に可溶; ヘキサンに難溶

文献

- Birch, A.J. et al., J.C.S., 1961, 1407, (構造決定)  
Bentley, T.W. et al., J.C.S.(C), 1967, 2234, (Mass)  
Asaka, Y. et al., Tetrahedron, 1970, 26, 2365, (Syringopicroside)  
Battersby, A.R., Alkaloids (London), 1971, 1, 31, (生合成)  
Bhakuni, D.S. et al., Indian J. Chem., 1972, 10, 454, (分離)  
Partridge, J.J. et al., J.A.C.S., 1973, 95, 532, (合成法)  
Büchi, G. et al., J.A.C.S., 1973, 95, 540, (合成法)  
Bisset, N.G. et al., Phytochemistry, 1974, 13, 265, (分離)  
Heckendorf, A.H. et al., J.O.C., 1976, 41, 2045, (C13-NMR)  
Au-Yeung, B.-W. et al., Chem. Comm., 1977, 81, (合成法)  
Bianco, A. et al., Phytochemistry, 1981, 20, 1873, (8-Epiloganin)  
Kon, K. et al., Helv. Chim. Acta, 1983, 66, 755, (合成法)  
Calis, I. et al., Helv. Chim. Acta, 1984, 67, 160, (Periclymenoside)  
Ikeshiro, Y. et al., Planta Med., 1984, 50, 485; 1987, 158, (Swertiaaside A, Senburiside II)  
Chulia, A.J. et al., J. Nat. Prod., 1985, 48, 54, (Depressoside)  
Calis, I. et al., J. Nat. Prod., 1985, 48, 108, (Periclymenosidic acid)  
Hewson, A.T. et al., J.C.S. Perkin 1, 1985, 2625, (合成法)  
Koenig, G. et al., Phytochemistry, 1985, 24, 1245, (Phenylpentadienoylepiloganin)  
Vandewalle, M. et al., Tetrahedron, 1986, 42, 4035, (合成法)  
Srivastava, V. et al., J. Nat. Prod., 1990, 53, 303, (Arborside B)  
Rasoanaivo, P. et al., Planta Med., 1991, 57, 486, (7-Caffeoylloganin)  
Young, M.C.M. et al., Phytochemistry, 1992, 31, 3433, (Loganetin)  
Garlaschelli, L. et al., Tetrahedron, 1992, 48, 9495, (合成法)  
Hsu, L.-F. et al., J.O.C., 1993, 58, 4756, (合成法)  
Itoh, A. et al., Phytochemistry, 1993, 33, 161, (7-Benzoylloganin acid)  
Lahloub, M.-F. et al., Phytochemistry, 1993, 33, 401, (7-p-Hydroxybenzoyl-8-epiloganic acid)  
Damtoft, S. et al., Phytochemistry, 1993, 34, 1291, (生合成)  
Tanahashi, T. et al., Chem. Pharm. Bull., 1995, 43, 729, (Jasheomslosides, 分離, H-NMR, C13-NMR, UV)  
Abdullaer, U.A. et al., Khim. Prir. Soedin., 1996, 32, 62; Chem. Nat. Compd. (Engl. Transl.), 1996, 32, 50, (Mass)  
Tomita, H. et al., Phytochemistry, 1996, 42, 239, (6'-glucoside, H-NMR, C13-NMR)  
Otsuka, H. et al., Phytochemistry, 1996, 42, 1435, (feruloyl esters)  
Bergeron, C. et al., Phytochemistry, 1997, 44, 633, (Linearoside)  
Damtoft, S. et al., Phytochemistry, 1997, 45, 743, (Ketologanic acid)  
Node, M. et al., Chem. Pharm. Bull., 1998, 46, 736, (合成法)  
Miyase, T. et al., J. Nat. Prod., 1999, 62, 1079, (Scrophularoside A)  
Tai, H.-M. et al., J.O.C., 1999, 64, 659, (Loganin, 合成法)  
Peacuterez, J.A. et al., Nat. Prod. Lett., 1999, 13, 247, (7-Dehydrologanetin)  
Eichinger, D. et al., Phytochemistry, 1999, 51, 223, (Loganin, 生合成)  
Carbonezi, C.A. et al., Phytochemistry, 1999, 51, 781, (Albosides)  
Helfrich, E. et al., Phytochemistry, 2000, 54, 191, (Gmephiloside)

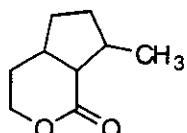
§ Mitsugashiwalactone; 8-Epimer

[化学名・別名] Onikulactone

[CAS No.] 60363-04-4

[化合物分類] テルペノイド (Iridoid monoterpenoids)

[構造式]



C<sub>9</sub>H<sub>14</sub>O<sub>2</sub>

[分子式]

[分子量] 154.208

[正確な分子量] 154.09938

[基原] 次の植物から分離: *Menyanthes trifoliata*

[用途] ネコ誘因物質

[性状] オイル

-----文献-----

- Sakan, T. et al., Nippon Kagaku Kaishi, 1969, 90, 507, (分離)  
Ohta, H. et al., J.O.C., 1977, 42, 1231, (合成法, IR, H-NMR, Mass)  
Marini-Bettolo, G.B. et al., Tetrahedron, 1983, 39, 323, (分離, 結晶構造, Boonein)  
Lee, T.V. et al., Chem. Comm., 1985, 371, (合成法, Boonein)  
Nugent, W.A. et al., J.O.C., 1986, 51, 3376  
Amri, M. et al., Tet. Lett., 1987, 28, 5521, (合成法)  
Weinges, K. et al., Annalen, 1993, 1029, (合成法, 絶対構造)  
Yamane, T. et al., Synthesis, 1995, 444, (合成法)  
Nangia, A. et al., Tetrahedron, 1996, 52, 3435, (合成法)  
Nangia, A. et al., Tetrahedron, 1997, 53, 14507, (レビュー, 合成法)

\*\*\*\*\*ハッコウシュ (Fermented alcoholic beverages) \*\*\*\*\*

§ § ワイン, シードル, マラスキーノ, シエリー, ビール, 清酒, ミリンなどの発酵酒。

\*\*\*\*\*ハッコウニュウ (Fermented milk) \*\*\*\*\*

§ § 家畜の乳汁(「ミルク」の項参照)を発酵して得られた発酵乳。

\*\*\*\*\*ハッコウミエキ (Fermented seasoning solution) \*\*\*\*\*

§ § 味液。

\*\*\*\*\*パッションフルーツ (Passion fruit) \*\*\*\*\*

§ § トケイソウ科クダモノトケイソウ (*Passiflora edulis* Sims) の果実, 花および葉。

§ 6-O- $\alpha$ -L-Arabinopyranosyl-D-glucose;  $\beta$ -Pyranose-form, Benzyl glycoside

[化学名・別名] Benzyl  $\beta$ -vicianoside

[CAS No.] 148031-67-8

[化合物分類] 炭水化物(Disaccharides), 单環芳香族(Simple benzyl alcohols)

[構造式] 有効な構造式はない

[分子式]  $C_{18}H_{26}O_{10}$

[分子量] 402.397

[正確な分子量] 402.1526

[基原] *Passiflora edulis* の果実

-----文献-----

- Helferich, B. et al., Annalen, 1928, 465, 166, (合成法)  
Kochetkov, N.K. et al., Zh. Obshch. Khim., 1967, 37, 338; CA, 67, 108856f, (合成法)  
Psenak, M. et al., Planta Med., 1972, 22, 93; CA, 77, 149673u, (分離)  
Balan, N.F. et al., Bioorg. Khim., 1980, 5, 1657; CA, 94, 103719m, (hepta-Ac)  
Bartlett, P.A. et al., J.A.C.S., 1980, 102, 337, (合成法)  
Paterson, I. et al., Tetrahedron, 1985, 41, 3569, (レビュー)  
Pearson, A.J. et al., Chem. Comm., 1988, 442, (合成法, 成書)

Chassagne, D. et al., Phytochemistry, 1996, 41, 1497, (benzyl glycoside)

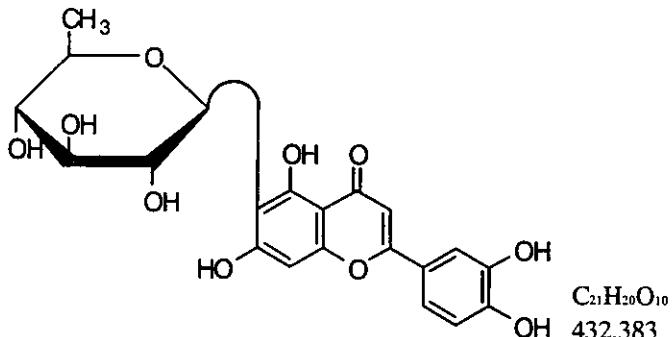
§ 6-C-(6-Deoxyglucopyranosyl)-3',4',5,7-tetrahydroxyflavone

[化学名・別名] 6-C-Chinovosylluteolin. 6-C-Quinovosylluteolin

[CAS No.] 132368-05-9

[化合物分類] フラボノイド(Flavones; 4 × O-置換基)

[構造式]



[分子式]

[分子量]

[正確な分子量] 432.10565

[基原] 次の植物から分離: *Passiflora edulis* *flavicarpa*

文献

Mareck, U. et al., Phytochemistry, 1991, 30, 3486, (分離, H-NMR, C13-NMR)

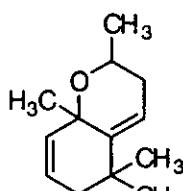
§ 5,9-Epoxy-3,6-megastigmadiene; ( $5\beta,9\alpha$ )-form

[化学名・別名] Edulan I

[CAS No.] 41678-29-9

[化合物分類] テルペノイド(Megastigmene norterpenoids)

[構造式]



[基原] Key

[性状] 才イ

[比旋光度]:  $[\alpha]_D +82.8$  (c, 0.39 in CH<sub>2</sub>Cl<sub>2</sub>)

文献

Prestwich, G.D. et al., Tetrahedron, 1970, 32, 2945, (Dihydroedulans)

Adams, D.R. et al., J.C.S. Perkin 1, 1975, 1736, (合成法)

Whitfield, F.B. et al., Aust. J. Chem., 1977, 30, 1073, (構造決定)

Winter, M. et al., Helv. Chim. Acta, 1979, 62, 131, (Epoxide)

Etoh, H. et al., Agric. Biol. Chem., 1980, 44, 2871

Winterhalter, P. et al., Chem. Ind. (London), 1990, 463, (分離)

Sugai, T. et al., Tetrahedron, 1991, 47, 7227, (合成法)

Weyerstahl, P. et al., Annalen, 1994, 415, (合成法)

Schmidt, G. et al., J. Agric. Food Chem., 1995, 43, 185, (合成法, H-NMR, 絶対構造)

Honda, T. et al., Tetrahedron: Asymmetry, 1997, 8, 837, (合成法, 絶対構造)

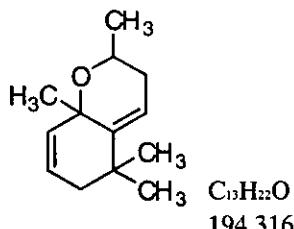
§ 5,9-Epoxy-3,6-megastigmadiene; ( $5\beta,9\alpha$ )-form, 6  $\beta$ ,7-Dihydro

[化学名・別名] 5,9-Epoxy-3-megastigmene. Dihydroedulan I

[CAS No.] 63335-66-0

[化合物分類] テルペノイド(Megastigmene norterpenoids)

[構造式]



[分子式]

C<sub>15</sub>H<sub>22</sub>O

[分子量]

194.316

[正確な分子量] 194.167065

[基原] *Passiflora edulis*

-----文献-----

Prestwich, G.D. et al., Tetrahedron, 1970, 32, 2945, (Dihydroedulans)

Adams, D.R. et al., J.C.S. Perkin 1, 1975, 1736, (合成法)

Whitfield, F.B. et al., Aust. J. Chem., 1977, 30, 1073, (構造決定)

Winter, M. et al., Helv. Chim. Acta, 1979, 62, 131, (Epoxide)

Etoh, H. et al., Agric. Biol. Chem., 1980, 44, 2871

Winterhalter, P. et al., Chem. Ind. (London), 1990, 463, (分離)

Sugai, T. et al., Tetrahedron, 1991, 47, 7227, (合成法)

Weyerstahl, P. et al., Annalen, 1994, 415, (合成法)

Schmidt, G. et al., J. Agric. Food Chem., 1995, 43, 185, (合成法, H-NMR, 絶対構造)

Honda, T. et al., Tetrahedron: Asymmetry, 1997, 8, 837, (合成法, 絶対構造)

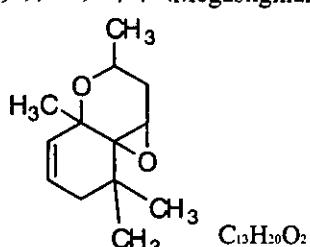
§ 5,9-Epoxy-3,6-megastigmadiene; (5 beta,9 alpha)-form, 6 alpha,7 alpha-Epoxide

[化学名・別名] 5,9:6,7-Diepoxy-3-megastigmene. 6,7-Epoxyedulan. Riesling acetal

[CAS No.] 69979-86-8

[化合物分類] テルペノイド (Megastigmene norterpenoids)

[構造式]



[分子式]

C<sub>15</sub>H<sub>20</sub>O<sub>2</sub>

[分子量]

208.3

[正確な分子量] 208.14633

[基原] 次の植物から分離: *Passiflora edulis*

[性状] オイル

-----文献-----

Prestwich, G.D. et al., Tetrahedron, 1970, 32, 2945, (Dihydroedulans)

Adams, D.R. et al., J.C.S. Perkin 1, 1975, 1736, (合成法)

Whitfield, F.B. et al., Aust. J. Chem., 1977, 30, 1073, (構造決定)

Winter, M. et al., Helv. Chim. Acta, 1979, 62, 131, (Epoxide)

Etoh, H. et al., Agric. Biol. Chem., 1980, 44, 2871

Winterhalter, P. et al., Chem. Ind. (London), 1990, 463, (分離)

Sugai, T. et al., Tetrahedron, 1991, 47, 7227, (合成法)

Weyerstahl, P. et al., Annalen, 1994, 415, (合成法)

Schmidt, G. et al., J. Agric. Food Chem., 1995, 43, 185, (合成法, H-NMR, 絶対構造)

Honda, T. et al., Tetrahedron: Asymmetry, 1997, 8, 837, (合成法, 絶対構造)

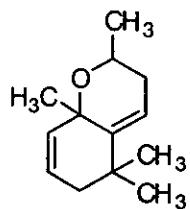
§ 5,9-Epoxy-3,6-megastigmadiene; (5 alpha,9 alpha)-form

[化学名・別名] Edulan II

[CAS No.] 41678-30-2

[化合物分類] テルペノイド (Megastigmene norterpenoids)

[構造式]



[基原] Key

[性状] オイ

[比旋光度]:  $[\alpha]_D +73.4$  ( $c, 0.39$  in  $\text{CH}_2\text{Cl}_2$ )

文献

Prestwich, G.D. et al., Tetrahedron, 1970, 32, 2945, (Dihydroedulans)

Adams, D.R. et al., J.C.S. Perkin 1, 1975, 1736, (合成法)

Whitfield, F.B. et al., Aust. J. Chem., 1977, 30, 1073, (構造決定)

Winter, M. et al., Helv. Chim. Acta, 1979, 62, 131, (Epoxide)

Etoh, H. et al., Agric. Biol. Chem., 1980, 44, 2871

Winterhalter, P. et al., Chem. Ind. (London), 1990, 463, (分離)

Sugai, T. et al., Tetrahedron, 1991, 47, 7227, (合成法)

Weyerstahl, P. et al., Annalen, 1994, 415, (合成法)

Schmidt, G. et al., J. Agric. Food Chem., 1995, 43, 185, (合成法, H-NMR, 絶対構造)

Honda, T. et al., Tetrahedron: Asymmetry, 1997, 8, 837, (合成法, 絶対構造)

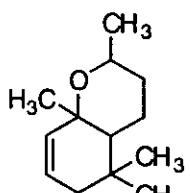
§ 5,9-Epoxy-3,6-megastigmadiene; ( $5\alpha,9\alpha$ )-form,  $6\alpha,7$ -Dihydro

[化学名・別名] Dihydroedulan II

[CAS No.] 41678-32-4

[化合物分類] テルペノイド (Megastigmene norterpenoids)

[構造式]



[分子式]

[分子量]

$\text{C}_{15}\text{H}_{22}\text{O}$

194.316

[正確な分子量] 194.167065

[基原] *Passiflora edulis*

文献

Prestwich, G.D. et al., Tetrahedron, 1970, 32, 2945, (Dihydroedulans)

Adams, D.R. et al., J.C.S. Perkin 1, 1975, 1736, (合成法)

Whitfield, F.B. et al., Aust. J. Chem., 1977, 30, 1073, (構造決定)

Winter, M. et al., Helv. Chim. Acta, 1979, 62, 131, (Epoxide)

Etoh, H. et al., Agric. Biol. Chem., 1980, 44, 2871

Winterhalter, P. et al., Chem. Ind. (London), 1990, 463, (分離)

Sugai, T. et al., Tetrahedron, 1991, 47, 7227, (合成法)

Weyerstahl, P. et al., Annalen, 1994, 415, (合成法)

Schmidt, G. et al., J. Agric. Food Chem., 1995, 43, 185, (合成法, H-NMR, 絶対構造)

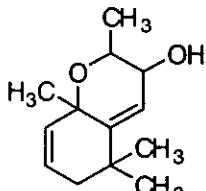
Honda, T. et al., Tetrahedron: Asymmetry, 1997, 8, 837, (合成法, 絶対構造)

§ 5,9-Epoxy-3,6-megastigmadien-8-ol; ( $5\alpha,8\beta,9\beta$ )-form

[CAS No.] 69927-26-0

[化合物分類] テルペノイド (Megastigmene norterpenoids)

[構造式]



[基原]

[性状] オイ

*Passiflora edulis*  
ル

文献

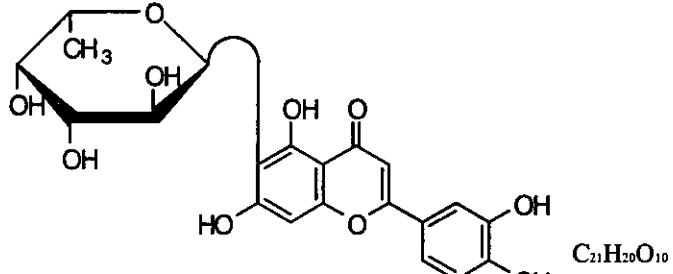
Winter, M. et al., Helv. Chim. Acta, 1979, 62, 131

§ 6-C-Fucopyranosyl-3',4',5,7-tetrahydroxyflavone

[化学名・別名] 6-C-Fucosylluteolin

[化合物分類] フラボノイド (Flavones; 4 × O-置換基)

[構造式]



[分子式]

[分子量]

[正確な分子量] 432.10565

[基原] 次の植物から分離: *Passiflora edulis*

文献

Mareck, U. et al., Phytochemistry, 1991, 30, 3486, (分離, H-NMR, C13-NMR)

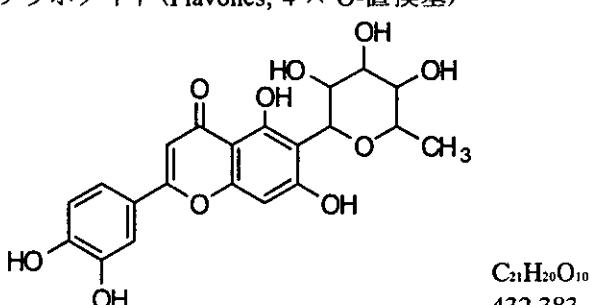
§ 6-C-Galactopyranosyl-3',4',5,7-tetrahydroxyflavone; 6''-Deoxy

[化学名・別名] 6-C-(6-Deoxygalactopyranosyl)-3',4',5,7-tetrahydroxyflavone. 6-C-Fucopyranosylluteolin

[CAS No.] 132368-06-0

[化合物分類] フラボノイド (Flavones; 4 × O-置換基)

[構造式]



[分子式]

[分子量]

[正確な分子量] 432.10565

[基原] *Passiflora edulis flavicarpa* の果汁

文献

Peterson, P.M. et al., Biochem. Syst. Ecol., 1987, 15, 647, (分離)

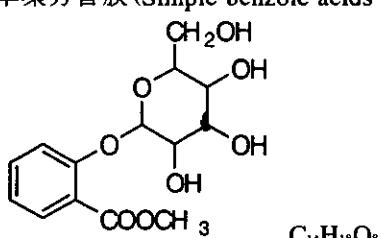
Herrara, Y. et al., Biochem. Syst. Ecol., 1991, 19, 665, (分離)

§ 2-Hydroxybenzoic acid; O- $\beta$ -D-Glucopyranoside, Me ester

[CAS No.] 10019-60-0

[化合物分類] 单環芳香族 (Simple benzoic acids and esters)

[構造式]



[分子式]

[分子量] 314.291

[正確な分子量] 314.10017

[基原] *Passiflora edulis*, *Pluchea indica*

[性状] 結晶 (EtOH)

[融点] Mp 106-108 °C

[比旋光度]:  $[\alpha]_D -67.7$  (c, 0.9 in H<sub>2</sub>O)

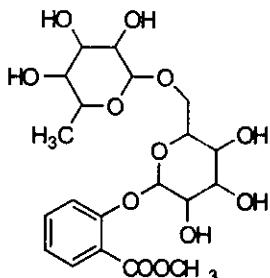
文献

- Levy, G., Drug Metab. Rev., 1979, 9, 1, (レビュー, 代謝)  
Goldsmith, L.A., Int. J. Dermatol., 1979, 18, 32, (レビュー, 薬理)  
Babhair, S.A. et al., Anal. Profiles Drug Subst., 1984, 13, 521, (レビュー)  
Brune, K. et al., Arzneim.-Forsch., 1984, 34, 1060, (レビュー, 薬理)  
Klicke, S. et al., Phytochemistry, 1988, 27, 2177, (生育, 配糖体)  
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, 21, 601, (レビュー)  
Vane, J.R. et al., Aspirin and Other Salicylates, Chapman and Hall, 1992, (専門書)  
Grynkiewicz, G. et al., Pol. J. Chem. (Roczn. Chem.), 1993, 63, 1251, (配糖体, 合成法)  
Abounassif, M.A. et al., Anal. Profiles Drug Subst., 1994, 23, 421, (レビュー)  
Raskin, I., Plant Horm. (2nd edn.), 1995, 188, (レビュー)

§ 2-Hydroxybenzoic acid; *O*-[ $\alpha$ -L-Rhamnopyranosyl-(1  $\rightarrow$  6)- $\beta$ -D-glucopyranoside], Me ester

[化合物分類] 单環芳香族 (Simple benzoic acids and esters)

[構造式]



[分子式]  $C_{20}H_{28}O_{12}$

[分子量] 460.43

[正確な分子量] 460.15808

[基原] *Passiflora edulis* の果実

文献

- Levy, G., Drug Metab. Rev., 1979, 9, 1, (レビュー, 代謝)  
Goldsmith, L.A., Int. J. Dermatol., 1979, 18, 32, (レビュー, 薬理)  
Babhair, S.A. et al., Anal. Profiles Drug Subst., 1984, 13, 521, (レビュー)  
Brune, K. et al., Arzneim.-Forsch., 1984, 34, 1060, (レビュー, 薬理)  
Klicke, S. et al., Phytochemistry, 1988, 27, 2177, (生育, 配糖体)  
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, 21, 601, (レビュー)  
Vane, J.R. et al., Aspirin and Other Salicylates, Chapman and Hall, 1992, (専門書)  
Grynkiewicz, G. et al., Pol. J. Chem. (Roczn. Chem.), 1993, 63, 1251, (配糖体, 合成法)  
Abounassif, M.A. et al., Anal. Profiles Drug Subst., 1994, 23, 421, (レビュー)  
Raskin, I., Plant Horm. (2nd edn.), 1995, 188, (レビュー)  
Liu, J.H. et al., J. Chromatogr., B: Biomed. Appl., 1996, 675, 61, (HPLC)

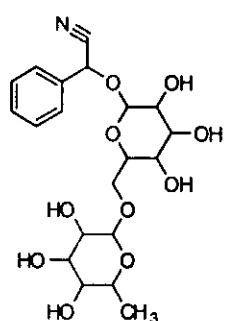
§ 2-Hydroxy-2-phenylacetonitrile; (*R*)-form, *O*-[ $\alpha$ -L-Rhamnopyranosyl-(1  $\rightarrow$  6)- $\beta$ -D-glucopyranoside]

[化学名・別名] Mandelonitrile rutinoside

[CAS No.] 184002-37-7

[化合物分類] 单環芳香族 (Phenylacetic acid derivatives), 炭水化物 (Cyanogenic glycosides)

[構造式]



[分子式]  $C_{20}H_{27}NO_{10}$

[分子量] 441.434

[正確な分子量] 441.163499

[基原] *Passiflora edulis* の果実

文献

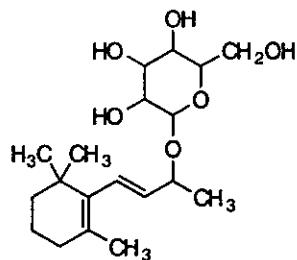
- Jones, M.B. et al., Science (Washington, D.C.), 1961, 134, 284, (分離, (±)-form)  
Towers, G.H.N. et al., Tetrahedron, 1964, 20, 71, (H-NMR, 配糖体)  
Turczan, J.W. et al., J. Assoc. Off. Anal. Chem., 1978, 61, 192; 1979, 62, 190, (H-NMR, 誘導体)

§ 5,7-Megastigmadien-9-ol; (*7E,9*  $\xi$ )-form, *O*- $\beta$ -D-Glucopyranoside

[CAS No.] 146610-77-7

[化合物分類] テルペノイド (Megastigmene norterpenoids)

[構造式]



[分子式] C<sub>19</sub>H<sub>32</sub>O<sub>6</sub>

[分子量] 356.458

[正確な分子量] 356.21989

[基原] *Passiflora edulis*

[用途] 4,6,8-megastigmatrienes の前駆体 (4,6,8-Megastigmatriene を参照)

文献

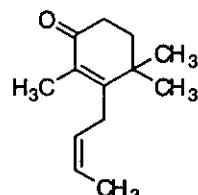
Herderich, M. et al., Nat. Prod. Lett., 1993, 2, 227, (分離, H-NMR, C13-NMR, 合成法)

### § 5,8-Megastigmadien-4-one; (E)-form

[CAS No.] 67401-26-7

[化合物分類] テルペノイド (Megastigmene norterpenoids)

[構造式]



[基原] *Nicotiana tabacum*, *Passiflora edulis*

[性状] オイル

文献

Demole, E. et al., Helv. Chim. Acta, 1979, 62, 67

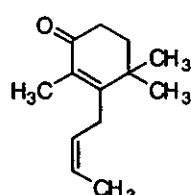
Boulin, B. et al., Tetrahedron, 2000, 56, 3927, (合成法)

### § 5,8-Megastigmadien-4-one; (Z)-form

[CAS No.] 67401-25-6

[化合物分類] テルペノイド (Megastigmene norterpenoids)

[構造式]



[基原] *Passiflora edulis*

[性状] オイル

文献

Demole, E. et al., Helv. Chim. Acta, 1979, 62, 67

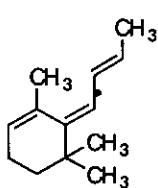
Boulin, B. et al., Tetrahedron, 2000, 56, 3927, (合成法)

### § 4,6,8-Megastigmatriene; (6E,8E)-form

[CAS No.] 51468-86-1

[化合物分類] テルペノイド (Megastigmene norterpenoids)

[構造式]



[基原] *Passiflora edulis*

[性状] オイル

文献

Barjot, J. et al., Bull. Soc. Chim. Fr., 1973, 3187, (合成法)

Whitfield, F.B. et al., Aust. J. Chem., 1979, 32, 891, (分離)

### § 4,6,8-Megastigmatriene; (6Z,8E)-form

[CAS No.] 51468-85-0

[化合物分類] テルペノイド (Megastigmene norterpenoids)

[構造式]



[基原] *Passiflora edulis*

[性状] オイル

文献

Barjot, J. et al., Bull. Soc. Chim. Fr., 1973, 3187, (合成法)

Whitfield, F.B. et al., Aust. J. Chem., 1979, 32, 891, (分離)

### § 3-Mercapto-1-hexanol; ( $\xi$ )-form, S-Me

[化合物分類] 脂肪族化合物 (Saturated unbranched alcohols)

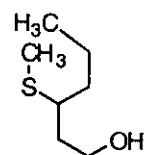
[構造式]

[分子量] 148.269

[正確な分子量] 148.092185

[基原] 次の植物から分離: yellow passion fruit *Passiflora edulis* f. *flavicarpa*

[性状] 緑色, 脂肪, 硫黄臭を持つオイル



文献

Aldrich Library of  $^{13}\text{C}$  and  $^1\text{H}$  FT NMR Spectra, 1992, 1, 442C, (NMR)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, 3, 361C, (IR)

Ger. Pat., 1974, 2 338 680; CA, 80, 132786, (合成法)

Winter, M. et al., Helv. Chim. Acta, 1976, 59, 1613, (分離, H-NMR, Mass, 合成法)

Heusinger, G. et al., Tet. Lett., 1984, 25, 507

Engel, K.H. et al., J. Agric. Food Chem., 1991, 39, 2249, (S-Me, Ac)

Weber, B. et al., Z. Lebensm.-Unters. -Forsch., 1992, 195, 426, (S-Me, Ac)

### § 3-Mercapto-1-hexanol; ( $\xi$ )-form, S-Me, O-Ac

[CAS No.] 51755-85-2

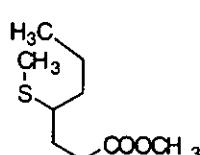
[構造式]

[分子式]  $\text{C}_9\text{H}_{14}\text{O}_2\text{S}$

[分子量] 190.306

[正確な分子量] 190.10275

[基原] Identified in *Passiflora edulis* の揮発性オイル



文献

Winter, M. et al., Helv. Chim. Acta, 1976, 59, 1613, (分離, H-NMR, Mass, 合成法)

Heusinger, G. et al., Tet. Lett., 1984, 25, 507

Engel, K.H. et al., J. Agric. Food Chem., 1991, 39, 2249, (S-Me, Ac)

Weber, B. et al., Z. Lebensm.-Unters. -Forsch., 1992, 195, 426, (S-Me, Ac)

### § 7-Methoxy-1-methyl- $\beta$ -carboline

[化学名・別名] 7-Methoxy-1-methyl-9*H*-pyrido[3,4-*b*]indole (CAS名). Harmine. Telepathine. Yageine. Banisterine

[CAS No.] 442-51-3

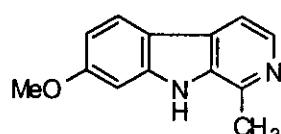
[化合物分類] アルカロイド化合物 ( $\beta$ -Carboline alkaloids), 薬物: 抗パーキンソン薬 (Antiparkinsonian agents), 薬物: 中枢神経興奮薬 (Central stimulants)

[構造式]

[分子式]  $\text{C}_{13}\text{H}_{12}\text{N}_2\text{O}$

[分子量] 212.251

[正確な分子量] 212.094963



[基原] 次の植物から得られるアルカロイド: *Peganum harmala*, いくつかの *Banisteriopsis* spp., *Passiflora edulis*, いくつかの他の属 (ハマビシ科, キントラノオ科, トケイソウ科)

[用途] 抗パーキンソン薬, 中枢神経興奮薬, 酸塩基の蛍光指示薬として使われる (pH 7.2-8.9 で色が青→黄色に変化). 南アメリカの幻覚を起こさせる飲み物の成分

[性状] 結晶

[融点] Mp 264-265 °C (257-259 °C)

[PKa 値] pK<sub>a</sub> 7.61 (20 °C)

[Log P 計算値] Log P 3.12 (計算値)

[UV]: [neutral]  $\lambda_{\text{max}}$  210 (); 240 (); 300 (); 338 () (MeOH)

[傷害・毒性] 筋肉内ルートにより人の胃腸及び中枢神経系に作用する. 50 % 致死量 (LD<sub>50</sub>) (マウス, 皮下) 243 mg/kg

[化学物質毒性データ総覧 (RTECS) 登録番号] UV0175000

文献

Ismailov, N.A. et al., Farm. Farmakol, 1938, 4, 8, (用途)

Schlittler, E. et al., Helv. Chim. Acta, 1953, 36, 996, (合成法)

Bishop, E., Indicators, Pergamon, Oxford, 1972, 695, (用途)