

[比旋光度]:  $[\alpha]_D^{26} +80$  (c, 0.3 in CHCl<sub>3</sub>)

-----文献-----

Chandra, A. et al., *Phytochemistry*, 1987, 26, 3077

§ 4,6-Tetradecadiene-8,10,12-triyn-1-ol; (*E, E*)-form, Ac

[化学名・別名] 1-Acetoxy-4,6-tetradecadiene-8,10,12-triyne

[CAS No.] 6581-87-9

[化合物分類] 脂肪族化合物 (Acetylenic acid and ester)

[構造式]

[分子式] C<sub>16</sub>H<sub>16</sub>O<sub>2</sub>

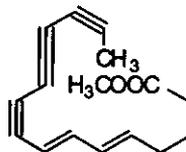
[分子量] 240.301

[正確な分子量] 240.11503

[基原] 次の植物から分離: *Tanacetum vulgare* と *Rudbeckia fulgida* の根, *Anthemis*, *Artemisia*, *Chrysanthemum* spp.

[性状] 結晶 (petrol)

[融点] Mp 36-37 °C (31.5 °C)



-----文献-----

Bohlmann, F. et al., *Chem. Ber.*, 1960, 93, 1937; 1962, 95, 1733; 1964, 97, 1179; 1965, 98, 1411; 1966, 99, 1830; 2096, (分離, UV, H-NMR, 構造決定)

Bohlmann, F. et al., *Phytochemistry*, 1982, 21, 1793, (分離, epoxide)

Herz, W. et al., *Phytochemistry*, 1985, 24, 89, (分離)

§ 2,8,9-Trihydroxy-1(10),4,11(13)-germacatrien-12,6-olide; (1(10)*E*,2 $\beta$ ,4*E*,6 $\alpha$ ,8 $\xi$ )-form, 9-Ketone

[化学名・別名] 2 $\beta$ ,9 $\xi$ -Dihydroxy-8-oxo-1(10),4,11(13)-germacatrien-12,6 $\alpha$ -olide

[化合物分類] テルペノイド (12,6-Germacranolide sesquiterpenoid)

[構造式]

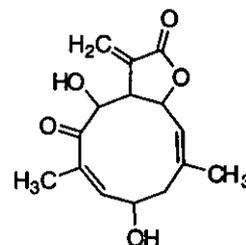
[分子式] C<sub>15</sub>H<sub>18</sub>O<sub>5</sub>

[分子量] 278.304

[正確な分子量] 278.115425

[基原] 次の植物から分離: *Tanacetum vulgare*

[性状] オイル



-----文献-----

Quijano, L. et al., *Phytochemistry*, 1979, 18, 843, (Montafusin A)

Bohlmann, F. et al., *Phytochemistry*, 1985, 24, 2029, (分離, H-NMR, Mas)

Quijano, L. et al., *Phytochemistry*, 1986, 25, 695, (Montafusin B, 結晶構造)

Chandra, A. et al., *Phytochemistry*, 1987, 26, 1463, (ketone)

§ *Vulgarolide*

[CAS No.] 120674-40-0

[化合物分類] テルペノイド (Miscellaneous monocyclic sesquiterpenoid)

[構造式]

[分子式] C<sub>15</sub>H<sub>20</sub>O<sub>5</sub>

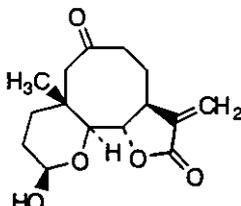
[分子量] 280.32

[正確な分子量] 280.131075

[基原] *Tanacetum vulgare*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{25} -45$  (c, 1 in CHCl<sub>3</sub>)



-----文献-----

Appendino, G. et al., *Gazz. Chim. Ital.*, 1988, 118, 55, (分離, H-NMR, C13-NMR)

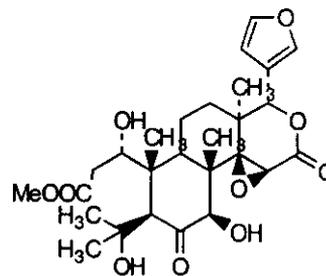
Paquette, L.A. et al., *Tet. Lett.*, 1995, 36, 673, (合成法)

\*\*\*\*\*タンジェリン (Tangerine, Mandarin) \*\*\*\*\*

§ § ミカン科タンジェリン (マンダリン) (*Citrus reticulata* Blanco) の果実。

§ Calamin

[CAS No.] 74751-40-9  
 [化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)  
 [構造式]  
 [分子式]  $C_{27}H_{36}O_{10}$   
 [分子量] 520.575  
 [正確な分子量] 520.23085  
 [基原] calamondin の種子 (*Citrus reticulata*)  
 [性状] 結晶 (MeOH)  
 [融点] Mp 162-165 °C

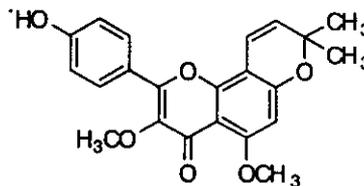


-----文献-----

Bennett, R.D. et al., *Tetrahedron*, 1981, 37, 17

§ Citrusinol; 3,6-Di-Me ether

[化学名・別名] 2-(4-Hydroxyphenyl)-3,6-dimethoxy-8,8-dimethyl-4H,8H-benzo[1,2-b:3,4-b']dipyran-4-one  
 [CAS No.] 157072-30-5  
 [化合物分類] フラボノイド (Flavonol; 4 × O-置換基), フラボノイド (Cyclised C-isopentenylated flavonoid)  
 [構造式]  
 [分子式]  $C_{22}H_{20}O_6$   
 [分子量] 380.396  
 [正確な分子量] 380.12599  
 [基原] tangerine (*Citrus reticulata* cv. blanco) の果実  
 [融点] Mp 225-226 °C

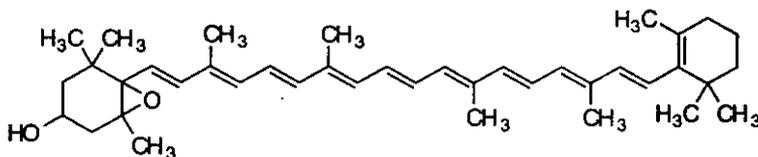


-----文献-----

Wu, T.S. et al., *Phytochemistry*, 1987, 26, 3094, (分離)  
 Fukai, T. et al., *Phytochemistry*, 1988, 27, 259, (Ikarisoside E)  
 Hu, B.H. et al., *Yaoxue Xuebao*, 1992, 27, 397; *CA*, 117, 167659, (Acuminatin)  
 Saxena, V.K. et al., *Phytochemistry*, 1994, 36, 1039, (di-Me ether)

§  $\beta$ -Cryptoxanthin; 5R,6S-Epoxy

[化学名・別名] 5,6-Epoxy-5,6-dihydro- $\beta$ ,  $\beta$ -caroten-3-ol. Cryptoxanthin epoxide  
 [CAS No.] 188116-19-0  
 [その他の CAS No.] 29291-23-4  
 [化合物分類] テルペノイド (Tetraterpenoid)  
 [構造式]  
 [分子式]  $C_{40}H_{56}O_2$   
 [分子量] 568.881  
 [正確な分子量] 568.42803  
 [基原] 次の植物から分離: *Capsicum annuum*, 熟した persimmon (*Diospyros kaki*) の皮, *Prunus persica* の成熟した果実, mandarin hybrid (*Citrus reticulata*) の熟した皮  
 [性状] 結晶 ( $C_6H_6$ /petrol)  
 [融点] Mp 154 °C



-----文献-----

Karrer, P. et al., *Helv. Chim. Acta*, 1946, 29, 229, (合成法)  
 Subbarayan, C. et al., *Anal. Biochem.*, 1965, 12, 275  
 Lassertois, D. et al., *Phytochemistry*, 1978, 17, 411, (分離)  
 Farin, D. et al., *Phytochemistry*, 1983, 22, 403, (分離)  
 Ebert, G. et al., *Phytochemistry*, 1985, 24, 29, (分離)

§  $\beta$ -Cryptoxanthin; 5  $\xi$ , 6  $\xi$ -Epoxide

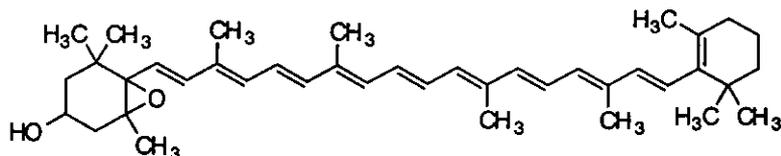
[化学名・別名] 5',6'-Epoxy-5',6'-dihydro- $\beta$ , $\beta$ -caroten-3-ol

[CAS No.] 29291-23-4

[化合物分類] テルペノイド

(Tetraterpenoid)

[構造式]



[分子式]  $C_{40}H_{56}O_2$

[分子量] 568.881

[正確な分子量] 568.42803

[基原] 次の植物から分離: *Citrus reticulata*

[性状] 結晶 ( $C_6H_6$ /petrol)

[融点] Mp 158-160 °C

-----文献-----

Karrer, P. et al., *Helv. Chim. Acta*, 1946, 29, 229, (合成法)

Lassertois, D. et al., *Phytochemistry*, 1978, 17, 411, (分離)

Farin, D. et al., *Phytochemistry*, 1983, 22, 403, (分離)

Ebert, G. et al., *Phytochemistry*, 1985, 24, 29, (分離)

§ Cyclocalamin

[CAS No.] 74751-39-6

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)

[構造式]

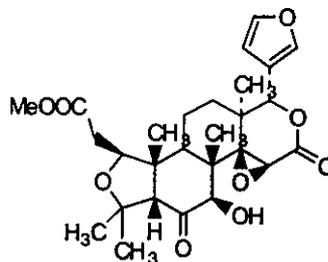
[分子式]  $C_{27}H_{34}O_9$

[分子量] 502.56

[正確な分子量] 502.220285

[基原] calamondin の種子 (*Citrus reticulata*)

[性状] ガム



-----文献-----

Bennett, R.D. et al., *Tetrahedron*, 1981, 37, 17, (Cyclocalamin)

Herman, Z. et al., *Phytochemistry*, 1987, 26, 2247, (Isocyclocalamin)

Hasegawa, S. et al., *Phytochemistry*, 1988, 27, 1349, (生合成)

§ Cyclocalamin; 7-Ketone, 6  $\beta$ -alcohol

[化学名・別名] Isocyclocalamin

[CAS No.] 111004-32-1

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)

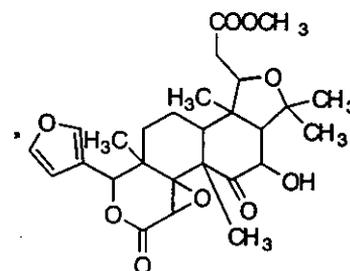
[構造式]

[分子式]  $C_{27}H_{34}O_9$

[分子量] 502.56

[正確な分子量] 502.220285

[基原] *Citrus reticulata* / *Fortunella hybrid*



-----文献-----

Herman, Z. et al., *Phytochemistry*, 1987, 26, 2247, (Isocyclocalamin)

Hasegawa, S. et al., *Phytochemistry*, 1988, 27, 1349, (生合成)

§ 3,4-Di-O-caffeoylquinic acid; 3''-Me ether

[化学名・別名] 5-Hydroxy-3,3',7,8-tetramethoxy-4',5'-methylenedioxyflavone

[CAS No.] 161697-25-2

[化合物分類] 脂肪族化合物 (Monocarbocyclic carboxylic acid and lactone)

[構造式]

[分子式]  $C_{26}H_{26}O_{12}$

[分子量] 530.484

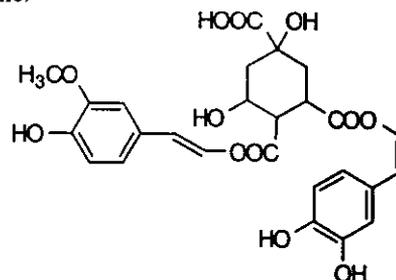
[正確な分子量] 530.14243

[基原] *Citrus reticulata* の果実

[性状] 無定型の黄色の塊

[比旋光度]:  $[\alpha]_D^{25} -24.7$  (c, 0.1 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  206 (); 216 (); 233 (); 328 () (EtOH)



-----文献-----

Scarpati, M.L., Tet. Lett., 1964, 2851-2853, (分離)

Taylor, A.O., Phytochemistry, 1968, 7, 63-71, (分離)

Timmermann, B.N. et al., J. Nat. Prod., 1983, 46, 365-368, (分離, H-NMR, C13-NMR, Mas)

Iwahashi, H. et al., Phytochemistry, 1985, 24, 630-632, (Caffeoylferuloylquinic acid)

Nishizawa, M. et al., Chem. Pharm. Bull., 1986, 34, 1419-1421; 1987, 35, 2133-2135, (誘導體)

Chen, M. et al., Yaoxue Xuebao, 1994, 29, 617-620, (Macroantoin F)

Lin, L.-C. et al., J. Nat. Prod., 1999, 62, 405-408, (分離, H-NMR, C13-NMR)

Choi, E.M. et al., Phytochemistry, 2001, 56, 733-739, (3-Caffeoyl-4-feruloylquinic acid)

### § 3,4-Di-O-caffeoylquinic acid; 3'-Me ether, Me ester

[化学名・別名] 5-Hydroxy-3,3',7,8-tetramethoxy-4',5'-methylenedioxyflavone

[化合物分類] 脂肪族化合物 (Monocarbocyclic carboxylic acid and lactone)

[構造式]

[分子式]  $C_{27}H_{28}O_{12}$

[分子量] 544.511

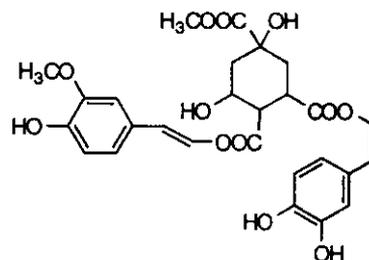
[正確な分子量] 544.15808

[基原] *Citrus reticulata* の果実

[性状] 無定型の塊

[比旋光度]:  $[\alpha]_D^{25} -171$  (c, 0.1 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  219 (); 236 (); 328 () (EtOH)



-----文献-----

Scarpati, M.L., Tet. Lett., 1964, 2851-2853, (分離)

Taylor, A.O., Phytochemistry, 1968, 7, 63-71, (分離)

Timmermann, B.N. et al., J. Nat. Prod., 1983, 46, 365-368, (分離, H-NMR, C13-NMR, Mas)

Iwahashi, H. et al., Phytochemistry, 1985, 24, 630-632, (Caffeoylferuloylquinic acid)

Nishizawa, M. et al., Chem. Pharm. Bull., 1986, 34, 1419-1421; 1987, 35, 2133-2135, (誘導體)

Chen, M. et al., Yaoxue Xuebao, 1994, 29, 617-620, (Macroantoin F)

Lin, L.-C. et al., J. Nat. Prod., 1999, 62, 405-408, (分離, H-NMR, C13-NMR)

Choi, E.M. et al., Phytochemistry, 2001, 56, 733-739, (3-Caffeoyl-4-feruloylquinic acid)

### § 3,3',4',5,5',7,8-Heptahydroxyflavone; 3,3',7,8-Tetra-Me, 4',5'-methylene ether

[化学名・別名] 5-Hydroxy-3,3',7,8-tetramethoxy-4',5'-methylenedioxyflavone

[CAS No.] 161697-25-2

[化合物分類] フラボノイド (Flavonol; 7 × O-置換基)

[構造式]

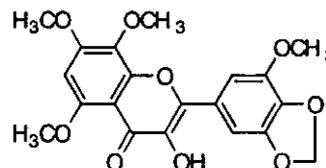
[分子式]  $C_{20}H_{18}O_9$

[分子量] 402.357

[正確な分子量] 402.095085

[基原] *Citrus reticulata* の果実

[用途] 抗ウイルス薬



-----文献-----

Saxena, V.K. et al., J. Inst. Chem. (India), 1994, 66, 62, (3,3',7,8-tetra-Me, 4',5'-methylene ether)

### § 3,3',4',5,6,8-Hexahydroxyflavone; Hexa-Me ether

[化学名・別名] 3,3',4',5,6,8-Hexamethoxyflavone

[CAS No.] 218945-14-3

[化合物分類] フラボノイド (Flavonol; 6 × O-置換基)

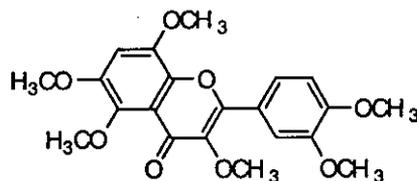
[構造式]

[分子式]  $C_{21}H_{22}O_8$

[分子量] 402.4

[正確な分子量] 402.13147

[基原] *Citrus reticulata*



-----文献-----

Abdel-Alim, M.A. et al., Egypt. J. Pharm. Sci., 1997, 38, 131

§ 3',4',5,6,7,8-Hexahydroxyflavone; 4',5,6,7,8-Penta-Me ether

[化学名・別名] 3'-Hydroxy-4',5,6,7,8-pentamethoxyflavone

[CAS No.] 112448-39-2

[化合物分類] フラボノイド (Flavone; 6 × O-置換基)

[構造式]

[分子式]  $C_{20}H_{20}O_8$

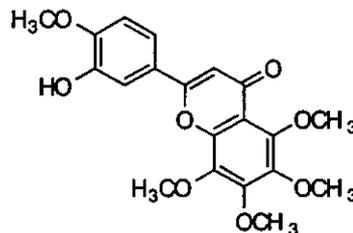
[分子量] 388.373

[正確な分子量] 388.11582

[基原] mandarin orange (*Citrus reticulata*)

[性状] 結晶 (EtOAc/hexane)

[融点] Mp 139-140 °C



-----文献-----

Mizuno, M. et al., Chem. Pharm. Bull., 1987, 35, 3125, (3'-Hydroxy-4',5,6,7,8-pentamethoxyflavone)

Mizuno, M. et al., J. Nat. Prod., 1987, 50, 751, (分離, 合成法)

§ 3',4',5,6,7,8-Hexahydroxyflavone; 3',5,6,7,8-Penta-Me ether

[化学名・別名] 4'-Hydroxy-3',5,6,7,8-pentamethoxyflavone

[CAS No.] 34810-62-3

[化合物分類] フラボノイド (Flavone; 6 × O-置換基)

[構造式]

[分子式]  $C_{20}H_{20}O_8$

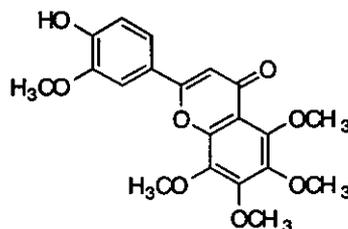
[分子量] 388.373

[正確な分子量] 388.11582

[基原] *Eupatorium leucolepis*, *Citrus reticulata*

[性状] 結晶 (MeOH 溶液) (またガムとも記載される)

[融点] Mp 147-148 °C



-----文献-----

Wagner, H. et al., Chem. Ber., 1971, 104, 3357, (4'-Hydroxy-3',5,6,7,8-pentamethoxyflavone)

Iinuma, M. et al., Chem. Pharm. Bull., 1980, 23, 717, (4'-Hydroxy-3',5,6,7,8-pentamethoxyflavone)

33, 46, (Estragonoside)

§ 3',4',5,6,7,8-Hexahydroxyflavone; 3',4',5,6,8-Penta-Me ether

[化学名・別名] 7-Hydroxy-3',4',5,6,8-pentamethoxyflavone

[CAS No.] 149402-88-0

[化合物分類] フラボノイド (Flavone; 6 × O-置換基)

[構造式]

[分子式]  $C_{20}H_{20}O_8$

[分子量] 388.373

[正確な分子量] 388.11582

[基原] mandarin orange (*Citrus reticulata*)

[性状] 針状結晶 (MeOH)

[融点] Mp 190-191 °C



-----文献-----

Sugiyama, S. et al., Chem. Pharm. Bull., 1993, 41, 714, (7-Hydroxy-3',4',5,6,8-pentamethoxyflavone)

§ *p*-Mentha-1,8-dien-7-ol; (*R*)-form

[CAS No.] 5503-12-8

[化合物分類] テルペノイド (*p*-Menthane monoterpene)

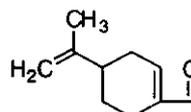
[構造式]

[基原] 次の植物から分離: *Siler trilobum*, *Sium latifolium*, *Citrus reticulata*, その他の植物

[性状] オイル

[沸点] Bp, 99-104 °C

[比旋光度]:  $[\alpha]_D +137$



-----文献-----

Acton, E.M. et al., *Experientia*, 1970, 26, 473, (構造決定)

Suga, T. et al., *Bull. Chem. Soc. Jpn.*, 1972, 45, 545, (stereochem)

Fujita, T. et al., *Phytochemistry*, 1993, 34, 1545, (Perilloside B)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DKX100; PCJ000

§ *p*-Mentha-1,8-dien-6-ol

[化学名・別名] 2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-ol. 5-Isopropenyl-2-methyl-2-cyclohexen-1-ol.

Carveol. FEMA 2247

[CAS No.] 99-48-9

[関連 CAS No.] 1197-06-4, 1197-07-5

[化合物分類] テルペノイド (*p*-Menthane monoterpene)

[構造式]

[分子式] C<sub>10</sub>H<sub>16</sub>O

[分子量] 152.236

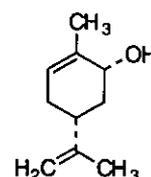
[正確な分子量] 152.120115

[基原] 次の植物に存在する: グレープフルーツ (*Citrus paradisi*) のオイル, mandarin (*Citrus reticulata*), *Heracleum canescens*, *Cymbopogon martini* and present in blackcurrant berries, セロリー, ブラックティ, dill, caraway seed and lamb's lettuce

[用途] 香水に使われる. 香気成分

[傷害・毒性] 50%致死量 (LD<sub>50</sub>) (ラット, 経口) 3000 mg/kg

[化学物質毒性データ総覧 (RTEC) 登録番号] OS8400000



(4*R*,6*R*)-form

-----文献-----

Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1973, 11, 1055, (レビュー, 毒性)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 107, (レビュー)

Bouwmeester, H.J. et al., *Phytochemistry*, 1999, 50, 243, (生合成)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MKY250

\*\*\*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

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-)] 11, 1055, 1973

\*\*\*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 : 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

FCTXAV Food and Cosmetics Toxicology. (London, UK) V.1-19, 1963-81. For publisher information, see FCTOD7. [Vol.,頁,年(19-)]11,1055,1973

§ 2-(4-Methylphenyl)-2-propanol

[化学名・別名]  $\alpha, \alpha, 4$ -Trimethylbenzenemethanol (CAS 名).  $\alpha, \alpha, 4$ -Trimethylbenzyl alcohol (旧 CAS 名). Dimethyl-*p*-tolylcarbinol.  $\alpha$ -Hydroxy-*p*-cymene. *p*-(Hydroxyisopropyl) toluene. 8-*p*-Cymenol.

*p*-Mentha-1,3,5-trien-8-ol

[CAS No.] 1197-01-9

[化合物分類] テルペノイド (*p*-Menthane monoterpene)

[構造式]

[分子式]  $C_{10}H_{14}O$

[分子量] 150.22

[正確な分子量] 150.104465

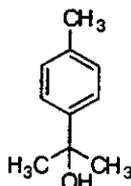
[基原] 精油に存在する, 例えば, *Citrus reticulata*

[融点] Mp 9 °C

[沸点] Bp<sub>75</sub> 145 °C. Bp<sub>16</sub> 112 °C

[濃度]  $d^{20}_D$  0.975

[屈折率]  $n^{20}_D$  1.5173



-----文献-----

Oki, M. et al., Bull. Chem. Soc. Jpn., 1963, 36, 1, (H-NMR)

Kugler, E. et al., Helv. Chim. Acta, 1963, 46, 1480, (分離)

§ 3',4',5,6,7-Pentahydroxyflavone; 3',4',5,6-Tetra-Me ether

[化学名・別名] 7-Hydroxy-3',4',5,6-tetramethoxyflavone

[CAS No.] 40983-99-1

[化合物分類] フラボノイド (Flavone; 5 × O-置換基)

[構造式]

[分子式]  $C_{19}H_{16}O_7$

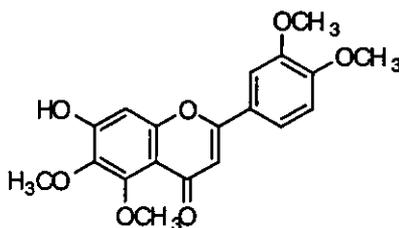
[分子量] 358.347

[正確な分子量] 358.105255

[基原] 次の植物から分離: *Citrus reticulata*

[性状] 針状結晶 (CHCl<sub>3</sub>/hexane)

[融点] Mp 205-208 °C



-----文献-----

Laux, D.O. et al., Phytochemistry, 1985, 24, 1081, (7-Hydroxy-3',4',5,6-tetramethoxyflavone, Bausplendin)

Mizuno, M. et al., J. Nat. Prod., 1987, 50, 751, (7-Hydroxy-3',4',5,6-tetramethoxyflavone)

§ 3',4',5,6,8-Pentahydroxyflavone; Penta-Me ether

[化学名・別名] 3',4',5,6,8-Pentamethoxyflavone

[CAS No.] 62953-03-1

[化合物分類] フラボノイド (Flavonol; 5 × O-置換基)

[構造式]

[分子式]  $C_{20}H_{20}O_7$

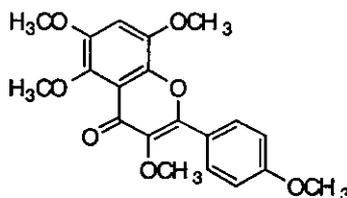
[分子量] 372.374

[正確な分子量] 372.120905

[基原] *Citrus reticulata*

[性状] 針状結晶 (EtOH)

[融点] Mp 142-144 °C



-----文献-----

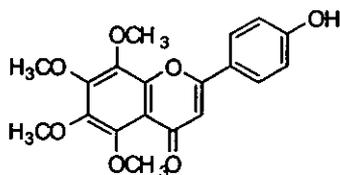
Horie, T. et al., Bull. Chem. Soc. Jpn., 1982, 55, 2933, (合成法, 構造決定)

Abdel-Alim, M.A. et al., Egypt. J. Pharm. Sci., 1997, 38, 131, (Pentamethoxyflavone, 分離)

§ 4',5,6,7,8-Pentahydroxyflavone; 5,6,7,8-Tetra-Me ether

[化学名・別名] 4'-Hydroxy-5,6,7,8-tetramethoxyflavone

[CAS No.] 36950-98-8  
 [化合物分類] フラボノイド (Flavone; 5 × O-置換基)  
 [構造式]  
 [分子式]  $C_{19}H_{18}O_7$   
 [分子量] 358.347  
 [正確な分子量] 358.105255  
 [基原] *Citrus reticulata*  
 [性状] 針状結晶 ( $C_6H_6$ )  
 [融点] Mp 196-198 °C

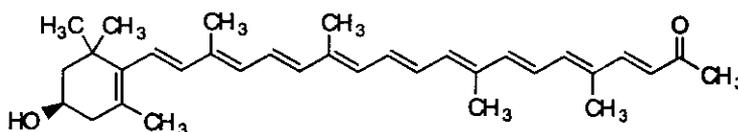


-----文献-----

Iinuma, M. et al., Chem. Pharm. Bull., 1980, 28, 708; 717, (C13-NMR, Gardenin B, 4'-Hydroxy-5,6,7,8-tetramethoxyflavone)

### § Reticulataxanthin

[化学名・別名] 3-Hydroxy-6'-methyl-6'-apo-β-caroten-6'-one. Reticulaxanthin. 3-Hydroxycitraniaxanthin  
 [CAS No.] 28368-09-4  
 [化合物分類] テルペノイド (Apocarotenoid)  
 [構造式]  
 [分子式]  $C_{39}H_{44}O_2$   
 [分子量] 472.709  
 [正確な分子量] 472.33413  
 [基原] *Citrus reticulata*, *Minneola*



*tangor*

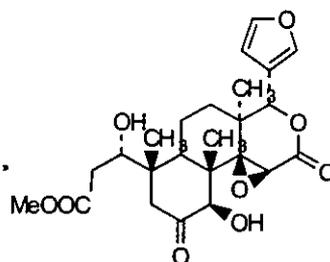
[性状] 橙-赤色の結晶 (Et<sub>2</sub>O/petrol)  
 [融点] Mp 171-172 °C  
 [その他のデータ] 非天然物

-----文献-----

Yokoyama, H. et al., J.O.C., 1965, 30, 2482, (分離, 構造決定, H-NMR)  
 Yokoyama, H. et al., Phytochemistry, 1966, 5, 1159, (8'-hydroxy-7',8'-dihydroreticulataxanthin)  
 de Ville, T.E. et al., Chem. Comm., 1969, 1311, (絶対構造)

### § Retrocalamin

[CAS No.] 74729-98-9  
 [化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)  
 [構造式]  
 [分子式]  $C_{23}H_{30}O_9$   
 [分子量] 462.496  
 [正確な分子量] 462.188985  
 [基原] calamondin の種子 (*Citrus reticulata*)  
 [性状] 結晶 ( $C_6H_6$ )  
 [融点] Mp 197-199 °C

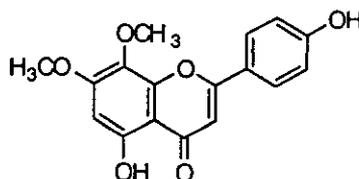


-----文献-----

Bennett, R.D. et al., Tetrahedron, 1981, 37, 17

### § 4',5,7,8-Tetrahydroxyflavone; 7,8-Di-Me ether

[化学名・別名] 4',5-Dihydroxy-7,8-dimethoxyflavone  
 [CAS No.] 6608-33-9  
 [化合物分類] フラボノイド (Flavone; 4 × O-置換基)  
 [構造式]  
 [分子式]  $C_{17}H_{14}O_6$   
 [分子量] 314.294  
 [正確な分子量] 314.07904  
 [基原] *Scutellaria* spp. の葉と茎, また *Citrus reticulata* の皮から得られる  
 [性状] 結晶 (EtOH)  
 [融点] Mp 292-294 °C

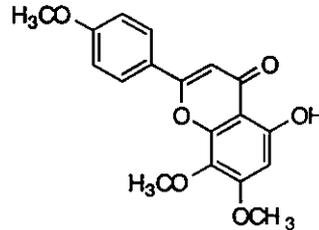


-----文献-----

- C.Djerassi et al., Dictionary of Natural Products, Chapman, Hall, 2002  
 Tatum, J.H. et al., *Phytochemistry*, 1978, 17, 447, (4',5,7,8-Tetramethoxyflavone)  
 Transl.), 1982, 18, 235, (Acetylisostachyflaside)  
 Tomimori, T. et al., *Yakugaku Zasshi*, 1982, 102, 388, (4',5,7-Trihydroxy-8-methoxyflavone)  
 Reynaud, J. et al., *Pharmazie*, 1983, 38, 628, (4',5,7-Trihydroxy-8-methoxyflavone)  
 Markham, K.R. et al., *Phytochemistry*, 1983, 22, 143, (分離)

§ 4',5,7,8-Tetrahydroxyflavone; 4',7,8-Tri-Me ether

[化学名・別名] 5-Hydroxy-4',7,8-trimethoxyflavone  
 [CAS No.] 57096-03-4  
 [化合物分類] フラボノイド (Flavone; 4 × O-置換基)  
 [構造式]  
 [分子式] C<sub>18</sub>H<sub>16</sub>O<sub>6</sub>  
 [分子量] 328.321  
 [正確な分子量] 328.09469  
 [基原] *Citrus reticulata*  
 [性状] 黄色の針状結晶 (EtOAc)  
 [融点] Mp 220-221 °C

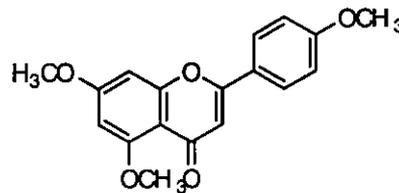


-----文献-----

- Tatum, J.H. et al., *Phytochemistry*, C.Djerassi et al., Dictionary of Natural Products, Chapman, Hall, 2002  
 1978, 17, 447, (4',5,7,8-Tetramethoxyflavone)  
 Reynaud, J. et al., *Pharmazie*, 1983, 38, 628, (4',5,7-Trihydroxy-8-methoxyflavone)  
 Ramesh, P. et al., *J. Nat. Prod.*, 1995, 58, 1242, (5,8-Dihydroxy-4',7-dimethoxyflavone)

§ 4',5,7-Trihydroxyflavone; Tri-Me ether

[化学名・別名] 4',5,7-Trimethoxyflavone  
 [CAS No.] 5631-70-9  
 [化合物分類] フラボノイド (Flavone; 3 × O-置換基)  
 [構造式]  
 [分子式] C<sub>18</sub>H<sub>16</sub>O<sub>5</sub>  
 [分子量] 312.321  
 [正確な分子量] 312.099775  
 [基原] *Cassia siamea* の葉に存在する, また *Citrus reticulata*, *Boesenbergia pandurata*, *Garcinia kola* から  
 も得られる  
 [性状] 針状結晶 (EtOH)  
 [融点] Mp 156-157 °C

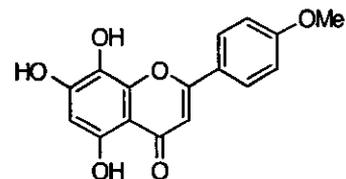


-----文献-----

- Matsuura, S. et al., *Chem. Pharm. Bull.*, 1978, 26, 305, (合成法, 4',5,7-Trimethoxyflavone)  
 Jaipetch, T. et al., *Phytochemistry*, 1983, 22, 625, (4',5,7-Trimethoxyflavone)

§ 5,7,8-Trihydroxy-4'-methoxyflavone

[化学名・別名] 5,7,8-Trihydroxy-2-(4-methoxyphenyl)-4H-1-benzopyran-4-one (CAS 名). Takakin. Isoscutellarein 4'-methyl ether  
 [CAS No.] 51876-19-8  
 [化合物分類] フラボノイド (Flavone; 4 × O-置換基)  
 [構造式]  
 [分子式] C<sub>16</sub>H<sub>12</sub>O<sub>6</sub>  
 [分子量] 300.267  
 [正確な分子量] 300.06339  
 [基原] 次の植物から分離: *Stachys inflata* の地上部, *Takakia* spp., *Citrus reticulata*, *Veronica filiformis*, *Scutellaria baicalensis*  
 [性状] 黄色の針状結晶 (MeOH)



[融点] Mp 275-277 °C で分解

-----文献-----

Transl.), 1978, 14, 445, (分離, H-NMR)  
Markham, K.R. et al., *Phytochemistry*, 1979, 18, 611, (分離)  
Inuma, M. et al., *Yakugaku Zasshi*, 1980, 100, 657, (分離)  
Chari, M.M. et al., *Phytochemistry*, 1981, 20, 1977, (分離)  
Chen, Z.-T. et al., *Heterocycles*, 1994, 38, 1399, (8-glucuronide)  
Sharaf, M. et al., *Fitoterapia*, 1998, 69, 47, (8-glucoside)

§ 3',5,7-Trihydroxy-4',6,8-trimethoxyflavone (旧 CAS 名)

[化学名・別名] 5,7-Dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-6,8-dimethoxy-4H-1-benzopyran-4-one (CAS 名). Acerosin

[CAS No.] 15835-74-2

[化合物分類] フラボノイド (Flavone; 6 × O-置換基)

[構造式]

[分子式] C<sub>18</sub>H<sub>16</sub>O<sub>8</sub>

[分子量] 360.32

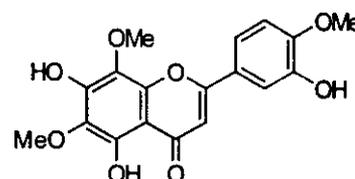
[正確な分子量] 360.08452

[基原] 次の植物から分離: *Iva acerosa*, *Vitex negundo*, *Helianthus strumosus*, *Gardenia* spp., *Citrus reticulata* の果実の皮

[用途] エストロゲン性を示す

[性状] 結晶 (CHCl<sub>3</sub>/Et<sub>2</sub>O/hexane)

[融点] Mp 239-241 °C



-----文献-----

Gupta, S.R. et al., *Indian J. Chem.*, 1975, 13, 785, (分離)  
Subramanian, P.M. et al., *J. Nat. Prod.*, 1979, 42, 540, (配糖体)  
Inuma, M. et al., *Chem. Pharm. Bull.*, 1980, 28, 717, (分離)  
Herz, W. et al., *Phytochemistry*, 1984, 23, 1453, (分離)  
Bhargava, S.K., *Plant. Med. Phytother.*, 1984, 18, 74, (分離, 性質)

\*\*\*\*\*タンポポ (Dandelion) \*\*\*\*\*

§ § キク科セイヨウタンポポ (*Taraxacum officinale* Weber) の根 (焙煎) または全草。

§ 1,3-Dihydroxy-12,6-eudesmanolide; (1 β, 3 β, 4 β, 6 α, 11 α H)-form

[化学名・別名] 4,11,13,15-Tetrahydroorientin B

[CAS No.] 75991-58-1

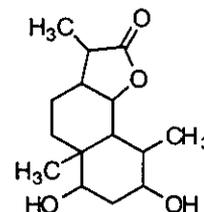
[化合物分類] テルペノイド (12,6-Eudesmanolide sesquiterpenoid)

[構造式]

[基原] *Taraxacum officinale*

[性状] 結晶 (Et<sub>2</sub>O/petrol)

[融点] Mp 141-142 °C



-----文献-----

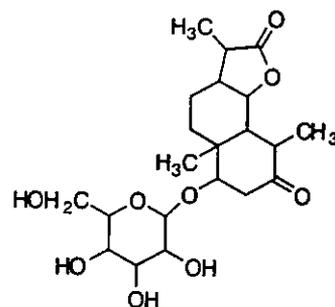
Haensel, R. et al., *Phytochemistry*, 1980, 19, 837; 857, (Tetrahydroorientin B, Arsanin glucoside)  
Banerjee, A.K. et al., *Tetrahedron*, 1993, 43, 4761, (合成法, レビュー)

§ 1,3-Dihydroxy-12,6-eudesmanolide; (1 β, 4 α, 6 α, 11 α H)-form, 3-Ketone, 1-O-β-D-glucopyranoside

[CAS No.] 75911-12-5

[化合物分類]テルペノイド(12,6-Eudesmanolide sesquiterpenoid)  
[構造式]

[分子式]  $C_{21}H_{32}O_9$   
[分子量] 428.478  
[正確な分子量] 428.204635  
[基原] *Taraxacum officinale*  
[性状] 無定型の結晶 (as tetra-Ac)  
[融点] Mp 192 °C (tetra-Ac)

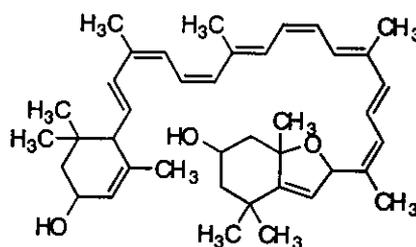


-----文献-----

Haensel, R. et al., *Phytochemistry*, 1980, 19, 837; 857, (Tetrahydroorientin B, Arsanin glucoside)  
Banerjee, A.K. et al., *Tetrahedron*, 1993, 43, 4761, (合成法, レビュー)  
Yang, D.S. et al., *Arch. Pharmacol. Res.*, 1996, 19, 507; *CA*, 126, 190812g, (配糖体)

§ 5,8-Epoxy-5,8-dihydro- $\beta, \epsilon$ -carotene-3,3'-diol; (3*S*,3'*R*,5*R*,6'*R*,8*R*)-form

[化学名・別名] Flavoxanthin  
[CAS No.] 512-29-8  
[化合物分類]テルペノイド(Tetraterpenoid)  
[構造式]  
[基原] 次の植物から分離: *Taraxacum officinale*, *Ranunculus acer*,  
*Senecio vernalis*, その他の植物  
[性状] 赤色結晶 (MeOH)  
[融点] Mp 175.5-177.5 °C  
[比旋光度]:  $[\alpha]_D^{25} +265$

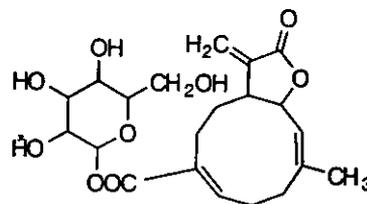


-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 1847  
Cadosch, H. et al., *Helv. Chim. Acta*, 1978, 61, 783, (分離, CD, H-NMR, C13-NMR)  
Straub, O. et al., *Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 248; 249, (成書)

§ 1(10),4,11(13)-Germacatrien-12,6-olid-14-oic acid; (1(10)*Z*,4*E*,6  $\alpha$ )-form,  $\beta$ -D-Glucopyranosyl ester

[化合物分類]テルペノイド(12,6-Germacranolide sesquiterpenoid)  
[構造式]  
[分子式]  $C_{21}H_{32}O_9$   
[分子量] 424.447  
[正確な分子量] 424.173335  
[基原] *Taraxacum officinale*  
[性状] 結晶 ( $CH_2Cl_2$ /MeOH)  
[融点] Mp 84-86 °C

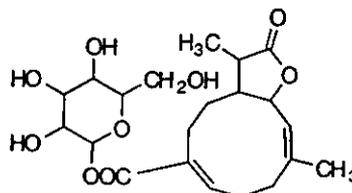


-----文献-----

Hansel, R. et al., *Phytochemistry*, 1980, 19, 857  
Jin, H., *Yakugaku Zasshi*, 1982, 102, 911, (Taraxinic acid)  
Miyase, T. et al., *Chem. Pharm. Bull.*, 1984, 32, 3043, (Ainsliaside B)  
Maldonado, E. et al., *Phytochemistry*, 1987, 26, 205, (Perydiscolic acid)

§ 1(10),4,11(13)-Germacatrien-12,6-olid-14-oic acid; (1(10)*Z*,4*E*,6  $\alpha$ )-form, 11,13-Dihydro,  $\beta$ -D-glucopyranosyl ester

[化合物分類]テルペノイド(12,6-Germacranolide sesquiterpenoid)  
[構造式]  
[分子式]  $C_{21}H_{30}O_9$   
[分子量] 426.463  
[正確な分子量] 426.188985  
[基原] *Taraxacum officinale*



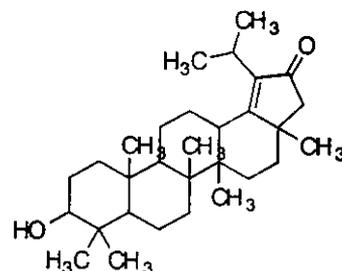
[性状] 結晶  
[融点] Mp 84-86 °C

-----文献-----

Hansel, R. et al., *Phytochemistry*, 1980, 19, 857  
Jin, H., *Yakugaku Zasshi*, 1982, 102, 911, (Taraxinic acid)  
Miyase, T. et al., *Chem. Pharm. Bull.*, 1984, 32, 3043, (Ainsliaside B)  
Maldonado, E. et al., *Phytochemistry*, 1987, 26, 205, (Perydiscolic acid)

§ 3-Hydroxy-18-lupen-21-one; 3 β -form

[CAS No.] 29367-66-6  
[化合物分類] テルペノイド (Lupane triterpenoid)  
[構造式]



[基原] *Taraxacum officinale*

-----文献-----

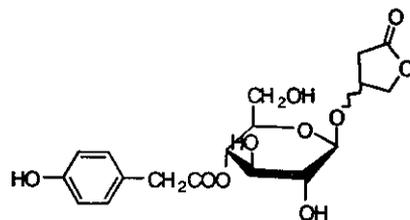
Kisiel, W. et al., *Pol. J. Chem. (Rocz. Chem.)*, 2000, 74, 281; *CA*, 132, 191798t, (分離, H-NMR, C13-NMR)

§ Taraxacoside

[CAS No.] 98449-40-2  
[化合物分類] 炭水化物 (gluco-Hexose), 含酸素複素環式化合物 (Butanolide)  
[構造式]

[分子式] C<sub>18</sub>H<sub>22</sub>O<sub>10</sub>  
[分子量] 398.366  
[正確な分子量] 398.1213

[基原] *Taraxacum officinale*  
[性状] 結晶 (CHCl<sub>3</sub>/EtOH/Me<sub>2</sub>CO)  
[融点] Mp 178-180 °C



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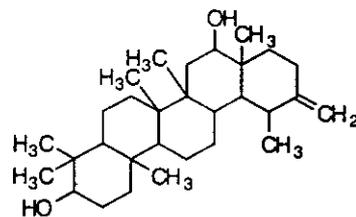
Rauwald, H.-W. et al., *Phytochemistry*, 1985, 24, 1557

§ 20(30)-Taraxastene-3,16-diol; (3 β, 16 β)-form

[化学名・別名] Arnidenediol, Arnidiol  
[CAS No.] 6750-30-7  
[化合物分類] テルペノイド (Taraxastane triterpenoid)  
[構造式]

[基原] *Taraxacum officinale* と *Arnica montana* を含む多くの植物にみられる

[融点] Mp 257 °C  
[比旋光度]: [α]<sub>D</sub> +81.2



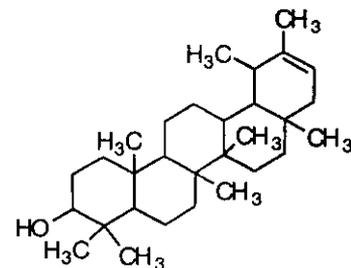
-----文献-----

Santer, J.O. et al., *J.O.C.*, 1962, 27, 3204, (分離)  
Kasprzyk, Z. et al., *Phytochemistry*, 1972, 11, 1961, (生合成)  
St. Pyrek, J. et al., *Tet. Lett.*, 1973, 809, (構造決定)  
St. Pyrek, J.S. et al., *Pol. J. Chem. (Rocz. Chem.)*, 1977, 51, 2331, (分離, H-NMR)  
Cassady, J.M. et al., *Phytochemistry*, 1978, 17, 324

§ 20-Taraxasten-3-ol; 3 β -form

[化学名・別名] ψ-Taraxasterol, Heterolupeol, Calendol, Pseudotaraxasterol  
[CAS No.] 464-98-2  
[化合物分類] テルペノイド (Taraxastane triterpenoid)  
[構造式]

[基原] *Taraxacum officinale*, *Calendula officinalis*. また *Doona* spp., *Arnica montana*, *Sonchus* spp., その他からも得られる



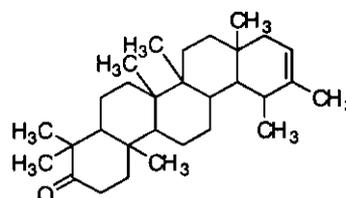
[性状] 結晶 (EtOH)  
[融点] Mp 217-219 °C  
[比旋光度]:  $[\alpha]_D^{25} +50$  (CHCl<sub>3</sub>)

-----文献-----

Ames, T.R. et al., J.C.S., 1954, 1905, (構造決定)  
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 2013, (生育)  
Kasprzyk, Z. et al., Phytochemistry, 1972, 11, 1961, (生合成)  
Reynolds, W.F. et al., Tetrahedron, 1986, 42, 3419, (H-NMR, C13-NMR)

§ 20-Taraxasten-3-ol; 3 β -form, Ketone

[化学名・別名] 20-Taraxasten-3-one. ψ-Taraxasterone. Pseudotaraxasterone  
[CAS No.] 16054-73-2  
[化合物分類] テルペノイド (Taraxastane triterpenoid)  
[構造式]  
[分子式] C<sub>30</sub>H<sub>48</sub>O  
[分子量] 424.709  
[正確な分子量] 424.370515  
[基原] *Shorea negrosensis*, *Verbesina encelioides*, *Taraxacum officinale*

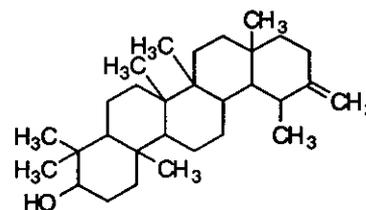


-----文献-----

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 2013, (生育)  
Kasprzyk, Z. et al., Phytochemistry, 1972, 11, 1961, (生合成)  
Reynolds, W.F. et al., Tetrahedron, 1986, 42, 3419, (H-NMR, C13-NMR)

§ 20(30)-Taraxasten-3-ol; (3 β, 18 α, 19 α)-form

[化学名・別名] Taraxasterol. α-Lactuceryl. α-Anthesterin. Taraxasterin. Inusterol A. Pyrethrol. Saussurol  
[化合物分類] テルペノイド (Taraxastane triterpenoid)  
[構造式]  
[基原] *Taraxacum officinale* の根, *Anthemis nobilis* の花. その他の多くの植物  
[性状] 結晶 (EtOH)  
[融点] Mp 225.5-226 °C  
[比旋光度]:  $[\alpha]_D^{17} +95.9$  (CHCl<sub>3</sub>)

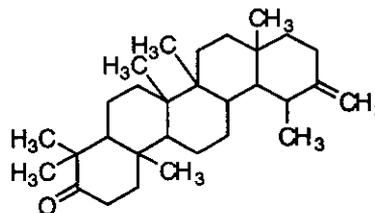


-----文献-----

Arthur, H.R. et al., Aust. J. Chem., 1969, 22, 597, (分離)  
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 2012, (生育)  
Reynolds, W.F. et al., Tetrahedron, 1986, 42, 3419, (C13-NMR)  
Anjaneyulu, V. et al., Phytochemistry, 1989, 28, 1471, (分離, H-NMR, C13-NMR)

§ 20(30)-Taraxasten-3-ol; (3 β, 18 α, 19 α)-form, 3-Ketone

[化学名・別名] 20(30)-Taraxasten-3-one. Taraxasterone  
[CAS No.] 6786-16-9  
[化合物分類] テルペノイド (Taraxastane triterpenoid)  
[構造式]  
[分子式] C<sub>30</sub>H<sub>48</sub>O  
[分子量] 424.709  
[正確な分子量] 424.370515  
[基原] 次の植物から分離: *Piptolepis leptospermoides*, *Balanophora indica*, *Pterocaulon virgatum*, *Taraxacum officinale*, その他  
[性状] 結晶 (Me<sub>2</sub>CO)  
[融点] Mp 182-183 °C



-----文献-----

Arthur, H.R. et al., Aust. J. Chem., 1969, 22, 597, (分離)

Kasprzyk, Z. et al., *Phytochemistry*, 1972, 11, 1961, (生合成)  
 Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 2012, (生育)  
 Anjaneyulu, V. et al., *Phytochemistry*, 1989, 28, 1471, (分離, H-NMR, C13-NMR)

§ 14-Taraxeren-3-ol; 3 β -form

[化学名・別名] Taraxerol. Skimmiol. Alnulin

[CAS No.] 127-22-0

[化合物分類] テルペノイド (Taraxerane triterpenoid), 薬物: 抗薬 (Antiulcerogenic agent)

[構造式]

[基原] *Taraxacum officinale*, *Alnus* spp., *Skimmia japonica*, *Rhododendron* spp., *Euphorbia* spp., その他の植物. 広く分布する. また *Pertusaria ophthalmiza* にも含まれる (本来の地衣類には含まれない)

[用途] 強い抗潰瘍性

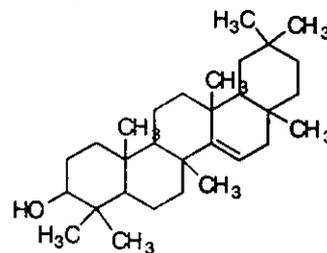
[性状] 結晶 (C<sub>30</sub>H<sub>48</sub>)

[融点] Mp 282-283 °C

[比旋光度]: [α]<sub>D</sub><sup>20</sup> +0.72 (c, 0.974 in CHCl<sub>3</sub>)

[Log P 計算値] Log P 10.66 (未確認値) (計算値)

[その他のデータ] 地衣類 *Pertusaria communis* から得られた Pertusarin と同定された (Hesse, 1898)



-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 1970, (生育)

Parvez, M. et al., *Acta Cryst. C*, 1999, 55, 213, (Taraxerone, 分離, 結晶構造)

Billodeaux, D.R. et al., *Acta Cryst. C*, 1999, 55, 2129, (Taraxerol Ac, 結晶構造)

\*\*\*\*\*チェリモラ (Cherimoya) \*\*\*\*\*

§ § パンレイシ科チェリモヤ (*Annona cherimolia* Miller) の果実.

§ Annocherin

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式] C<sub>33</sub>H<sub>52</sub>O<sub>7</sub>

[分子量] 594.871

[正確な分子量] 594.449555

[基原] *Annona cherimolia* の種子成分

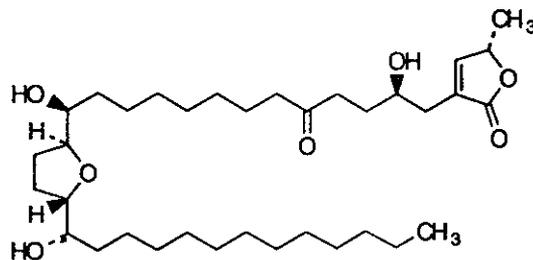
[用途] 細胞毒

[性状] 粉末

[融点] Mp 80.2-81.5 °C

[比旋光度]: [α]<sub>D</sub><sup>20</sup> +1.1 (c, 0.01 in CH<sub>2</sub>Cl<sub>2</sub>)

[UV]: [neutral] λ<sub>max</sub> 227 (log ε 3.4) (MeOH)



-----文献-----

Woo, M.-H. et al., *J. Nat. Prod.*, 1999, 62, 1250

§ Annocherinone

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式] C<sub>33</sub>H<sub>52</sub>O<sub>7</sub>

[分子量] 594.871

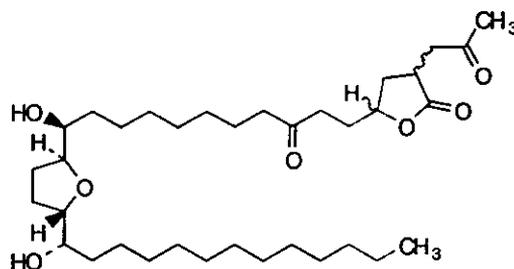
[正確な分子量] 594.449555

[基原] *Annona cherimolia* の種子成分

[用途] 細胞毒

[性状] 粉末

[融点] Mp 76.1-78 °C



[比旋光度]: $[\alpha]_D^{22} -1.3$  (c, 0.005 in  $\text{CH}_2\text{Cl}_2$ )

[UV]:[neutral]  $\lambda_{\text{max}} 205$  (log  $\epsilon$  3.6) (MeOH)

-----文献-----

Woo, M.-H. et al., J. Nat. Prod., 1999, 62, 1250

§ **Annogalene; 20-Epimer, 23,24-dihydro**

[化学名・別名] Annosenegalin

[CAS No.] 176200-77-4

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $\text{C}_{37}\text{H}_{66}\text{O}_7$

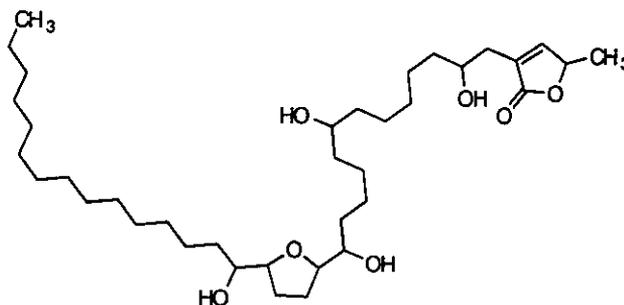
[分子量] 624.94

[正確な分子量] 624.496505

[基原] *Annona cherimolia*, *Annona senegalensis*

[性状] 無定型

[比旋光度]: $[\alpha]_D +15$  (c, 0.3 in  $\text{CHCl}_3$ )



-----文献-----

Colman-Saizarbitoria, T. et al., J. Nat. Prod., 1994, 57, 1661, (Xylomatenin)

Sahpaz, S. et al., Phytochemistry, 1996, 42, 103, (分離, H-NMR, C13-NMR, Mas)

§ **Annomolin**

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $\text{C}_{35}\text{H}_{64}\text{O}_7$

[分子量] 596.886

[正確な分子量] 596.465205

[基原] *Annona cherimolia* の種子

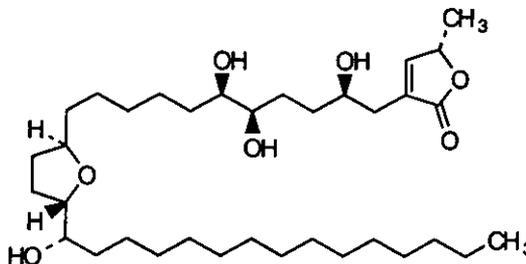
[用途] 細胞毒

[性状] 粉末

[融点] Mp 60.5-61.2 °C

[比旋光度]: $[\alpha]_D^{23} +4$  (c, 0.02 in  $\text{CH}_2\text{Cl}_2$ )

[UV]:[neutral]  $\lambda_{\text{max}} 230$  (log  $\epsilon$  3.2) (MeOH)



-----文献-----

Kim, D.H. et al., J. Nat. Prod., 2001, 64, 502-506

§ **Bullatanocin**

[化学名・別名] Annonin IV. Cherimolin 2. Crassiflorin. Purpureacin 1. Squamostatin C

[関連 CAS No.] 125882-64-6

[その他の CAS No.] 150134-21-7, 151637-38-6, 157184-02-6, 159249-82-8

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $\text{C}_{37}\text{H}_{66}\text{O}_8$

[分子量] 638.924

[正確な分子量] 638.47577

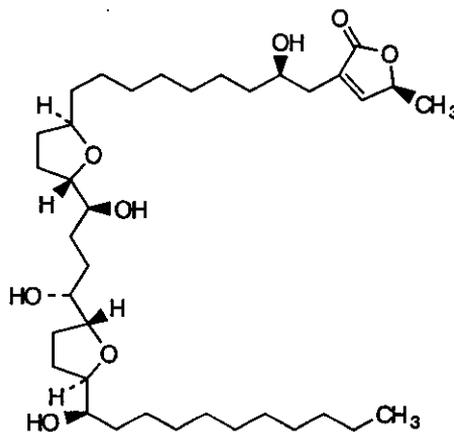
[基原] *Annona squamosa*, *Annona bullata*, *Annona cherimolia*,  
*Annona glabra*, *Annona crassiflora*, *Annona purpurea*

[性状] 無定型のワックス

[融点] Mp 107-109 °C (95-97 °C)

[比旋光度]: $[\alpha]_D^{25} +13.6$  (c, 0.28 in  $\text{CH}_2\text{Cl}_2$ )

[UV]:[neutral]  $\lambda_{\text{max}} 215$  ( $\epsilon$  5000) (EtOH)



-----文献-----

Cepleanu, F. et al., *Helv. Chim. Acta*, 1993, 76, 1379, (Purpureacin 1)  
 Cortes, D. et al., *Phytochemistry*, 1993, 32, 1467; 1475, (レビュー)  
 Fujimoto, Y. et al., *Chem. Pharm. Bull.*, 1994, 42, 1175, (Squamostatin)  
 Pinheiro-Santos, L. et al., *Quim. Nova*, 1994, 17, 387, (Crassiflorin)  
 Shimada, H. et al., *Tet. Lett.*, 1994, 35, 3961, (絶対構造, Squamostatin)  
 Marshall, J.A. et al., *J.O.C.*, 1998, 63, 7066, (合成法, Squamostatin D)  
 Chang, F.-R. et al., *Phytochemistry*, 1999, 51, 883, (*cis*-Squamostatin D)

§ **Bullatanocin; 24-Epimer**

[化学名・別名] Bullatalicin. Annonin VIII. Cherimolin 1. Squamostatin B

[CAS No.] 152323-84-7

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $C_{37}H_{66}O_8$

[分子量] 638.924

[正確な分子量] 638.47577

[基原] *Annona squamosa*, *Annona bullata*, *Annona cherimolia*

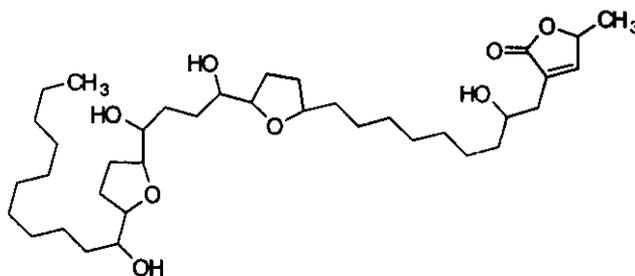
[性状] 無定型のワックス

[融点] Mp 120-121 °C (113-116 °C)

[比旋光度]:  $[\alpha]_D^{25} +64$  (c, 0.3 in MeOH).  $[\alpha]_D^{25}$

+9.8 (c, 0.29 in  $CH_2Cl_2$ )

[UV]: [neutral]  $\lambda_{max}$  215 ( $\epsilon$  5000) (EtOH)



-----文献-----

Cortes, D. et al., *Phytochemistry*, 1993, 32, 1467; 1475, (レビュー)  
 Fujimoto, Y. et al., *Chem. Pharm. Bull.*, 1994, 42, 1175, (Squamostatin)  
 Shimada, H. et al., *Tet. Lett.*, 1994, 35, 3961, (絶対構造, Squamostatin)  
 Gu, Z.-M. et al., *J. Nat. Prod.*, 1995, 41, 229, (*cis*-Bullatanocin, *cis*-Bullatalicin)  
 Martin, J.M. et al., *J. Nat. Prod.*, 1999, 62, 2, (活性, Bullatalicin)

§ **Isomolvizarin 1**

[CAS No.] 161169-72-8

[関連 CAS No.] 158018-15-6, 158252-74-5

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $C_{35}H_{62}O_7$

[分子量] 594.871

[正確な分子量] 594.449555

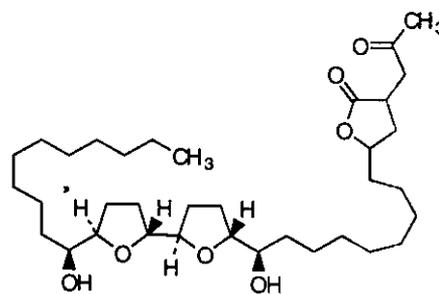
[基原] *Annona cherimolia* (バンレイシ科) の根の成分

[性状] ワックス

[比旋光度]:  $[\alpha]_D^{25} +24$  (c, 0.3 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  206 ( $\epsilon$  3325) (MeOH)

[その他のデータ] 非天然物. 2,4-*cis*- と *trans*-isomers の混合物として分離



-----文献-----

Duret, P. et al., *Heterocycles*, 1994, 39, 741, (分離, 構造決定)  
 Duret, P. et al., *J. Nat. Prod.*, 1994, 57, 911, (分離, UV, IR, H-NMR, C13-NMR, Mas)

§ **Isomolvizarin 1; 22-Epimer**

[化学名・別名] Isomolvizarin 2

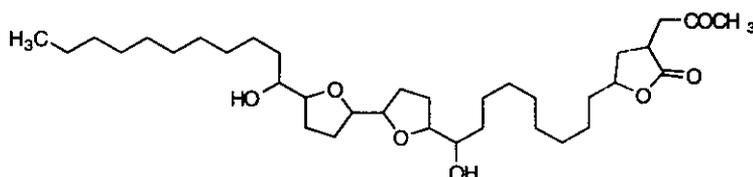
[CAS No.] 158252-75-6

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $C_{35}H_{62}O_7$

[分子量] 594.871



[正確な分子量] 594.449555

[基原] *Annona cherimolia* の根の成分

[UV]: [neutral]  $\lambda_{max}$  204 ( $\epsilon$  3674) (MeOH)

[その他のデータ] 非天然物. 2,4-*cis*- と *trans*-isomers の混合物

-----文献-----

Duret, P. et al., *Heterocycles*, 1994, 39, 741, (分離, 構造決定)

Duret, P. et al., *J. Nat. Prod.*, 1994, 57, 911, (分離, UV, IR, H-NMR, C13-NMR, Mas)

### § Itrabin

[CAS No.] 139294-54-5

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $C_{35}H_{66}O_7$

[分子量] 596.886

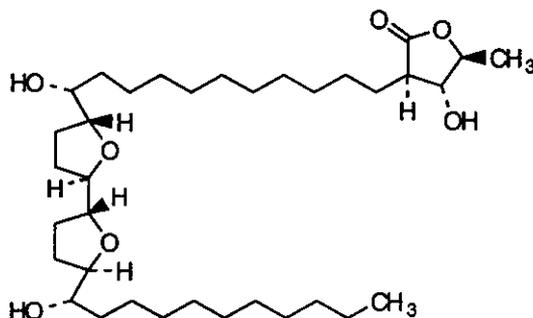
[正確な分子量] 596.465205

[基原] *Annona cherimolia*

[性状] 塊

[融点] Mp 38-40 °C

[比旋光度]:  $[\alpha]_D^{25} +21$  (c, 0.2 in MeOH)



-----文献-----

Cortes, D. et al., *Tet. Lett.*, 1991, 32, 6133, (分離, H-NMR, C13-NMR, Mas)

Cortes, D. et al., *Phytochemistry*, 1993, 32, 1475, (分離)

Warmerdam, E. et al., *Tet. Lett.*, 1998, 39, 8077, (構造決定)

### § Jetein

[CAS No.] 139294-55-6

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $C_{35}H_{66}O_7$

[分子量] 598.902

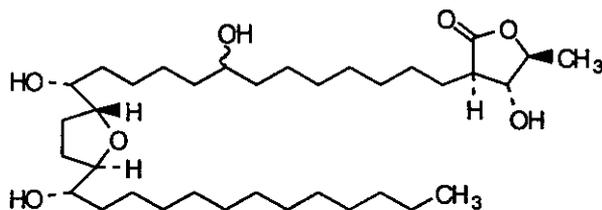
[正確な分子量] 598.480855

[基原] *Annona cherimolia*

[性状] 塊

[融点] Mp 58-60 °C

[比旋光度]:  $[\alpha]_D^{25} +9$  (c, 0.03 in MeOH)



-----文献-----

Cortes, D. et al., *Tet. Lett.*, 1991, 32, 6133, (分離, H-NMR, C13-NMR, Mas)

Cortes, D. et al., *Phytochemistry*, 1993, 32, 1475, (分離)

Warmerdam, E. et al., *Tet. Lett.*, 1998, 39, 8077, (構造決定)

### § Laherradurin

[CAS No.] 125276-75-7

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $C_{37}H_{68}O_7$

[分子量] 624.94

[正確な分子量] 624.496505

[基原] 次の植物の種子から分離: *Annona cherimolia*

[用途] 細胞毒

[融点] Mp 85-86 °C

[比旋光度]:  $[\alpha]_D^{25} +21$  (c, 0.1 in MeOH)

[その他のデータ] 化学構造は次の物質と似ている: 3-[2,13-Dihydroxy-13-[octahydro-5'-(1-hydroxyundecyl) [2,2'-bifuran]-5-yl] tridecyl]-5-methyl-2(5H)-furanone

-----文献-----

Rios, J.L. et al., *Planta Med.*, 1989, 55, 321, (分離)

Cortes, D. et al., *Phytochemistry*, 1993, 32, 1467; 1475, (レビュー, 構造決定)  
Laprevote, O. et al., *Tetrahedron*, 1994, 50, 8479, (Mass, 構造決定)  
Warmerdam, E. et al., *Tet. Lett.*, 1998, 39, 8077, (構造決定)

#### § 4-Methylbenzo[g]quinoline-5,10-dione (CAS 名)

[化学名・別名] Cleistopholine

[CAS No.] 96889-94-0

[化合物分類] アルカロイド化合物 (Azaanthracene alkaloid)

[構造式]

[分子式]  $C_{14}H_9NO_2$

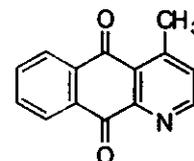
[分子量] 223.231

[正確な分子量] 223.063329

[基原] 次の植物から得られるアルカロイド: *Cleistopholis patens* の根皮, *Annona cherimolia* の種子, *Oncodistigma monosperma* (バンレイシ科) の茎皮

[性状] 青白い黄色の無定型の塊

[融点] Mp 185-190 °C



#### -----文献-----

Waterman, P.G. et al., *Phytochemistry*, 1985, 24, 523, (分離, UV, IR, H-NMR, C13-NMR, Mass, 構造決定)  
Koyama, J. et al., *Heterocycles*, 1989, 29, 1649, (合成法)  
Bou-Abdallah, E. et al., *J. Nat. Prod.*, 1989, 52, 273, (分離)  
Ríos, J.L. et al., *Planta Med.*, 1989, 55, 321, (分離)

#### § Molvizarin

[CAS No.] 138551-26-5

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $C_{35}H_{62}O_7$

[分子量] 594.871

[正確な分子量] 594.449555

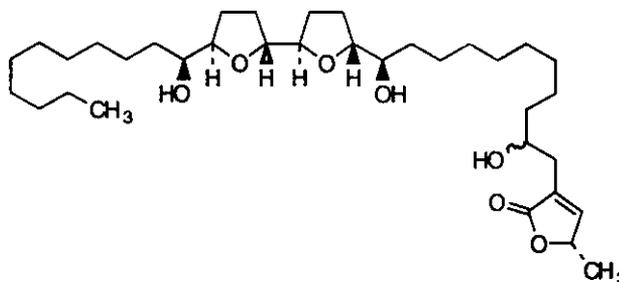
[基原] 次の植物から分離: *Annona cherimolia*, その他の *Annona* spp.- and *Asimina parviflora*

[用途] 細胞毒

[融点] Mp 36-38 °C

[比旋光度]:  $[\alpha]_D +9.7$  (c, 0.13 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  215 ( $\epsilon$  6800) (EtOH)



#### -----文献-----

Cortes, D. et al., *Tetrahedron*, 1991, 47, 8195, (分離, H-NMR, C13-NMR)  
Cave, A. et al., *Prog. Chem. Org. Nat. Prod.*, 1997, 70, 81, (レビュー)

#### § Motrilin

[化学名・別名] Annonin III. Squamocin C

[CAS No.] 138551-27-6

[関連 CAS No.] 141505-62-6

[その他の CAS No.] 157084-75-8

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $C_{37}H_{66}O_7$

[分子量] 622.924

[正確な分子量] 622.480855

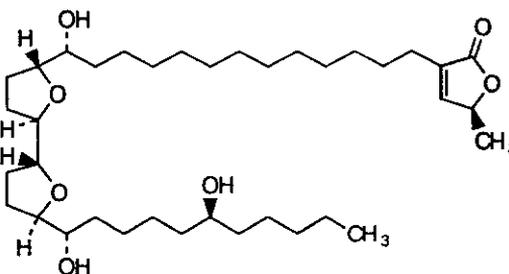
[一般的性質] 化学構造は Narumicin I と Squamostatin A によく似ている

[基原] 次の植物から分離: *Annona cherimolia*, *Annona squamosa*, *Asimina triloba*

[用途] 細胞毒

[融点] Mp 50-51 °C

[比旋光度]:  $[\alpha]_D +19.5$  (c, 0.9 in MeOH)



[UV]:[neutral]  $\lambda_{\max}$  210 ( $\epsilon$  7000) (MeOH) [neutral]  $\lambda_{\max}$  211 ( $\epsilon$  11800) (EtOH)

-----文献-----

Cortes, D. et al., Tetrahedron, 1991, 47, 8195, (分離, H-NMR, C13-NMR)

Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163, (Squamocin C)

Zhao, G.-X. et al., J. Med. Chem., 1994, 37, 1971, (Asiminecin)

Cave, A. et al., Prog. Chem. Org. Nat. Prod., 1997, 70, 81, (レビュー)

### § Otivarin

[CAS No.] 92280-15-4

[化合物分類] ポリケチド (Annonaceae acetogenin)

[構造式]

[分子式]  $C_{37}H_{66}O_8$

[分子量] 640.939

[正確な分子量] 640.49142

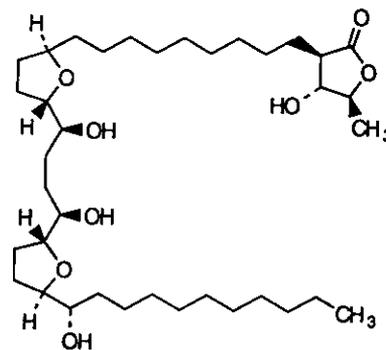
[基原] 次の植物の種子から分離: *Annona cherimolia*

[用途] 細胞毒

[比旋光度]:  $[\alpha]_D^{25} +13$  (c, 0.1 in MeOH)

[溶解性] BERDY SOL: アセトン, ヘキサンに可溶; 水に難溶

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



-----文献-----

Cortes, D. et al., Tet. Lett., 1984, 25, 3199, (分離)

Cortes, D. et al., Phytochemistry, 1993, 32, 1467; 1475, (レビュー)

Warmerdam, E. et al., Tet. Lett., 1998, 39, 8077, (構造決定)

### \*\*\*\*\*チェリーローレル (Cherry laurel) \*\*\*\*\*

§ § バラ科セイヨウバクチノキ (*Prunus laurocerasus* L.) の葉。

§ Benzyl alcohol; *O*-[ $\beta$ -D-Xylopyranosyl-(1  $\rightarrow$  6)-D-glucopyranoside]

[化学名・別名] Benzyl  $\beta$ -primeveroside

[CAS No.] 130622-31-0

[化合物分類] 単環芳香族 (Simple benzyl alcohol)

[構造式]

[分子式]  $C_{18}H_{26}O_{10}$

[分子量] 402.397

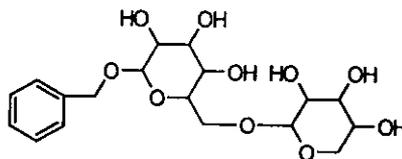
[正確な分子量] 402.1526

[基原] *Alangium platanifolium*, *Camellia sinensis*, *Panax ginseng*, *Prunus laurocerasus*

[性状] 結晶 (EtOH)

[融点] Mp 188-189 °C

[比旋光度]:  $[\alpha]_D^{20} -71.2$  (c, 1 in H<sub>2</sub>O)



-----文献-----

Guo, W. et al., Biosci., Biotechnol., Biochem., 1994, 58, 1532, (primeveroside)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, BDX500

§ 2-Hydroxy-2-phenylacetonitrile; ( $\pm$ )-form, *O*- $\beta$ -D-Glucopyranoside

[化学名・別名] Prulaurasin

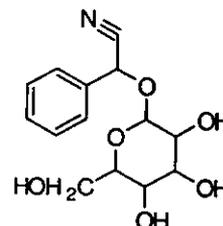
[CAS No.] 138-53-4

[化合物分類] 単環芳香族 (Phenylacetic acid derivative), 炭水化物 (Cyanogenic glycoside)

[構造式]

[分子式]  $C_{14}H_{17}NO_6$

[分子量] 295.291



[正確な分子量] 295.105589

[基原] 次の植物から分離: *Prunus laurocerasus*, *Cotoneaster* spp., その他の植物

[性状] 針状結晶 (EtOAc)

[融点] Mp 122-123 °C

[比旋光度]:  $[\alpha]_D^{20}$  -53 (H<sub>2</sub>O)

[化学物質毒性データ総覧 (RTEC) 登録番号] UL3200000

-----文献-----

Caldwell, R.J. et al., J.C.S., 1907, 91, 671, (*Sambunigrin*, *Prulaurasin*)

\*\*\*RTECS (化学物質毒性データ)\*\*\*

\*\*\*健康障害に関するデータ\*\*\*

\*\*\*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 : 560 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

JTSCDR Journal of Toxicological Sciences. (Japanese Soc. of Toxicological Sciences, 4th Floor, Gakkai Center Bldg., 4-16, Yayoi 2-chome, Bunkyo-ku, Tokyo 113, Japan) V.1- 1976- [Vol.,頁,年(19-)] 12,47,1987

§ 6-O-β-D-Xylopyranosyl-D-glucose; β - PyranosE-form, Benzyl glycoside

[化学名・別名] 1-O-Benzyl-β-D-primeveroside

[化合物分類] 炭水化物 (Disaccharide)

[構造式]

[分子式] C<sub>18</sub>H<sub>26</sub>O<sub>10</sub>

[分子量] 402.397

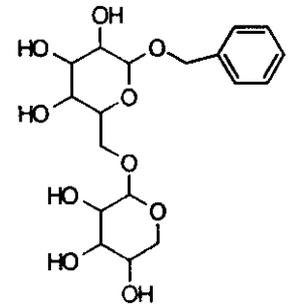
[正確な分子量] 402.1526

[基原] 次の植物の緑の果実から分離: *Prunus laurocerasus*

[性状] 結晶 (EtOH)

[融点] Mp 188-189 °C

[比旋光度]:  $[\alpha]_D^{20}$  -71.2 (c, 1 in H<sub>2</sub>O)



-----文献-----

Tollens, B. et al., Kurzes Handbuch der Kohlenhydrate, Edwards Bros. Inc., Ann Arbor, 4th Ed., 1935, 425

Begbie, R. et al., Carbohydr. Res., 1966, 2, 272, (分離, 構造決定)

Weinges, K. et al., Annalen, 1991, 703, (benzyl glycoside)

\*\*\*\*\*チェリーワイルド (Wild cherry) \*\*\*\*\*

§ §バラ科ブラックチェリー (*Prunus serotina* Ehrhart) の樹皮。

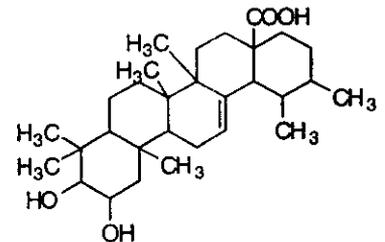
§ 2,3-Dihydroxy-12-ursen-28-oic acid; (2α,3α)-form

[CAS No.] 52213-27-1

[化合物分類] テルペノイド (Ursane triterpenoid)

[構造式]

[基原] *Prunus serotina*, *Prunus lusitanica*, *Pseudopanax arboreum*



-----文献-----

Glen, A.T. et al., J. Solution Chem., 1967, 510, (分離)

Biessels, H.W.A. et al., Phytochemistry, 1974, 13, 203, (分離)

Bowden, B.F. et al., Aust. J. Chem., 1975, 28, 91, (分離)

Seo, S. et al., Chem. Comm., 1975, 270; 954, (生合成, H-NMR)

Blandari, S.P.S. et al., Phytochemistry, 1990, 29, 3956, (Nepetoic acid)

Lontsi, D. et al., Planta Med., 1990, 56, 287, (Cecropic acid)