

Feheacuter, F. et al., Z. Naturforsch., B, 1969, 24, 1485, (合成法)
 Feheacuter, F. et al., CA, 1976, 85, 54924c, (結晶構造)

§ 1,2,3,5,6,8-Hexathionane (CAS 名)

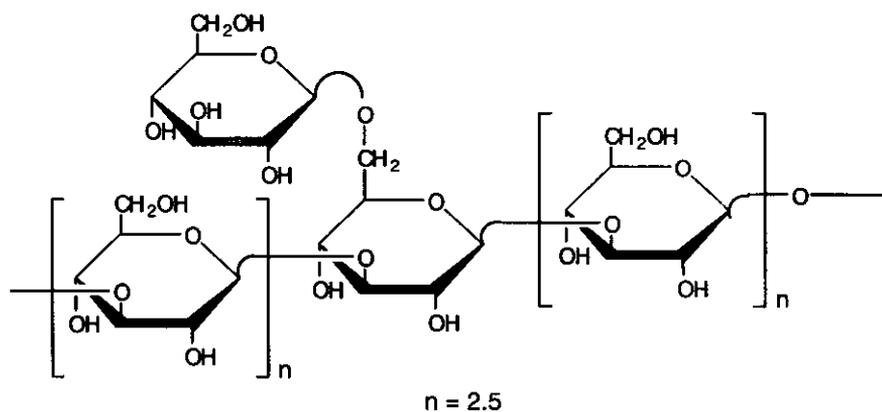
[CAS No.] 103439-80-1
 [化合物分類] 脂肪族化合物 (Simple heteroalicyclics (miscellaneous heteroatom))
 [構造式]
 [分子式] $C_3H_6S_6$
 [分子量] 234.476
 [正確な分子量] 233.87937
 [基原] マッシュルーム *Lentinus edodes*

-----文献-----

Chen, C.C. et al., ACS Symp. Ser., 1986, 317, 176, (生育)
 Chen, C.C. et al., J. Agric. Food Chem., 1986, 34, 830, (生育)

§ Lentinan

[CAS No.] 37339-90-5
 [関連 CAS No.] 114285-68-6
 [化合物分類] 炭水化物 (Polysaccharide), 薬物: 免疫刺激剤 (Immunostimulant)
 [構造式]
 [一般的性質] A highly (1 → 6) branched (1 → 3) β-D-glucan
 [基原] Elaborated by the fungus *Lentinus edodes*
 [用途] 免疫刺激剤.
 [性状] 粉末
 [開発状況] 1986 年に開発開始
 [溶解性] 水, DMSO に可溶; 水に易溶; エタノール, ヘキサンに難溶
 [UV]: [neutral] λ_{max} (MeOH)

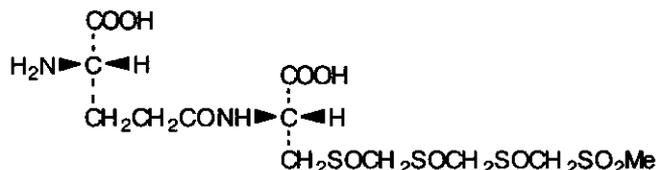


-----文献-----

Chihara, G. et al., Nature (London), 1969, 222, 687; 1971, 229, 634, (分離, 薬理)
 Sasaki, T. et al., Carbohydr. Res., 1976, 47, 99, (薬理)
 Bluhm, T.L. et al., ACS Symp. Ser., 1977, 48, 105, (結晶構造)
 Saito, H. et al., Carbohydr. Res., 1979, 74, 227, (C13-NMR, 構造決定)
 Saito, H. et al., Bull. Chem. Soc. Jpn., 1986, 59, 2093, (conform, C13-NMR)
 Tsukagoshi, S., Drugs of Today (Barcelona), 1988, 24, 91, (レビュー)
 Suzuki, M. et al., Int. J. Immunopharmacol., 1994, 16, 463, (レビュー)
 Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1721
 Gordon, M. et al., J. Med. (Westbury, N.Y.), 1998, 29, 305, (薬理)

§ Lenticinic acid

[CAS No.] 12705-98-5
 [化合物分類], アミノ酸とペプチド (Dipeptide)
 [構造式]
 [分子式] $C_{17}H_{22}N_2O_{10}S_4$
 [分子量] 482.577
 [正確な分子量] 482.015728
 [基原] 次の植物から分離: マッシュルーム *Lentinus edodes*



[用途] 1,2,3,5,6-Pentathiepane の前駆物質

-----文献-----

Yasumoto, K. et al., Agric. Biol. Chem., 1971, 35, 2059

Gmelin, R. et al., Phytochemistry, 1980, 19, 553

§ Nicotianine; (S)-form

[化学名・別名] L-form

[CAS No.] 19701-79-2

[化合物分類] アミノ酸とペプチド (Non-protein α -aminoacid)

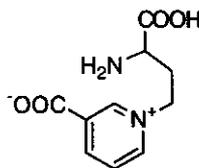
[構造式]

[基原] *Nicotiana tabacum*, *Lentinus edodes*

[性状] 結晶 (MeOH 溶液)

[融点] Mp 241-243 °C で分解

[比旋光度]: $[\alpha]_D^{24} +24$ (c, 2.0 in H₂O)



-----文献-----

Noma, M. et al., Phytochemistry, 1968, 7, 1861, (分離, 構造決定)

§ 7-Nonene-3,5-diyn-1-ol (CAS 名)

[CAS No.] 90535-88-9

[化合物分類] 脂肪族化合物 (Acetylenic alcohol)

[構造式] $H_3CCH=CHC \equiv CC \equiv CCH_2CH_2OH$

[分子式] C₉H₁₆O

[分子量] 134.177

[正確な分子量] 134.073165

[基原] *Lentinus edodes* と 病原性 *Trichoderma* の混合培養物から分離

-----文献-----

Tokimoto, K. et al., Proc. Jpn. Acad., Ser. B, 1987, 63, 277, (分離)

§ 2,3-Octadiene-5,7-diyn-1-ol (CAS 名)

[関連 CAS No.] 64753-26-0

[化合物分類] 脂肪族化合物 (Acetylenic alcohol)

[構造式] $HC \equiv CC \equiv CCH=C=CHCH_2OH$

[分子式] C₈H₆O

[分子量] 118.135

[正確な分子量] 118.041865

[基原] 次の植物から分離: *Lentinus edodes*

-----文献-----

Bew, R.E. et al., J.C.S. (C), 1966, 129, (分離, UV, IR)

Landor, P.D. et al., J.C.S. Perkin 1, 1975, 1628, (合成法, UV, IR)

Kleijn, H. et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.), 1982, 101, 97, (合成法)

Tokimoto, K. et al., Proc. Jpn. Acad., Ser. B, 1987, 63, 277, (分離)

§ 3,5,7-Octatriyn-1-ol (CAS 名)

[CAS No.] 6071-20-1

[化合物分類] 脂肪族化合物 (Acetylenic alcohol)

[構造式] $HC \equiv CC \equiv CC \equiv CCH_2CH_2OH$

[分子式] C₈H₆O

[分子量] 118.135

[正確な分子量] 118.041865

[基原] 次の植物から分離: *Lentinus edodes*

[その他のデータ] λ_{max} 209 nm

-----文献-----

Bew, R.E. et al., J.C.S. (C), 1966, 129, (合成法, IR, UV)

Tokimoto, K. et al., Proc. Jpn. Acad., Ser. B, 1987, 63, 277, (分離)

§ 7-Octene-3,5-diyn-1-ol (CAS 名)

[化学名・別名] Lentialexin

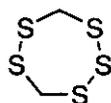
[CAS No.] 114020-45-0
[化合物分類] 脂肪族化合物 (Acetylenic alcohol)
[構造式] $\text{H}_2\text{C}=\text{CHC}\equiv\text{CC}\equiv\text{CCH}_2\text{CH}_2\text{OH}$
[分子式] $\text{C}_8\text{H}_8\text{O}$
[分子量] 120.151
[正確な分子量] 120.057515
[基原] 次の植物から分離: *Lentinus edodes*
[溶解性] 水, エーテルに可溶
[UV]: [neutral] λ_{max} 238 ; 251 ; 264 ; 282 (MeOH)

-----文献-----

Tokimoto, K. et al., Proc. Jpn. Acad., Ser. B, 1987, 63, 277, (分離)

§ 1,2,3,5,6-Pentathiepane (CAS 名) (旧 CAS 名)

[化学名・別名] Lenthionine
[CAS No.] 292-46-6
[化合物分類] 脂肪族化合物 (Simple heteroalicyclics (miscellaneous heteroatom))
[構造式]
[分子式] $\text{C}_2\text{H}_4\text{S}_5$
[分子量] 188.384
[正確な分子量] 187.89165
[基原] 食用キノコシイタケ *Lentinus edodes*, responsible for its characteristic odour. Also a volatile prod. of cooked mutton and found in the alga *Chondria californica*. また *Parkia speciosa* から分離される
[用途] グラム陽性・陰性菌, *Candida albicans* に対して抗菌性を有する
[性状] 結晶 (CH_2Cl_2)
[融点] Mp 60-61 °C
[溶解性] 水, polar 有機溶媒に難溶; オイルに可溶



-----文献-----

Morita, K. et al., Chem. Pharm. Bull., 1967, 15, 988, (合成法, 分離, Mas)
Wada, S. et al., J. Food Sci., 1967, 32, 559, (分離, 合成法)
Wratten, S.J. et al., J.O.C., 1976, 41, 2465, (分離)
Iwami, K., CA, 1978, 89, 161546, (レビュー, 成書)
Nixon, L.N. et al., J. Agric. Food Chem., 1979, 27, 355, (分離)
Gmelin, R. et al., Phytochemistry, 1981, 20, 2521, (分離, 性質)
Still, I.W.J. et al., Tet. Lett., 1981, 1939, (合成法)
Holzmann, G. et al., Org. Mass Spectrom., 1982, 17, 165, (Mas)
Bannister, R.M. et al., J.C.S. Perkin 1, 1990, 509, (合成法)
Ritzau, M. et al., Annalen, 1993, 871, (分離)

§ 1,2,4,5,7-Pentathiocane (CAS 名)

[化学名・別名] 1,2,4,5,7-Pentathiacyclooctane
[CAS No.] 81531-39-7
[関連 CAS No.] 81531-40-0
[化合物分類] 脂肪族化合物 (Simple heteroalicyclics (miscellaneous heteroatom))
[構造式]
[分子式] $\text{C}_2\text{H}_4\text{S}_5$
[分子量] 202.41
[正確な分子量] 201.9073
[基原] *Parkia speciosa* の種子, マッシュルーム *Lentinus edodes*
[性状] プリズム結晶 ($\text{CHCl}_3/\text{hexane}$)
[融点] Mp 102-104 °C

-----文献-----

Gmelin, R. et al., Phytochemistry, 1981, 20, 2521, (分離)
Holzmann, G. et al., Org. Mass Spectrom., 1982, 17, 165, (Mas)
Chen, C.C. et al., J. Agric. Food Chem., 1986, 34, 830, (生育)

§ 3,5,9,14-Tetrahydroxyergosta-7,22-dien-6-one; (3 β ,5 α ,9 α ,14 α ,22E,24R)-form

[CAS No.] 211486-14-5

[化合物分類] ステロイド (Ergostane steroids; excluding withanolides and brassinolide). (C28)

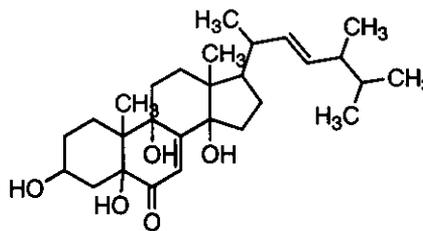
[構造式]

[基原] *Lentinus edodes*, *Hypsizigus marmoreus*, *Pleurotus ostreatus*, *Pholiota nameko*

[性状] 無定型の粉末

[比旋光度]: $[\alpha]_D^{25} -22.7$ (c, 0.04 in CHCl₃)

[UV]: [neutral] $\lambda_{max} 225$ (log ϵ 3.9) (MeOH)



-----文献-----

Yaoita, Y. et al., Chem. Pharm. Bull., 1998, 46, 944, (分離, H-NMR, C13-NMR)

§ 1,2,4,6-Tetrathiepane

[化学名・別名] 1,2,4,6-Tetrathiacycloheptane

[CAS No.] 292-45-5

[化合物分類] 脂肪族化合物 (Simple heteroalicyclics (miscellaneous heteroatom))

[構造式]

[分子式] C₇H₈S₄

[分子量] 170.344

[正確な分子量] 169.93523



[基原] 次の植物から分離: *Lentinus edodes* (マッシュルーム), *Chondria californica* (藻類), *Parkia speciosa*

[用途] グラム陽性・陰性細菌と *Candida albicans* に対して弱い活性を有する

[融点] Mp 79 °C

-----文献-----

Morita, K. et al., Chem. Pharm. Bull., 1967, 15, 998, (合成法, 分離)

Wratten, S.J. et al., J.O.C., 1976, 41, 2465, (分離)

Weissflog, E., Phosphorus Sulfur Relat. Elem., 1980, 8, 157, (合成法)

Gmelin, R. et al., Phytochemistry, 1981, 20, 2521

Still, I.W.J. et al., Tet. Lett., 1981, 1939, (合成法)

Holzmann, G. et al., Org. Mass Spectrom., 1982, 17, 165, (Mas)

§ 3,5,9-Trihydroxy-23-methylergosta-7,22-dien-6-one; (3 β ,5 α ,9 α ,22E,24R)-form

[CAS No.] 211486-12-3

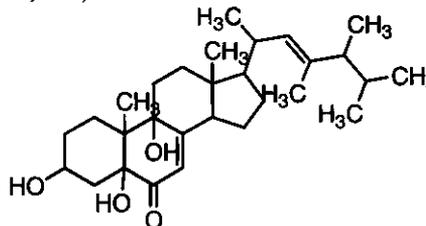
[化合物分類] ステロイド (Ergostane steroids; excluding withanolides and brassinolide). (C28)

[構造式]

[基原] *Lentinus edodes*

[性状] 無定型の粉末

[比旋光度]: $[\alpha]_D^{25} -40$ (c, 0.05 in CHCl₃)



-----文献-----

Yaoita, Y. et al., Chem. Pharm. Bull., 1998, 46, 944, (分離, H-NMR, C13-NMR)

§ 1,2,4-Trithiolane (CAS 名)

[化学名・別名] 1,2,4-Trithiacyclopentane

[CAS No.] 289-16-7

[化合物分類] 脂肪族化合物 (Simple heteroalicyclics (miscellaneous heteroatom))

[構造式]

[分子式] C₅H₆S₃

[分子量] 124.252



[基原] *Acacia pulchella*, *Parkia speciosa*. また藻類; *Chondria californica*, マッシュルーム *Lentinus edodes* から分離される. Excretion prod. of *Ochromonas danica*

[用途] マッシュルームの香気成分

[性状] 青白い黄色の液体

[沸点] Bp₁₀ 102-103 °C. Bp₃ 78-79 °C

[溶解性] ヘキサンに難溶

-----文献-----

Morita, K. et al., Chem. Pharm. Bull., 1967, 15, 988, (合成法)
Tjan, S.B. et al., Tetrahedron, 1972, 28, 3489, (合成法, Mas)
Wratten, S.J. et al., J.O.C., 1976, 41, 2465, (isol oxide)
Gmelin, R. et al., Phytochemistry, 1981, 20, 2521, (分離)
Holzmann, G. et al., Org. Mass Spectrom., 1982, 17, 165, (Mas)
Juettner, F. et al., Phytochemistry, 1982, 21, 2185, (分離)
Borseth, D.G. et al., J.A.C.S., 1984, 106, 841, (構造決定)
Chen, C.C. et al., J. Agric. Food Chem., 1986, 34, 830, (分離)

*****ジェネ (Genet) *****

§ § マメ科エニシダ (*Spartium junceum* L.) の花。

§ Cytisine; (-)-form, N-Me

[化学名・別名] N-Methylcytisine. Caulophylline

[CAS No.] 486-86-2

[化合物分類] アルカロイド化合物 (Quinolizidine alkaloids; 3 × ring)

[構造式]

[分子式] C₁₂H₁₆N₂O

[分子量] 204.271

[正確な分子量] 204.126263

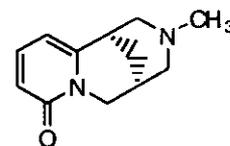
[基原] 次の植物から得られるアルカロイド: *Cytisus laburnum*, *Genista* spp., *Leontice* spp., *Spartium junceum*, その他とても多くの種, マメ科の種

[性状] プリズム結晶 (EtOH)

[融点] Mp 137 °C

[比旋光度]: [α]_D -221.6 (H₂O)

[化学物質毒性データ総覧 (RTECS) 登録番号] HA4400000



-----文献-----

Cockburn, W.F. et al., Can. J. Chem., 1952, 30, 92, (分離, 構造決定)
Monakhova, T.E. et al., Khim. Prir. Soedin., 1973, 9, 59; Chem. Nat. Compd. (Engl. Transl.), 1973, 9, 52, (N-(2-Hydroxyethyl) cytisine)
Gazaliev, A.M. et al., Khim. Prir. Soedin., 1991, 27, 301; Chem. Nat. Compd. (Engl. Transl.), 1991, 27, 259, (レビュー, 成書)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, CQL500; CQL750

***RTECS (化学物質毒性データ) ***

生体影響物質 : 医薬品.

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-マウス

投与量・期間 : 511 mg/kg

毒性影響 : [行動] 傾眠 (全身活動度の低下).

[行動] 痙攣または発作閾値への影響.

[行動] 筋収縮または痙直.

参照文献

BJPCBM British Journal of Pharmacology. (Macmillan Press Ltd., Houndmills, Basingstoke, Hants. RG21 2XS, UK) V.34- 1968- [Vol.,頁,年(19-)] 35,161,1969

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 腹腔内投与

被験動物 : げっ歯類-マウス
投与量・期間 : 51 mg/kg
毒性影響 : [行動] 傾眠(全身活動度の低下).
[行動] 痙攣または発作閾値への影響.
[行動] 筋収縮または痙直.

参考文献

BJPCBM British Journal of Pharmacology. (Macmillan Press Ltd., Houndmills, Basingstoke, Hants. RG21 2XS, UK) V.34- 1968- [Vol.,頁,年(19-)]35,161,1969

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 静脈注射
被験動物 : げっ歯類-マウス
投与量・期間 : 22 mg/kg
毒性影響 : [行動] 痙攣または発作閾値への影響.
参考文献

JPETAB Journal of Pharmacology and Experimental Therapeutics. (Williams & Wilkins Co., 428 E. Preston St., Baltimore, MD 21202) V.1- 1909/10- [Vol.,頁,年(19-)]79,334,1943

<<試験方法>> 認知されている最小致死量(LDL₀)試験.

曝露経路 : 報告なし.
被験動物 : げっ歯類-マウス
投与量・期間 : 160 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.
参考文献

JOETD7 Journal of Ethnopharmacology. (Elsevier Scientific Pub. Ireland Ltd., POB 85, Limerick, Ireland) V.1- 1979- [Vol.,頁,年(19-)]7,24,1983

§ Cytisine; (-)-form, N-Ethoxycarbonyl

[化学名・別名] 12-Ethoxycarbonylcytisine

[CAS No.] 132216-16-1

[化合物分類] アルカロイド化合物 (Quinolizidine alkaloids; 3 × ring)

[構造式]

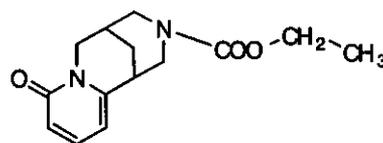
[分子式] C₁₄H₁₈N₂O₃

[分子量] 262.308

[正確な分子量] 262.131743

[基原] *Laburnum watereri*, *Spartium junceum* (マメ科)

[その他のデータ] 非天然物の可能性



-----文献-----

Greinwald, R. et al., *Phytochemistry*, 1990, 29, 3553, (12-Ethoxycarbonylcytisine)

§ 5,7-Dihydroxyflavone; 7-O-Gentiobioside

[CAS No.] 88640-89-5

[化合物分類] フラボノイド (Flavones; 2 × O-置換基)

[構造式]

[分子式] C₂₇H₃₀O₁₄

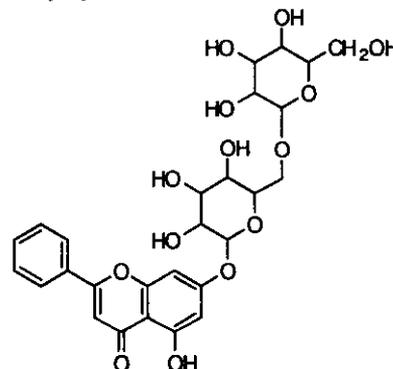
[分子量] 578.526

[正確な分子量] 578.16356

[基原] 次の植物の花から分離: *Spartium junceum*

[性状] 結晶 (EtOH)

[融点] Mp 185-188 °C



-----文献-----

De Rosa, S. et al., *Phytochemistry*, 1983, 22, 2323, (7-gentiobioside)

§ 1,26-Hexacosanediol

[CAS No.] 15541-01-2

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

[構造式] HOCH₂(CH₂)₂₄CH₂OH

[分子式] $C_{26}H_{34}O_2$

[分子量] 398.711

[正確な分子量] 398.41238

[基原] *Spartium junceum* の花, carnauba wax. Also from apple wax and in esterified form from oats (*Avena sativa*)

[性状] 結晶 (C_6H_6 /EtOAc)

[融点] Mp 110.5 °C (102-105 °C)

-----文献-----

Musgrave, O.C. et al., J.C.S., 1952, 4393, (分離, 合成法)

Murray, K.E. et al., Aust. J. Chem., 1955, 8, 432, (分離)

Mazliak, P., Phytochemistry, 1962, 1, 79, (分離)

Daniels, D.G.H. et al., Chem. Ind. (London), 1965, 1763, (分離)

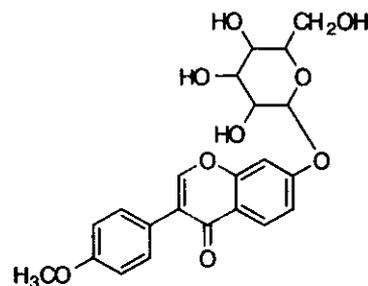
§ 7-Hydroxy-4'-methoxyisoflavone; 7-O-β-D-Glucopyranoside

[化学名・別名] Ononin. Ononoside

[CAS No.] 486-62-4

[化合物分類] フラボノイド (Isoflavones; 2 × O-置換基)

[構造式]



[分子式] $C_{22}H_{22}O_9$

[分子量] 430.41

[正確な分子量] 430.126385

[基原] マメ科亜科のマメ亜科に広く分布する, 例えば, *Amorpha*

fruticosa, *Baptisia* spp., *Cicer arietinum*, *Cladrastis* spp., *Dalbergia paniculata*, *Genista patula*, *Medicago sativa*, *Ononis* spp., *Piptanthus* spp., *Pueraria thunbergiana*, *Spartium junceum*, *Thermopsis* spp., *Trifolium* spp., *Wisteria floribunda*

[性状] 針状結晶 (dioxan 溶液)

[融点] Mp 218-219 °C

[溶解性] メタノール, エーテルに可溶; 水に難溶

[UV]: [neutral] λ_{max} 250 (MeOH)

-----文献-----

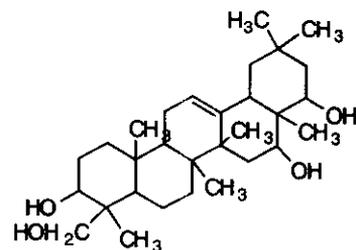
Lewis, P. et al., J.C.S. Perkin 1, 1998, 2481, (Ononin, 合成法, H-NMR, C13-NMR)

§ 12-Oleanene-3,16,22,24-tetrol; (3β,16β,22β)-form

[化学名・別名] Junceogenol

[化合物分類] テルペノイド (Oleanane triterpenoid)

[構造式]



[基原] Sapogenin from *Spartium junceum*

-----文献-----

Bilia, A.R. et al., Phytochemistry, 1993, 34, 847, (分離, H-NMR, C13-NMR)

Yecedilsilada, E. et al., Phytochemistry, 1999, 51, 903, (分離, H-NMR, C13-NMR)

§ 12-Oleanene-3,16,22,24-tetrol; (3β,16β,22β)-form,

3-O-[β-D-Glucopyranosyl-(1→2)-α

-L-rhamnopyranoside]

[化学名・別名] Junceoside

[CAS No.] 154159-19-0

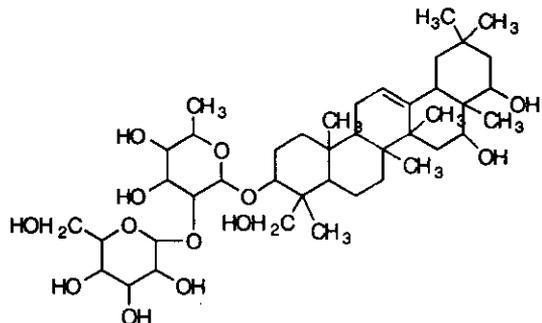
[化合物分類] テルペノイド (Oleanane triterpenoid)

[構造式]

[分子式] $C_{42}H_{70}O_{13}$

[分子量] 783.007

[正確な分子量] 782.481645



[基原] *Spartium junceum*

[比旋光度]: $[\alpha]_D^{20}$ -14.2 (c, 0.57 in CHCl₃)

-----文献-----

Bilia, A.R. et al., *Phytochemistry*, 1993, 34, 847, (分離, H-NMR, C13-NMR)

Yecedilsilada, E. et al., *Phytochemistry*, 1999, 51, 903, (分離, H-NMR, C13-NMR)

§ 12-Oleanene-3,16,22,24-tetrol; (3 β,16 β,22 β)-form, 3-O-[α-L-Rhamnopyranosyl-(1 → 2)-β-D-glucopyranosyl-(1 → 2)-β-D-glucuronopyranoside]

[CAS No.] 244140-10-1

[化合物分類] テルペノイド (Oleanane triterpenoid)

[構造式]

[分子式] C₃₈H₇₈O₁₉

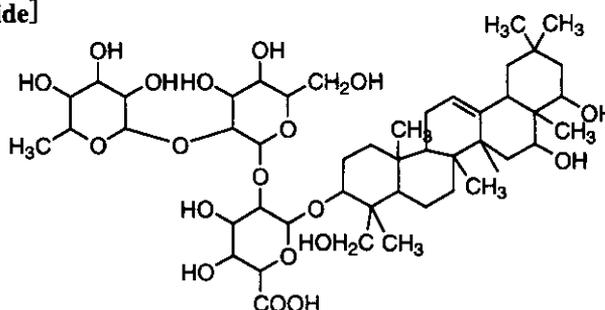
[分子量] 959.133

[正確な分子量] 958.513735

[基原] *Spartium junceum*

[性状] 粉末

[比旋光度]: $[\alpha]_D^{24}$ -5.95 (c, 0.23 in Py)



-----文献-----

Bilia, A.R. et al., *Phytochemistry*, 1993, 34, 847, (分離, H-NMR, C13-NMR)

Yecedilsilada, E. et al., *Phytochemistry*, 1999, 51, 903, (分離, H-NMR, C13-NMR)

§ 13(18)-Oleanen-3-ol; 3 β-form

[化学名・別名] δ-Amyrin. δ-Amyrenol

[CAS No.] 508-04-3

[化合物分類] テルペノイド (Oleanane triterpenoid)

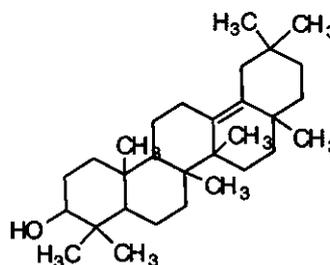
[構造式]

[基原] *Spartium junceum*, *Cistus quadrangularis*

[性状] 結晶 (MeOH)

[融点] Mp 212-213.5 °C

[比旋光度]: $[\alpha]_D^{20}$ -50.5 (CHCl₃)



-----文献-----

Wollenweber, E., *Z. Naturforsch., C*, 1974, 29, 362, (分離)

Bohlmann, F. et al., *Chem. Ber.*, 1975, 108, 433, (δ-Amyrin acetate)

Singh, R.S. et al., *J. Nat. Prod.*, 1984, 47, 368, (delta-Amyrin acetate)

Bhutani, K.K. et al., *Phytochemistry*, 1984, 23, 407, (分離)

Tanaka, R. et al., *Phytochemistry*, 1988, 27, 3579, (δ-Amyrin formate, C13-NMR, H-NMR)

He, A. et al., *Phytochemistry*, 1998, 49, 2607, (H-NMR, C13-NMR)

§ 4',5,6,7,8-Pentahydroxyisoflavone; 6,7-Methylene, 4'-Me ether

[化学名・別名] 5,8-Dihydroxy-4'-methoxy-6,7-methylenedioxyisoflavone

[CAS No.] 152367-39-0

[化合物分類] フラボノイド (Isoflavones; 5 × O-置換基)

[構造式]

[分子式] C₁₇H₁₂O₇

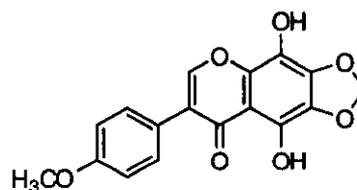
[分子量] 328.278

[正確な分子量] 328.058305

[基原] *Spartium junceum*

[性状] 青白い黄色の結晶 (MeOH)

[融点] Mp 233-237 °C



-----文献-----

Agarwal, V.K. et al., *Phytochemistry*, 1984, 23, 1342, (分離)

Bashir, A. et al., *Phytochemistry*, 1992, 31, 309, (誘導體)

Bilia, A.R. et al., *Phytochemistry*, 1993, 34, 847, (誘導體)

§ 4',5,7,8-Tetrahydroxyflavanone; (S)-form, 7-O-α-L-Rhamnopyranoside

[化学名・別名] Isocarthamidin 7-rhamnoside

[CAS No.] 152367-40-3

[化合物分類] フラボノイド (Flavanones; 4 × O-置換基)

[構造式]

[分子式] $C_{21}H_{22}O_{10}$

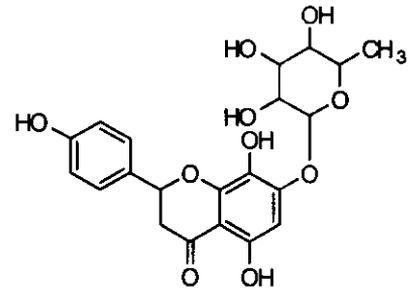
[分子量] 434.399

[正確な分子量] 434.1213

[基原] *Spartium junceum*

[性状] 無定形の黄色粉末 (MeOH 溶液)

[比旋光度]: $[\alpha]_D -41.9$ (c, 1.5 in MeOH)



-----文献-----

Bilia, A.R. et al., *Phytochemistry*, 1993, 34, 847, (7-rhamnoside)

§ 3',4',5,7-Tetrahydroxyflavone; 4'-O-β-D-Glucopyranoside

[化学名・別名] Luteolin 4'-glucoside. Juncin

[CAS No.] 6920-38-3

[化合物分類] フラボノイド (Flavones; 4 × O-置換基)

[構造式]

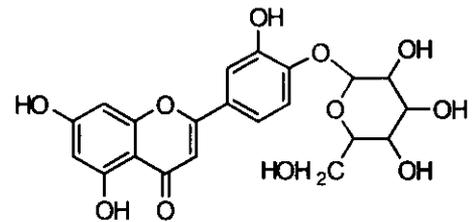
[分子式] $C_{21}H_{20}O_{11}$

[分子量] 448.382

[正確な分子量] 448.100565

[基原] 次の植物から分離: *Spartium junceum*, その他多くの植物種.

[融点] Mp 178-179 °C



-----文献-----

Perkin, A.G., *J.C.S.*, 1900, 77, 1315, (分離)

Diller, E., *Ber.*, 1901, 34, 1452, (分離)

Spada, A. et al., *Gazz. Chim. Ital.*, 1958, 88, 204, (4'-glucoside)

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhauser Verlag, Basel, 1972, nos. 1470; 1473, (生育)

Shamyrina, A.A. et al., *Khim. Prir. Soedin.*, 1977, 13, 577; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, 13, 482, (5-galactoside)

Plant Flavonoids in Biology and Medicine, (eds. Cody, V. et al), A. R. Liss, N. Y., 1986, (生化学的性質)

The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

§ 2',4',5,7-Tetrahydroxyisoflavone

[化学名・別名] 3-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one (CAS 名).

2'-Hydroxygenistein

[CAS No.] 1156-78-1

[化合物分類] フラボノイド (Isoflavones; 4 × O-置換基)

[構造式]

[分子式] $C_{15}H_{10}O_6$

[分子量] 286.24

[基原] 次の植物から分離: *Apios tuberosa*, *Argyrocytisus battandieri*, *Cajanus cajan*, *Crotalaria juncea*, *Dolichos biflorus*, *Hardenbergia violacea*, *Lablab niger*, *Laburnum anagyroides*, *Lupinus albus*, *Moghania macrophylla*, *Neonotonia wightii*, *Phaseolus vulgaris*, *Phaseolus coccineus*, *Spartium junceum*, *Stizolobium deeringianum* (全てマメ科, マメ亜科)

[性状] 結晶 (CHCl₃/MeOH)

[融点] Mp 270-273 °C

[UV]: [neutral] λ_{max} 209 ; 262 ; 288 (MeOH)

-----文献-----

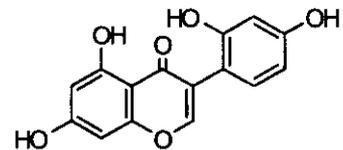
King, F.E. et al., *J.C.S.*, 1952, 4752, (合成法, 誘導體)

Farkas, L. et al., *J.C.S. (C)*, 1971, 10, 1994, (合成法)

Braz Filho, R. et al., *Phytochemistry*, 1976, 15, 1029, (分離, UV, IR, H-NMR, Mass, 誘導體)

Ingham, J.L., *Z. Naturforsch., C*, 1976, 31, 504; 1977, 32, 1018, (分離)

Prasad, J.S. et al., *Phytochemistry*, 1977, 16, 1120, (分離, UV, H-NMR, 構造決定)



Ingham, J.L., Prog. Chem. Org. Nat. Prod., 1983, 43, 1, (レビュー, 生育)
 Sanduja, R. et al., J. Chem. Res., Synop., 1985, 56, (分離, 誘導體)
 Parmar, V.S. et al., Org. Mass Spectrom., 1985, 20, 265, (Mas)
 Adesanya, S.A. et al., Phytochemistry, 1985, 24, 2699, (分離, 誘導體)

§ 2,3,9-Trihydroxypterocarpan; 2,3-Di-Me ether

[化学名・別名] 9-Hydroxy-2,3-dimethoxypterocarpan. Sparticarpin

[CAS No.] 73793-85-8

[化合物分類] フラボノイド (Simple pterocarpan flavonoid)

[構造式]

[分子式] C₁₇H₁₆O₅

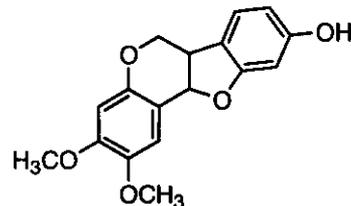
[分子量] 300.31

[正確な分子量] 300.099775

[基原] *Spartium junceum* の葉のストレス代謝物

[比旋光度]: [α]_D -170 (c, 0.01 in MeOH)

[UV]: [neutral] λ_{max} 211; 294 (EtOH) [base] λ_{max} 215; 299 (EtOH-NaOH)



-----文献-----

Kalra, V.K. et al., Indian J. Chem., 1967, 5, 607, (合成法)
 Pueppke, S.G. et al., J.C.S. Perkin 1, 1975, 946, (分離)
 Ingham, J.L. et al., Z. Naturforsch., C, 1980, 35, 197, (Sparticarpin)

*****シソ (Perilla) *****

§ § シソ科シソ (*Perilla frutescens* Britton var. *crispa* (Thunb.) Decene.) の茎葉, 果実。

§ 3-(3,4-Dihydroxyphenyl)-2-propenoic acid; (E)-form, Vinyl ester

[化学名・別名] Vinyl caffeate

[化合物分類] 単環芳香族 (Simple phenylpropanoid)

[構造式]

[分子式] C₁₁H₁₀O₄

[分子量] 206.198

[正確な分子量] 206.05791

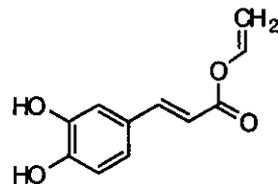
[基原] *Perilla frutescens* var. *crispa*

[用途] 抗酸化剤

[性状] 結晶

[融点] Mp 133-140 °C

[UV]: [neutral] λ_{max} 221 (ε 17000); 247 (ε 13000); 339 (ε 22000) (EtOH)



-----文献-----

Hermann, F.X., Pharmazie, 1956, 11, 433, (レビュー)
 Klosterman, H.J. et al., J.A.C.S., 1959, 81, 2188, (Linocaffein)
 Achenbach, H. et al., Chem. Ber., 1971, 104, 1468, (分離, 誘導體)
 Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhauser Verlag, Basel, 1972, no. 957
 IARC Monog., 1993, 56, 115, (Caffeic acid, レビュー, 毒性)
 Mellidis, A.S. et al., J. Nat. Prod., 1993, 56, 949, (分離, ester)
 Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, CAK375

§ *p*-Menth-8-en-7-ol; (1*RS*, 4*RS*)-form, 3,4-Dihydroxycinnamoyl (*E*-)

[化学名・別名] *p*-Menth-8-en-7-yl caffeate

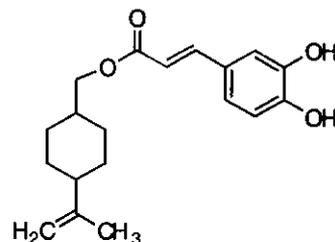
[CAS No.] 179694-78-1

[化合物分類] テルペノイド (*p*-Menthane monoterpene) 単環芳香族 (Simple phenylpropanoid)

[構造式]

[分子式] C₁₉H₂₄O₄

[分子量] 316.396
 [正確な分子量] 316.16746
 [基原] *Perilla frutescens* var. *crispa*
 [用途] 抗酸化剤
 [性状] 黄色の結晶
 [融点] Mp 155-156 °C
 [UV]: [neutral] λ_{\max} 217 (ϵ 15450); 236 (ϵ 9130); 245 (ϵ 9730)
 (EtOH)

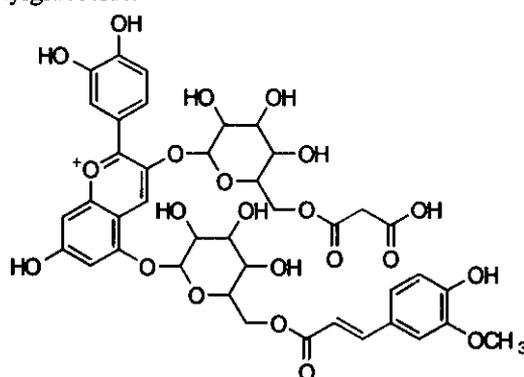


-----文献-----

Iskenderov, M.A., J. Gen. Chem. USSR (Engl. Transl.), 1937, 7, 1429, (合成法)
 Kayahara, H. et al., Agric. Biol. Chem., 1969, 33, 86, (合成法)
 Fujita, Y. et al., Bull. Chem. Soc. Jpn., 1970, 43, 2637, (分離)
 Fujita, T. et al., Phytochemistry, 1993, 34, 1545, (Perilloside C, Perilloside D)
 Tada, M. et al., Biosci., Biotechnol., Biochem., 1996, 60, 1093, (caffeate)

§ 3,3',4',5,7-Pentahydroxyflavylum (1+); 3-O-[4-Hydroxy-3-methoxycinnamoyl-(→ 6)-β-D-glucopyranoside] 5-O-(6-O-malonyl-β-D-glucopyranoside)

[化学名・別名] Cyanidin 3-(6-feruloylglucoside) 5-(6-malonylglucoside)
 [CAS No.] 123453-03-2
 [化合物分類] フラボノイド (Anthocyanidins and anthocyanins; 5 × O-置換基)
 [構造式]



[分子式] C₄₀H₄₁O₂₂⁽⁺⁾
 [分子量] 873.751
 [正確な分子量] 873.208955
 [基原] 次の植物から分離: *Perilla frutescens* var. *crispa*

-----文献-----

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhauser Verlag, Basel, 1972, nos. 1713; 1715; 1716, (生育)
 The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

§ § シソ科アオジソ (*Perilla frutescens* Britton var. *crispa* Decaisne f. *viridis* Makino) の茎 葉, 果実。

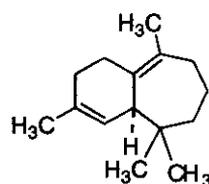
本調査研究では研究報告ない。

*****シダー (Cedar) *****

§ § マツ科レバノンスギ (*Cedrus libani* Barrel.) の葉または材。

§ 2,6-Himachaladiene

[化学名・別名] β-Himachalene
 [CAS No.] 1461-03-6
 [化合物分類] テルペノイド (Himachalane sesquiterpenoid)
 [構造式]
 [分子式] C₁₅H₂₄
 [分子量] 204.355
 [正確な分子量] 204.1878
 [基原] *Cedrus deodara*, *Cedrus atlantica*, *Cedrus libani*
 [性状] オイル
 [沸点] Bp₄ 121-122 °C



[比旋光度]: $[\alpha]_D^{25} +225.8$ (neat)

[屈折率] $n_D^{25} 1.5113$

-----文献-----

Challand, B.D. et al., Chem. Comm., 1967, 704, (合成法)

Joseph, T.C. et al., Tetrahedron, 1968, 24, 3809; 3841, (分離, 構造決定)

Wenkert, E. et al., Synth. Commun., 1973, 3, 45, (合成法)

Piers, E. et al., Chem. Comm., 1979, 166, (合成法)

Oppolzer, W. et al., Helv. Chim. Acta, 1981, 64, 2592, (合成法)

§ 2,7(14)-Himachaladiene

[化学名・別名] α -Himachalene

[CAS No.] 3853-83-6

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

[構造式]

[分子式] $C_{15}H_{24}$

[分子量] 204.355

[正確な分子量] 204.1878

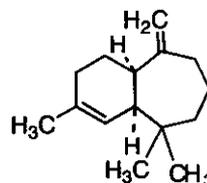
[基原] *Cedrus deodara*, *Cedrus atlantica*, *Cedrus libani*

[性状] オイル

[沸点] Bp_2 93-94 °C

[比旋光度]: $[\alpha]_D^{25} -187.1$ (neat)

[屈折率] $n_D^{25} 1.5082$



-----文献-----

Bredenberg, J.B. et al., Acta Chem. Scand., 1961, 15, 685, (分離, 構造決定)

Joseph, T.C. et al., Tetrahedron, 1968, 24, 3809; 3841, (分離, 構造決定)

Wenkert, E. et al., Synth. Commun., 1973, 3, 45, (合成法)

Oppolzer, W. et al., Helv. Chim. Acta, 1981, 64, 2592, (合成法)

Suginome, H. et al., Tetrahedron, 1994, 50, 7771, (合成法)

§ Libanotic acid

[化学名・別名] 4-(1-Methyl-3-oxobutyl)-1-cyclohexene-1-carboxylic acid (CAS 名).

11,12,13-Trinor-9-oxo-2-bisabolen-15-oic acid

[CAS No.] 119765-97-8

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

[構造式]

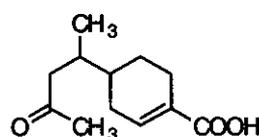
[分子式] $C_{12}H_{18}O_3$

[分子量] 210.272

[正確な分子量] 210.125595

[基原] *Cedrus libani*

[性状] オイル



-----文献-----

Avcibasi, H. et al., Phytochemistry, 1988, 27, 3967

§ 9-Oxo-2,7-bisaboladien-15-oic acid

[化学名・別名] 4-(1,5-Dimethyl-3-oxo-1-hexenyl)-1-cyclohexene-1-carboxylic acid (CAS 名). Atlantonc acid. Dehydrotodomatuic acid

[CAS No.] 120019-19-4

[関連 CAS No.] 17904-28-8

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

[構造式]

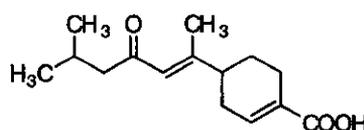
[分子式] $C_{15}H_{22}O_3$

[分子量] 250.337

[正確な分子量] 250.156895

[基原] *Cedrus libani*, *Cedrus deodara*

[性状] オイル



-----文献-----

Dev, S. et al., *Tetrahedron*, 1984, 40, 2961, (分離, H-NMR)
 Avcibasi, H. et al., *Phytochemistry*, 1988, 27, 3967

§ 9-Oxo-2-bisabolen-15-oic acid; (6R,7R)-form

[化学名・別名] Todomatuic acid. Dihydroatlantonic acid

[CAS No.] 6753-22-6

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

[構造式]

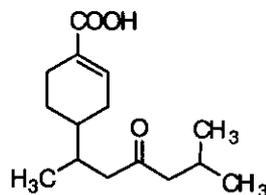
[基原] *Abies sachalinensis*, *Cedrus libani*

[性状] 結晶 (petrol)

[融点] Mp 58.5 °C

[沸点] Bp 200-215 °C

[比旋光度]: $[\alpha]_D^{32.5} +85.8$



-----文献-----

Manville, J.F. et al., *Can. J. Chem.*, 1977, 55, 2547, (分離, 構造決定, C13-NMR)

Bhan, P. et al., *Tetrahedron*, 1984, 40, 2961, (C13-NMR, H-NMR)

Numata, A. et al., *Phytochemistry*, 1992, 31, 3773, (分離, H-NMR, C13-NMR, 誘導體)

§ § ヒノキ科レッドシダー (*Juniperus procera* Hochstter ex Endl.) の葉または材。

§ 6,7-Dihydroxy-8,13-abietadiene-11,12-dione; (6 α ,7 β)-form, 6-Deoxy

[化学名・別名] 7 β -Hydroxy-8,13-abietadiene-11,12-dione

[CAS No.] 126979-82-6

[化合物分類] テルペノイド (Abietane diterpenoid)

[構造式]

[分子式] C₂₀H₂₈O₃

[分子量] 316.439

[正確な分子量] 316.203845

[基原] 次の植物から分離: *Salvia miltiorrhiza*, *Salvia nutans*, *Juniperus procera*

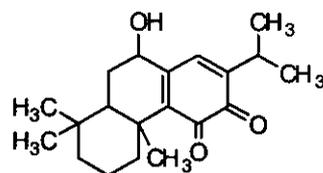
[性状] 黄色結晶 (EtOAc/hexane)

[融点] Mp 83-84 °C. Mp 156-158 °C

[比旋光度]: $[\alpha]_D -8.3$ (c, 0.084 in CHCl₃)

[UV]: [neutral] λ_{max} 210 (log ϵ 4.15); 270 (log ϵ 2.8) (MeOH) [neutral] λ_{max} 242; 283; 421

(CHCl₃) [neutral] λ_{max} 239 (sh); 295; 424 (MeOH) [neutral] λ_{max} 210 (ϵ 14125); 270 (ϵ 500) (MeOH)



-----文献-----

Hueso-Rodriguez, J.A. et al., *Phytochemistry*, 1983, 22, 2005

Chang, H.M. et al., *J.O.C.*, 1990, 55, 3537, (誘導體)

Muhammad, I. et al., *Phytother. Res.*, 1996, 10, 604, (分離, C13-NMR)

Nagy, G. et al., *Phytochemistry*, 1999, 51, 809, (6-deoxy, C13-NMR)

§ 14,15-Dinor-13-oxo-8(17),11-labdadien-19-oic acid; (11E)-form

[CAS No.] 98531-41-0

[化合物分類] テルペノイド (Norlabdane diterpenoid)

[構造式]

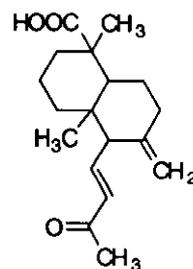
[基原] *Juniperus chinensis*, *Juniperus procera*, *Platycladus orientalis*

[性状] 塊 (EtOAc/hexane) (以前はオイルと記載されていた)

[融点] Mp 99-101 °C

[比旋光度]: $[\alpha]_D^{20} +24.1$ (c, 1 in MeOH)

[UV]: [neutral] λ_{max} 210 (log ϵ 3.95); 275 (log ϵ 2.6) (MeOH)



-----文献-----

Inoue, M. et al., *Phytochemistry*, 1985, 24, 1602, (分離, H-NMR)

Fang, J.-M. et al., *Phytochemistry*, 1996, 41, 1361, (分離)

Su, W.C. et al., *Phytochemistry*, 1996, 43, 255, (11,12-dihydro Me ester)
Muhammad, I. et al., *Phyther. Res.*, 1996, 10, 604, (分離, H-NMR, C13-NMR)

§ **Nootkatin; 2'',3''-Didehydro**

[化学名・別名] 2-Hydroxy-5-(3-methyl-2-butenyl)-4-(1-methylethenyl)-2,4,6-cycloheptatrien-1-one (CAS名). 4-Isopropenyl-5-prenyltropolone. 6-Isopropenyl-5-prenyltropolone. Procerin

[CAS No.] 552-96-5

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

[構造式]

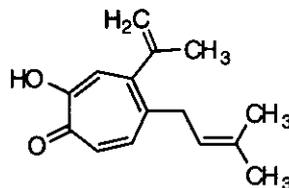
[分子式] $C_{15}H_{18}O_2$

[分子量] 230.306

[正確な分子量] 230.13068

[基原] 次の植物から分離: *Juniperus procera*

[融点] Mp 71-72 °C



-----文献-----

Duff, S.R. et al., *Chem. Ind. (London)*, 1954, 432, (構造決定)

Runeberg, J. et al., *Acta Chem. Scand.*, 1960, 14, 353; 797; 1985; 1991; 1961, 15, 645, (分離, IR, 合成法)

Kitahara, Y. et al., *Bull. Chem. Soc. Jpn.*, 1964, 37, 895, (合成法, Procerin)

Zavarin, E. et al., *Phytochemistry*, 1967, 6, 1387, (分離, 生育)

Senter, P. et al., *Phytochemistry*, 1975, 14, 2233, (分離)

§ § ヒノキ科エンピツバクシン (*Juniperus virginiana* L.) の葉または材。

本調査研究では研究報告ない。

§ § ヒノキ科ニオイヒバ (*Thuja occidentalis* L.) の葉または材。

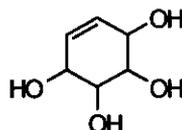
§ **5-Cyclohexene-1,2,3,4-tetrol; (1 α , 2 α , 3 β , 4 α)-form**

[化学名・別名] 1,2,4/3-form. Conduritol F. Leucanthemitol

[CAS No.] 4782-76-7

[化合物分類] 炭水化物 (Cyclitol)

[構造式]



[基原] *Chrysanthemum leucanthemum*, *Chrysanthemum maximum*, *Hoya carnososa*, *Thuja occidentalis*, *Chlorella fusca*. Found in opt. active form in nearly all green plants in small amts.

[融点] Mp 103-104 °C

[UV]: [neutral] λ_{max} 0 (end) (ϵ) (EtOH)

-----文献-----

Le Drian, C. et al., *Helv. Chim. Acta*, 1989, 72, 338; 1990, 73, 161, (合成法, 成書, 絶対構造)

Secen, H. et al., *Synth. Commun.*, 1994, 24, 2103, (合成法, C13-NMR, Conduritol F)

Patti, A. et al., *J.O.C.*, 1996, 61, 6458, (合成法, Conduritol F)

§ **Deoxypropodophyllic acid; 7',8'-Diepimer, lactone**

[化学名・別名] Isopicrodeoxypropodophyllotoxin

[化合物分類] リグナン化合物 (Aryltetralin lactone lignan)

[構造式]

[分子式] $C_{22}H_{22}O_7$

[分子量] 398.412

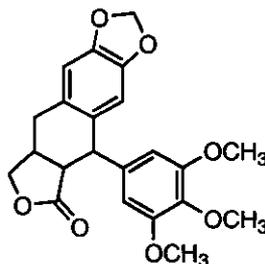
[正確な分子量] 398.136555

[基原] *Thuja occidentalis*

[性状] オイル

[比旋光度]: $[\alpha]_D^{20} +12.5$ (c, 0.06 in $CHCl_3$)

[UV]: [neutral] λ_{max} 217 (log ϵ 4); 241 (log ϵ 3.5); 291 (log ϵ 3.2) (MeOH)



-----文献-----

Hartwell, J.L. et al., *J.A.C.S.*, 1953, 75, 2138; 1954, 76, 4034, (構造決定, 合成法)

Novelo, M. et al., J. Nat. Prod., 1993, 56, 1728, (Isodeoxydopodophyllotoxin)
Chang, L.C. et al., J. Nat. Prod., 2000, 63, 1235, (Isopicrodeoxydopodophyllotoxin)

§ 2,7-Dihydroxy-4-isopropyl-2,4,6-cycloheptatrien-1-one; 7-Me ether

[化学名・別名] 2-Hydroxy-4-isopropyl-7-methoxy-2,4,6-cycloheptatrien-1-one.

4-Isopropyl-7-methoxytropolone

[CAS No.] 89647-85-8

[化合物分類] 単環芳香族 (Tropolone derivative), テルペノイド (Cycloheptane monoterpene)

[構造式]

[分子式] $C_{11}H_{14}O_3$

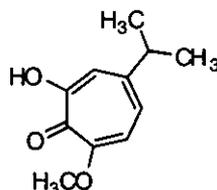
[分子量] 194.23

[正確な分子量] 194.094295

[基原] 次の植物から分離: *Thuja occidentalis*

[性状] 褐色の板状結晶 (CHCl₃/hexane)

[融点] Mp 81-83 °C (sealed tube)



-----文献-----

Gardner, J.A.F. et al., Can. J. Chem., 1957, 35, 1039, (分離, IR, UV, 構造決定)

Zavarin, E. et al., Phytochemistry, 1967, 6, 1387, (分離, 生育)

Witte, L. et al., Planta Med., 1983, 49, 216, (誘導体)

Banwell, M.G. et al., Aust. J. Chem., 1991, 44, 705, (合成法, 誘導体)

§ 2,7-Dihydroxy-4-isopropyl-2,4,6-cycloheptatrien-1-one; Di-Me ether

[化学名・別名] 2,7-Dimethoxy-4-isopropyl-2,4,6-cycloheptatrien-1-one. 2,7-Dimethoxy-4-isopropyltropolone

[CAS No.] 89659-30-3

[化合物分類] テルペノイド (Cycloheptane monoterpene) 単環芳香族 (Tropolone derivative)

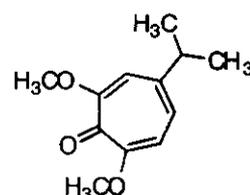
[構造式]

[分子式] $C_{12}H_{16}O_3$

[分子量] 208.257

[正確な分子量] 208.109945

[基原] 次の植物から分離: *Thuja occidentalis*



-----文献-----

Gardner, J.A.F. et al., Can. J. Chem., 1957, 35, 1039, (分離, IR, UV, 構造決定)

Zavarin, E. et al., Phytochemistry, 1967, 6, 1387, (分離, 生育)

Witte, L. et al., Planta Med., 1983, 49, 216, (誘導体)

Banwell, M.G. et al., Aust. J. Chem., 1991, 44, 705, (合成法, 誘導体)

§ 9,11-Epoxy-3,10(14)-guaidiene; (1 β, 5 α, 7 β H, 9 α)-form

[CAS No.] 176435-25-9

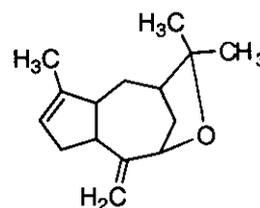
[化合物分類] テルペノイド (Simple guaiane sesquiterpenoid)

[構造式]

[基原] *Thuja occidentalis*

[性状] オイル

[比旋光度]: $[\alpha]_D^{20} +62$ (c, 0.15 in CHCl₃)



-----文献-----

Weyerstahl, P. et al., Annalen, 1996, 99, (分離, H-NMR, C13-NMR)

§ 1,3-Eudesmadien-11-ol; (5 α, 7 β, 10 α)-form

[化学名・別名] Occidentalol

[CAS No.] 473-17-6

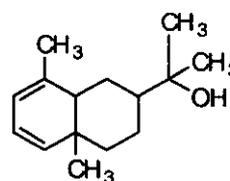
[化合物分類] テルペノイド (Simple eudesmane sesquiterpenoid)

[構造式]

[基原] *Thuja occidentalis*

[性状] 結晶 (petrol)

[融点] Mp 95 °C



[比旋光度]: $[\alpha]_D^{24} +361$ (c, 2.4 in CHCl₃)

-----文献-----

Suga, T. et al., Bull. Chem. Soc. Jpn., 1972, 45, 3502, (構造決定)

Hortmann, A.G. et al., J.O.C., 1973, 38, 728, (合成法)

Uegaki, R. et al., Phytochemistry, 1985, 24, 2445, (誘導體)

Banerjee, A.K. et al., Tetrahedron, 1993, 49, 4761, (合成法, レビュー)

§ 4-Eudesmen-11-ol; 7 β -form

[化学名・別名] γ-Eudesmol. Uncineol

[CAS No.] 1209-71-8

[化合物分類] テルペノイド (Simple eudesmane sesquiterpenoid)

[構造式]

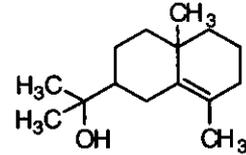
[基原] *Neocallitropsis araucaroides* (Araucaria oil), *Thuja occidentalis*, *Callitris columellaris*, その他のオイル

[性状] オイル

[沸点] Bp_{0.1} 83-86 °C

[比旋光度]: $[\alpha]_D^{25} +66.7$ (neat)

[屈折率] n_D²⁰ 1.5087



-----文献-----

Bates, R.B. et al., Chem. Ind. (London), 1962, 1759, (分離, 構造決定)

Su, W.-C. et al., Phytochemistry, 1995, 39, 603, (7-Epi-γ-eudesmol)

Raharivelomanana, P. et al., Phytochemistry, 1998, 47, 1085, (7-Epi-γ-eudesmol, H-NMR, C13-NMR, Mas)

§ Fenchone; (-)-form

[CAS No.] 4695-62-9

[化合物分類] テルペノイド (Fenchane monoterpene)

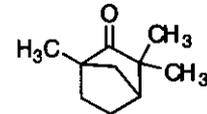
[構造式]

[基原] 次の植物から分離: 種々の精油, 例えば, *Thuja occidentalis*, *Artemisia frigida*

[用途] 香気成分

[比旋光度]: $[\alpha]_D -67$

[化学物質毒性データ総覧 (RTECS) 登録番号] RB7875200



-----文献-----

Opdyke, D.L.J., Food Cosmet. Toxicol., 1976, 14, 769, (レビュー, 毒性)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, 8, 228

Wijekoon, W.M.D. et al., J. Phys. Chem., 1983, 87, 3034, (H-NMR, C13-NMR, UV, CD)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 278, (レビュー)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, TLW250

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 : 6160 mg/kg

毒性影響 : [知覚組織と特異感覚] (嗅覚) 効果, その他特定すべき事象なし
[知覚組織と特異感覚] (眼) その他特定すべき事象なし
[行動] 傾眠 (全身活動度の低下).

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-)] 2,327,1964

米国に於ける状況

EPA TSCA Section 8(b) CHEMICAL INVENTORY

§ 3,10(14)-Guaiadien-11-ol; (1 α ,5 β ,7 α H)-form

[化学名・別名] Awabukinol

[CAS No.] 176435-26-0

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

[構造式] 構造式はまだ有効ではない

[基原] *Viburnum awabuki*, *Thuja occidentalis*

[性状] オイル

[比旋光度]: $[\alpha]_D^{24} +161$ (c, 0.74 in CHCl_3), $[\alpha]_D^{20} +103$ (c, 1.2 in CHCl_3)

[その他のデータ] 高い方の旋光度は Awabukinol に似ている

-----文献-----

Weyerstahl, P. et al., *Annalen*, 1996, 99, (分離, H-NMR, C13-NMR)

Fukuyama, Y. et al., *Phytochemistry*, 1996, 42, 741, (Awabukinol, 分離, H-NMR, C13-NMR, CD)

§ 12-Hydroxydodecanoic acid

[化学名・別名] 12-Hydroxylauric acid. Sabinic acid

[CAS No.] 505-95-3

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

[構造式] $\text{HOCH}_2(\text{CH}_2)_{10}\text{COOH}$

[分子式] $\text{C}_{12}\text{H}_{24}\text{O}_3$

[分子量] 216.32

[正確な分子量] 216.172545

[基原] *Juniperus oxycedrus* の葉。また, *Juniperus sabina*, *Thuja occidentalis*, *Pinus* spp., *Chamaecyparis* spp. and *Cycas revoluta*. 広範囲にわたる針葉樹のワックス

[性状] 結晶 (MeOH 溶液, C_6H_6 or EtOAc)

[融点] Mp 84-85 °C (78-79 °C)

-----文献-----

Aldrich Library of FT-IR Spectra, 1st edn., 1985, 1, 520B, (IR)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, 1, 810C; 1162C, (NMR)

Chuit, P. et al., *Helv. Chim. Acta*, 1929, 12, 463, (合成法)

Lycan, W.H. et al., *J.A.C.S.*, 1929, 51, 625, (合成法)

De Pascual, T.J. et al., *An. Quim.*, 1973, 69, 941, (分離)

Fan, L.L. et al., *Anal. Biochem.*, 1976, 71, 265, (HPLC)

Kurihara, T. et al., *Tet. Lett.*, 1976, 2455, (合成法)

Bidd, I. et al., *J.C.S. Perkin 1*, 1983, 1369, (lactone)

Alcaraz, M.-L. et al., *J.O.C.*, 1996, 61, 192, (Et ester, 合成法, H-NMR, C13-NMR, IR)

Menger, F.M. et al., *J.O.C.*, 1996, 61, 7382, (Me ether, 合成法, H-NMR, C13-NMR)

§ 2-Hydroxy-3-isopropyl-2,4,6-cycloheptatrien-1-one

[化学名・別名] 2-Hydroxy-3-(1-methylethyl)-2,4,6-cycloheptatrien-1-one (CAS 名). 3-Isopropyltropolone.

α -Thujaplicin

[CAS No.] 1946-74-3

[化合物分類] 単環芳香族 (Tropolone derivative), テルペノイド (Cycloheptane monoterpene) 薬物: 抗力ビ菌 (Antifungal agent), 薬物: 抗腫瘍薬 (Antineoplastic agent)

[構造式]

[分子式] $\text{C}_{10}\text{H}_{12}\text{O}_2$

[分子量] 164.204

[正確な分子量] 164.08373

[基原] *Juniperus conferta*, *Thuja plicata* の心材に存在する。また, *Thuja occidentalis*, *Thuja dolabrata*, *Thuja standishii*, *Cupressus* spp., *Juniperus* spp. から得られる

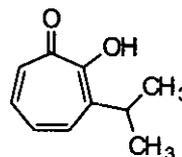
[用途] 抗カビ, 抗腫瘍薬。

[性状] 針状結晶 (petrol)

[融点] Mp 82 °C (34 °C)

[沸点] Bp_{0.001} 80 °C (bath)

[溶解性] メタノール, クロロホルムに可溶; 水に難溶



[Log P 計算値] Log P 0.87 (計算値)

[UV]: [neutral] λ_{\max} 235 ; 345 (EtOH) [base] λ_{\max} 235 ; 333 ; 390 (pH 12 buffer)

-----文献-----

- Gripenberg, J., Acta Chem. Scand., 1948, 2, 639, (分離)
Cook, J.W. et al., J.C.S., 1951, 695, (合成法)
Zavarin, E. et al., J.O.C., 1959, 24, 1318, (分離)
Bredenberg, J.B., Acta Chem. Scand., 1961, 15, 961, (分離)
Takaya, H. et al., J.A.C.S., 1978, 100, 1778, (合成法)
Weyerstahl, P. et al., Annalen, 1996, 99, (分離, H-NMR, Mas)

§ 2-Hydroxy-4(6)-isopropyl-2,4,6-cycloheptatrien-1-one

[化学名・別名] 2-Hydroxy-4(6)-(1-methylethyl)-2,4,6-cycloheptatrien-1-one (CAS 名).

4(6)-Isopropyltropolone. β -Thujaplicin. Hinokitiol

[CAS No.] 499-44-5

[化合物分類] 単環芳香族 (Tropolone derivative), テルペノイド (Cycloheptane monoterpene)

[構造式]

[分子式] $C_{10}H_{12}O_2$

[分子量] 164.204

[正確な分子量] 164.08373

[基原] *Juniperus conferta*, *Juniperus chinensis*, *Juniperus communis*, *Juniperus thurifera*, *Juniperus utahensis*, Hinoki tree (*Chamaecyparis obtusa*) の木部のオイル, *Thuja plicata*, *Thuja occidentalis* の心材. 広範囲にわたるヒノキ科植物

[用途] 抗カビ物質. 強い殺虫と植物成長抑制作用を示す

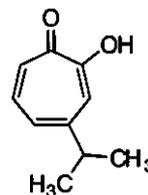
[性状] 結晶 (petrol)

[融点] Mp 52-52.5 °C

[PKa 値] pKa₁ 6.72 (25 °C, I 2.0)

[傷害・毒性] 50 % 致死量 (LD₅₀) (マウス, 腹腔内投与) 85 mg/kg

[化学物質毒性データ総覧 (RTECS) 登録番号] GU4200000



-----文献-----

- Anderson, A.B. et al., Acta Chem. Scand., 1948, 2, 644, (分離, 構造決定)
Tanaka, K. et al., Tetrahedron, 1971, 27, 4889, (合成法)
Derry, J.E. et al., J.C.S. Perkin 2, 1972, 694, (結晶構造)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhauser Verlag, Basel, 1972, no. 573, (生育)
Banwell, M.G. et al., Aust. J. Chem., 1991, 44, 705, (合成法)
Ohishi, H. et al., Acta Cryst. C, 1994, 50, 587, (結晶構造, 成書)
Madar, Z. et al., Phytochemistry, 1995, 38, 351, (Cupressotropolone A)
Ono, M. et al., Biosci., Biotechnol., Biochem., 1998, 62, 1653, (prodn)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, IRR000

RTECS (化学物質毒性データ)

生体影響物質 : 医薬品. 生殖影響物質. 天然物.

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>> 認知されている最小致死量 (LDLo) 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 : 500 mg/kg

毒性影響 : [行動] 傾眠 (全身活動度の低下).

[行動] 摂餌量 (動物).

[胃腸] その他の変化.

参照文献

NTIS** National Technical Information Service. (Springfield, VA 22161) Formerly U.S. Clearinghouse for Scientific & Technical Information. [Vol., 頁, 年 (19-)] OTS0570591

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 腹腔内投与

被験動物 : げっ歯類-マウス

投与量・期間 : 85 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

JMCMAR Journal of Medicinal Chemistry. (American Chemical Soc., Distribution Office Dept. 223, POB 57136, West End Stn., Washington, DC 20037) V.6- 1963- [Vol.,頁,年(19-)]6,755,1963

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 皮下投与.

被験動物 : げっ歯類-マウス

投与量・期間 : 541 mg/kg

毒性影響 : [行動] 痙攣または発作閾値への影響.

[行動] 鎮痛.

[栄養と総代謝] 体温低下.

参照文献

YKKZAJ Yakugaku Zasshi. Journal of Pharmacy. (Nippon Yakugakkai, 2-12-15 Shibuya, Shibuya-ku, Tokyo 150, Japan) No.1- 1881- [Vol.,頁,年(19-)]91,550,1971

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 静脈注射

被験動物 : げっ歯類-マウス

投与量・期間 : 128 mg/kg

毒性影響 : [行動] 痙攣または発作閾値への影響.

[行動] 鎮痛.

[栄養と総代謝] 体温低下.

参照文献

YKKZAJ Yakugaku Zasshi. Journal of Pharmacy. (Nippon Yakugakkai, 2-12-15 Shibuya, Shibuya-ku, Tokyo 150, Japan) No.1- 1881- [Vol.,頁,年(19-)]91,550,1971

<<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 : >2 gm/kg

毒性影響 : [行動] 傾眠(全身活動度の低下).

[行動] 摂餌量(動物).

参照文献

NTIS** National Technical Information Service. (Springfield, VA 22161) Formerly U.S. Clearinghouse for Scientific & Technical Information. [Vol.,頁,年(19-)]OTS0570591

<<試験方法>> 認知されている最小致死量(LDLo)試験.

曝露経路 : 皮下投与.

被験動物 : げっ歯類-モルモット.

投与量・期間 : 500 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

JAPMA8 Journal of the American Pharmaceutical Association, Scientific Edition. (Washington, DC) V.29-49, 1940-60. For publisher information, see JPMSAE. [Vol.,頁,年(19-)]48,722,1959

生殖に関するデータ

<<試験方法>> 最小毒性量(TDLo)試験.

曝露経路 : 経口投与.

被験動物 : げっ歯類-マウス

投与量 : 560 mg/kg

雌雄投与期間 : 雌 9 日間(交配後)

毒性影響 : [生殖] 生殖に関する傷害-胚または胎児に対する影響 : 胎児毒性

(死亡を除く. 例えば胎児の発育阻害)

[生殖] [特定の発育異常] 頭骸と顔(鼻と舌を含む).

[生殖] [特定の発育異常] 筋肉骨格系.

参照文献

FACTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- [Vol.,頁,年(19-)]37,1097,1999
米国に於ける状況

EPA TSCA Section 8(b) CHEMICAL INVENTORY
EPA TSCA TEST SUBMISSION (TSCATS) DATA BASE, JANUARY 2001

§ 8(14),15-Isopimaradiene-7,18-diol; 7 α -form, 18-Carboxylic acid, 7-ketone

[化学名・別名] 7-Oxo-8(14),15-isopimaradien-18-oic acid. 7-Oxosandaracopimaric acid

[化合物分類] テルペノイド (Isopimarane diterpenoid)

[構造式]

[分子式] $C_{20}H_{28}O_3$

[分子量] 316.439

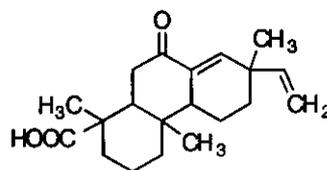
[正確な分子量] 316.203845

[基原] 次の植物から分離: *Salvia microphylla*, *Thuja occidentalis*

[性状] オイル

[比旋光度]: $[\alpha]_D^{20} +63.8$ (c, 0.3 in $CHCl_3$)

[UV]: [neutral] λ_{max} 248 (log ϵ 3.2) (MeOH)



-----文献-----

Esquivel, B. et al., J. Nat. Prod., 1987, 50, 738, (7-Oxosandaracopimaric acid)

Chang, L.C. et al., J. Nat. Prod., 2000, 63, 1235, (7-Oxo-8(14),15-isopimaradien-18-oic acid)

§ 8,15-Isopimaradiene-7,18-diol; 7 β -form, 18-Carboxylic acid, 7-k

[化学名・別名] 7-Oxo-8,15-isopimaradien-18-oic acid

[CAS No.] 114191-62-7

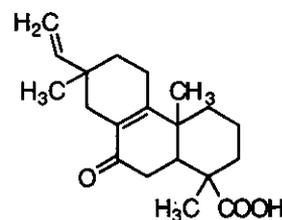
[化合物分類] テルペノイド (Isopimarane diterpenoid)

[構造式]

[基原] 次の植物から分離: *Juniperus communis*, *Thuja occidentalis*

[性状] オイル (as Me ester)

[比旋光度]: $[\alpha]_D +77.6$ (c, 0.8 in $CHCl_3$)



etone

-----文献-----

de Pascual Teresa, J. et al., Phytochemistry, 1980, 19, 1153-1156; 1987, 26, 1481

Urones, J.G. et al., Phytochemistry, 1988, 27, 523

Chang, L.C. et al., J. Nat. Prod., 2000, 63, 1235-1238, (7-Oxo-8,15-isopimaradien-18-oic acid)

§ *p*-Mentha-1,3,5-triene-2,8-diol; 2-Me ether

[化学名・別名] 2-Methoxy-*p*-mentha-1,3,5-trien-8-ol. 3-Methoxy- α , α ,4-benzyl alcohol

[CAS No.] 40180-62-9

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

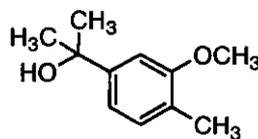
[構造式]

[分子式] $C_{11}H_{18}O_2$

[分子量] 180.246

[正確な分子量] 180.11503

[基原] 次の植物から分離: *Cupressus dupreziana*, *Thuja occidentalis* の培養細胞



-----文献-----

Leitich, J. et al., Monatsh. Chem., 1964, 95, 129, (合成法)

Pioveti, L. et al., Phytochemistry, 1980, 19, 2117, (分離, 2-Me ether)

Patwardhan, S.A. et al., Phytochemistry, 1983, 22, 2081, (分離)

§ Occidenol

[化学名・別名] Occidiol

[CAS No.] 27548-56-7

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

[構造式]

[分子式] $C_{15}H_{24}O_2$

