

Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 2039, (分離)
Camarda, L. et al., Heterocycles, 1983, 20, 39, (分離)
Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (Ophiopogonanone)

§ Spirost-5-ene-1,3-diol; (1 β , 3 α , 25R)-form, 1-O-[α -L-Rhamnopyranosyl-(1 \rightarrow 2)- β -D-fucopyranoside]

[化学名・別名] Ophiopogonin B. Prosapogenin D₃

[CAS No.] 38971-41-4

[化合物分類] ステロイド (Spirostane steroid).

(C₂₇)

[構造式]

[分子式] C₃₉H₆₂O₁₂

[分子量] 722.912

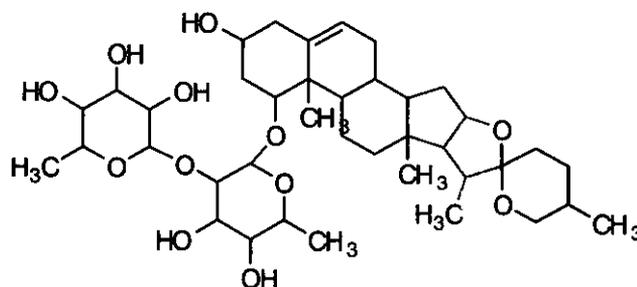
[正確な分子量] 722.42413

[基原] *Ophiopogon japonicus*

[性状] 結晶

[融点] Mp 269-271 °C

[比旋光度]: [α]_D²⁵ -105.5 (Py)



----- 文献 -----

Tada, A. et al., Chem. Pharm. Bull., 1972, 20, 1729; 1973, 21, 308, (分離, 構造決定)
Watanabe, Y. et al., Chem. Pharm. Bull., 1977, 25, 3049, (分離)
Kravets, S.D. et al., Khim. Prir. Soedin., 1986, 22, 188; Chem. Nat. Compd. (Engl. Transl.),
Kravets, S.D. et al., Khim. Prir. Soedin., 1986, 22, 589; Chem. Nat. Compd. (Engl. Transl.),
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1410
Mimaki, Y. et al., Phytochemistry, 1996, 42, 1609, (*Nolina recurvata* saponin)
Yu, B.-Y. et al., Phytochemistry, 1996, 43, 201, (Lirioprolisides, Ophiopogonin A, C13-NMR)

§ Spirost-5-ene-1,3-diol; (1 β , 3 α , 25R)-form, 1-O-[α -L-Rhamnopyranosyl-(1 \rightarrow 2)- β -D-xylopyranosyl-(1 \rightarrow 3)]- β -D-fucopyranoside]

[化学名・別名] Ophiopogonin D

[CAS No.] 41753-55-3

[化合物分類] ステロイド (Spirostane steroid). (C₂₇)

[構造式]

[分子式] C₄₄H₇₀O₁₆

[分子量] 855.027

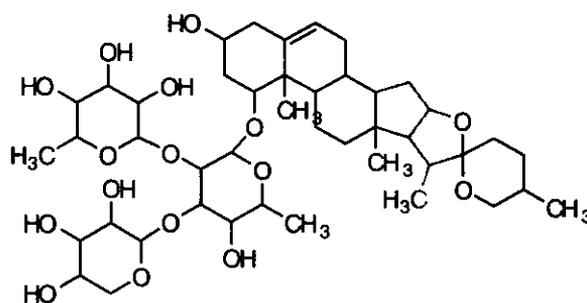
[正確な分子量] 854.46639

[基原] *Ophiopogon japonicus*

[性状] 結晶 (EtOH 溶液)

[融点] Mp 263-265 °C

[比旋光度]: [α]_D²⁴ -107.9 (c, 0.66 in Py)



----- 文献 -----

Shoppee, C.W. et al., J.C.S. (C), 1967, 339
Tada, A. et al., Chem. Pharm. Bull., 1972, 20, 1729; 1973, 21, 308, (分離, 構造決定)
Watanabe, Y. et al., Chem. Pharm. Bull., 1977, 25, 3049, (分離)
Takahira, M. et al., Tet. Lett., 1977, 3647
Bertani, W. et al., Fitoterapia, 1984, 55, 101, (HPLC)
1986, 22, 174, (Alliospiroside A)
Kravets, S.D. et al., Khim. Prir. Soedin., 1986, 22, 589; Chem. Nat. Compd. (Engl. Transl.), 1986, 22, 553,
(Alliospiroside B)
Yong, L.D. et al., Arch. Pharmacol Res., 1989, 12, 295, (Spicatoside A)
Yu, B.-Y. et al., Chem. Pharm. Bull., 1990, 38, 1931, (Liriope saponin)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1410
Yu, B.-Y. et al., Phytochemistry, 1996, 43, 201, (Lirioprolisides, Ophiopogonin A, C13-NMR)
Liu, M. et al., Tet. Lett., 1998, 39, 415, (Glycoside Lm-3)

§ Spirost-5-ene-1,3-diol; (1 β , 3 β , 25*R*)-form, 1-*O*-[3-*O*-Acetyl- α -L-rhamnopyranosyl-(1 \rightarrow 2)]- β -D-fucopyranoside]

[化学名・別名] Ophiopogonin A

[CAS No.] 11054-24-3

[化合物分類] ステロイド (Spirostane steroid). (C27)

[構造式]

[分子式] C₄₁H₆₄O₁₃

[分子量] 764.949

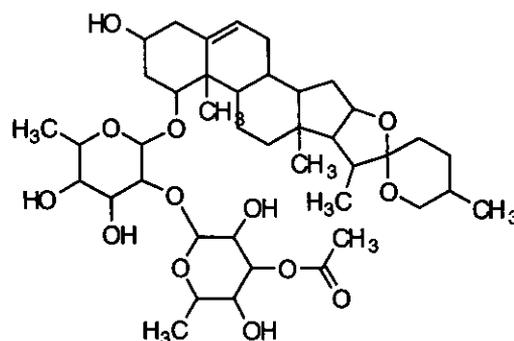
[正確な分子量] 764.434695

[基原] *Ophiopogon japonicus*

[性状] 結晶 (EtOH 溶液)

[融点] Mp 182-184 °C

[比旋光度]: [α]_D¹⁸ -89.7 (c, 0.27 in Py)



-----文献-----

Yu, B.-Y. et al., *Phytochemistry*, 1996, 43, 201, (Lirioprolisides, Ophiopogonin A, C13-NMR)

§ Spirost-5-ene-1,3-diol; (1 β , 3 β , 25*R*)-form, 1-*O*-[α -D-Rhamnopyranosyl-(1 \rightarrow 2)]-[3-*O*-acetyl- β -D-xylopyranosyl-(1 \rightarrow 3)]- β -D-fucopyranoside]

[化学名・別名] Ophiopogonin C

[CAS No.] 65586-25-6

[化合物分類] ステロイド (Spirostane steroid). (C27)

[構造式]

[分子式] C₄₆H₇₂O₁₇

[分子量] 897.065

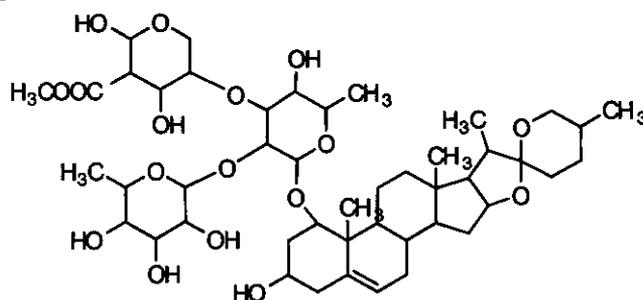
[正確な分子量] 896.476955

[基原] *Ophiopogon japonicus*

[性状] 結晶 (EtOH 溶液)

[融点] Mp 238-240 °C

[比旋光度]: [α]_D²⁸ -93.33 (c, 0.15 in Py)



-----文献-----

Tada, A. et al., *Chem. Pharm. Bull.*, 1972, 20, 1729; 1973, 21, 308, (分離, 構造決定)

Watanabe, Y. et al., *Chem. Pharm. Bull.*, 1977, 25, 3049, (分離)

Kravets, S.D. et al., *Khim. Prir. Soedin.*, 1986, 22, 188; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, 22, 174, (Alliospiroside A)

Kravets, S.D. et al., *Khim. Prir. Soedin.*, 1986, 22, 589; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, 22, 553, (Alliospiroside B)

Yu, B.-Y. et al., *Chem. Pharm. Bull.*, 1990, 38, 1931, (Liriope saponin)

Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, 1993, 1410

Yu, B.-Y. et al., *Phytochemistry*, 1996, 43, 201, (Lirioprolisides, Ophiopogonin A, C13-NMR)

Mimaki, Y. et al., *Phytochemistry*, 1998, 48, 485, (*Ruscus aculeatus* saponin)

Liu, M. et al., *Tet. Lett.*, 1998, 39, 415, (Glycoside Lm-3)

§ Spirost-5-en-3-ol; (3 β , 25*R*)-form, 3-*O*-[α -L-Rhamnopyranosyl-(1 \rightarrow 2)]- β -D-glucopyranoside]

[化学名・別名] Ophiopogonin C'. Prosapogenin A. Prosapogenin D'. Progenin III

[CAS No.] 19057-67-1

[化合物分類] ステロイド (Spirostane steroid). (C27)

[構造式]

[分子式] $C_{39}H_{62}O_{12}$

[分子量] 722.912

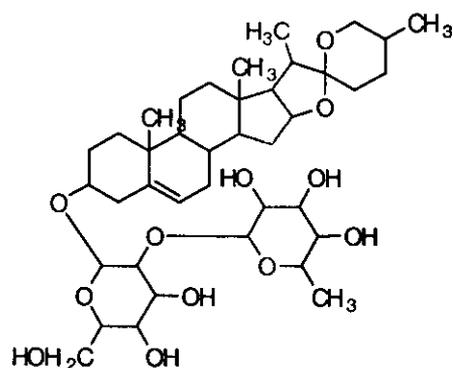
[正確な分子量] 722.42413

[基原] *Ophiopogon japonicus*, *Ophiopogon planiscapus*, *Allium vineale*

[性状] 結晶 (MeOH)

[融点] Mp 238-240 °C で分解

[比旋光度]: $[\alpha]_D^{21} -99.2$ (c, 0.21 in Py)



-----文献-----

Bite, P. et al., Acta Chim. Acad. Sci. Hung., 1967, 52, 79, (分離)

Madaeva, O.S. et al., Khim. Prir. Soedin., 1967, 3, 237; Chem. Nat. Compd. (Engl. Transl.), 1967, 3, 198, (Caucasaponin)

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhauser Verlag, Basel, 1972, no. 2095, (生育, Diosgenin)

Rajaraman, K. et al., Indian J. Chem., Sect. B, 1976, 14, 735, (配糖体)

Watanabe, Y. et al., Chem. Pharm. Bull., 1977, 25, 3049, (Ophiopogonin)

Espejo, O. et al., Phytochemistry, 1982, 21, 413, (Prosapogenin B)

§ Spirost-5-en-3-ol; (3β,25R)-form, 3-O-[α-L-Rhamnopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranoside]

[化学名・別名] Ophiopogonin D'

[CAS No.] 65604-80-0

[化合物分類] ステロイド (Spirostane steroid). (C27)

[構造式]

[分子式] $C_{44}H_{70}O_{16}$

[分子量] 855.027

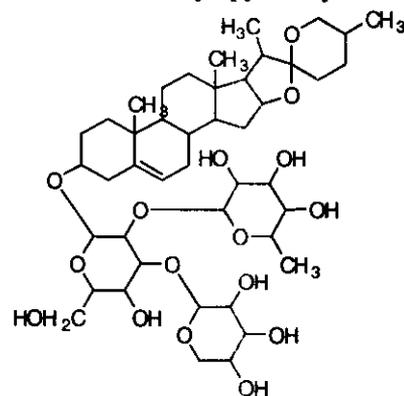
[正確な分子量] 854.46639

[基原] *Ophiopogon japonicus*

[性状] 結晶 (EtOH 溶液)

[融点] Mp 255-257 °C で分解

[比旋光度]: $[\alpha]_D^{18} -41.34$ (c, 0.17 in Py)



-----文献-----

Rajaraman, K. et al., Indian J. Chem., Sect. B, 1976, 14, 735, (配糖体)

Watanabe, Y. et al., Chem. Pharm. Bull., 1977, 25, 3049, (Ophiopogonin)

§ Spirost-5-en-3-ol; (3β,25R)-form, 3-O-[4-O-Acetyl-α-L-rhamnopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranoside]

[化学名・別名] Ophiopogonin B'

[CAS No.] 65604-79-7

[化合物分類] ステロイド (Spirostane steroid). (C27)

[構造式]

[分子式] $C_{46}H_{72}O_{17}$

[分子量] 897.065

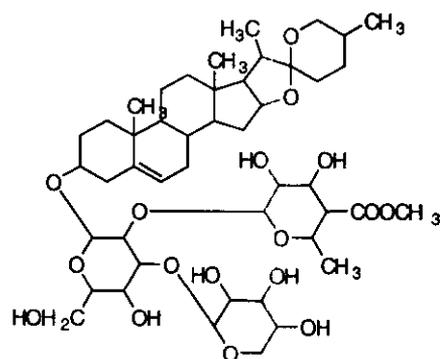
[正確な分子量] 896.476955

[基原] *Ophiopogon japonicus*

[性状] 結晶 (EtOH)

[融点] Mp 245-248 °C で分解

[比旋光度]: $[\alpha]_D^{20} -86.65$ (Py)



-----文献-----

Watanabe, Y. et al., Chem. Pharm. Bull., 1977, 25, 3049, (Ophiopogonin)

§ § ユリ科ナガバジャノヒゲ (*Ophiopogon phwii* Okuyan) の塊根。
本調査研究では研究報告ない。

§ § ユリ科コヤブラン (*Liliope koreana* Nakai) の塊根。
本調査研究では研究報告ない。

*****ジャボランジ (Jaborandi) *****

§ § ミカン科ジャボランジ (*Pilocarpus jaborandi* Holmskiold) の茎, 葉。

§ 5,9-Dimethyl-1-phenyl-5-vinyldecane

[化学名・別名] (5-Ethenyl-5,9-dimethyldecyl) benzene

[CAS No.] 213765-04-9

[化合物分類] テルペノイド (Meroterpenoid)

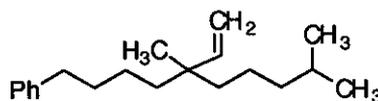
[構造式]

[分子式] $C_{20}H_{32}$

[分子量] 272.473

[正確な分子量] 272.2504

[基原] *Pilocarpus jaborandi* のワックス



-----文献-----

Negri, G. et al., *Phytochemistry*, 1998, 49, 127, (分離, H-NMR, C13-NMR)

§ 5,9-Dimethyl-5-vinyl-1-phenyldecane

[化学名・別名] (5-Ethenyl-5,9-dimethyldecyl) benzene. 3,7-Dimethyl-3-(4-phenylbutyl)-1-octene

[化合物分類] 脂肪族化合物 (Branched alkenic hydrocarbon), 単環芳香族 (Simple benzene derivative)

[構造式]

[分子式] $C_{20}H_{32}$

[分子量] 272.473

[正確な分子量] 272.2504

[基原] *Pilocarpus jaborandi* の葉のワックス

[UV]: [neutral] λ_{max} 235; 253 (sh); 274 (sh); 300 (sh); 322 (sh) (溶媒の報告はない)

[その他のデータ] 光学活性は示されていない

-----文献-----

Negri, G. et al., *Phytochemistry*, 1998, 49, 127, (分離, UV, H-NMR, C13-NMR, Mas)

§ Pilocarpine; (+)-form, N-De-Me

[化学名・別名] Pilocarpidine

[CAS No.] 127-67-3

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

[構造式]

[分子式] $C_{10}H_{14}N_2O_2$

[分子量] 194.233

[正確な分子量] 194.105528

[基原] 次の植物の葉から得られるアルカロイド: *Pilocarpus jaborandi* (ミカン科)

[用途] Pharmacol. resembles that of Pilocarpine, but weaker

[性状] シロップ

[比旋光度]: $[\alpha]_D +81.3$ (H₂O)

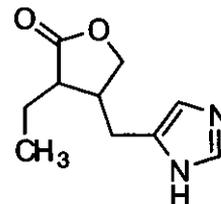
[溶解性] 水に可溶

[その他のデータ] 蒸留で分解

-----文献-----

Spaumlth, E. et al., *Ber.*, 1925, 58, 513, (構造決定, Pilocarpidine)

Burtles, R. et al., *J.C.S.*, 1925, 127, 581, (構造決定, Pilocarpidine)



Preobrashenski, N.A. et al., Ber., 1933, 66, 1536; 1936, 69, 1835, (合成法, Pilocarpidine)
 Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 4526; 4525
 Al-Badr, A.A. et al., Anal. Profiles Drug Subst., 1983, 12, 385, (レビュー, UV, IR, H-NMR, C13-NMR, Mass, 分析)
 Turski, L. et al., Synapse (N.Y.), 1989, 3, 154, (pharmacol, レビュー)
 Wiseman, L.R. et al., Drugs, 1995, 49, 143, (レビュー)
 Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, PIF000; PIF250; PIF500

*****シャロット (Shallot) *****

§ § ユリ科ワケギ (*Allium ascalonicum* L.) の鱗茎。

本調査研究では研究報告ない。

*****ジュウニヒトエ (Bugle) *****

§ § シソ科ジュウニヒトエ (*Ajuga nipponensis* Makino) の全草。

§ Ajugose

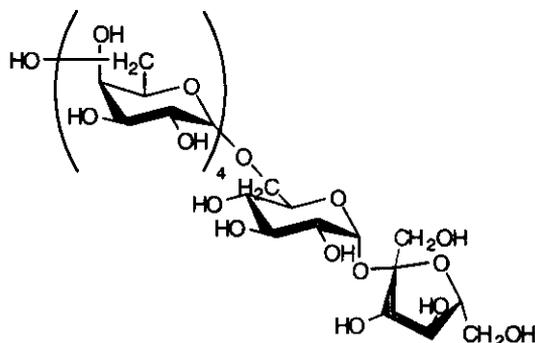
[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₃₆H₆₂O₃₁

[分子量] 990.867

[正確な分子量] 990.327515



[基原] *Ajuga nipponensis* と *Verbascum thapsiforme* の根

[融点] Mp 270 °C

[比旋光度]: [α]_D¹² +190.8 (H₂O). [α]_D¹⁸ +161.3 (H₂O)

-----文献-----

Murakami, S., Acta Phytochim., 1941, 12, 97

Anagnostopoulos, C. et al., Bull. Soc. Chim. Biol., 1954, 36, 1115

Herissey, H. et al., C. R. Hebd. Seances Acad. Sci., 1964, 259, 824, (分離)

§ 18-Chloro-1,4,6,12,19-pentahydroxy-13-cleroden-15,16-olide; (*ent*-1 α,4 β,6 β,12*R*)-form, 1-Tigloyl, 6,19-di-Ac

[化学名・別名] Ajugamarin chlorohydrin

[CAS No.] 85447-27-4

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

[構造式]

[分子式] C₂₉H₄₁ClO₁₀

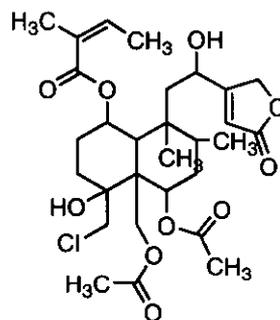
[分子量] 585.09

[正確な分子量] 584.238827

[基原] *Ajuga nipponensis*

[性状] 無定型の塊

[その他のデータ] 非天然物の可能性

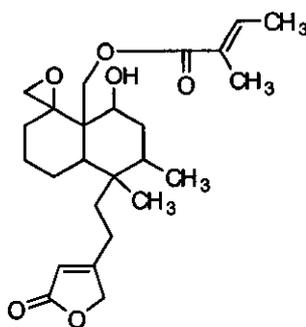


-----文献-----

Shimomura, H. et al., Chem. Pharm. Bull., 1983, 31, 2192, (分離, 構造決定)

§ 4,18-Epoxy-6,19-dihydroxy-13-cleroden-15,16-olide; (*ent*-4 β,6 β)-form, 19-Tigloyl

[化学名・別名] Ajugacumbin B. Ajugamarin L2
 [CAS No.] 124961-67-7
 [化合物分類] テルペノイド (Clerodane diterpenoid)
 [構造式]
 [分子式] $C_{25}H_{36}O_6$
 [分子量] 432.556
 [正確な分子量] 432.25119
 [基原] *Ajuga decumbens*, *Ajuga nipponensis*
 [用途] 茎葉を食する昆虫の予防剤
 [性状] 結晶 (EtOAc/cyclohexane)
 [融点] Mp 194-195 °C
 [比旋光度]: $[\alpha]_D^{25} +40.5$ (c, 0.74 in $CHCl_3$)

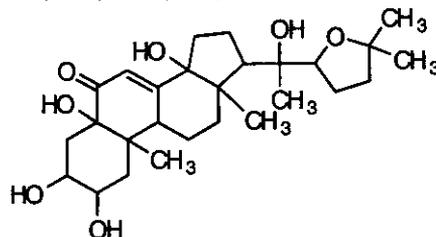


-----文献-----

Zhi-da, M. et al., Chem. Pharm. Bull., 1989, 37, 2505, (分離, H-NMR, C13-NMR, 結晶構造)
 Huan-ming, C. et al., Chem. Pharm. Bull., 1995, 43, 2253, (Ajugacumbin G)
 Liu, Z. et al., Chin. Chem. Lett., 1996, 6, 581, (Ajugamarin L 2, 結晶構造)

§ 22,25-Epoxy-2,3,5,14,20-pentahydroxycholest-7-en-6-one; (2 β ,3 β ,5 β ,14 α ,20R,22 ξ)-form

[化学名・別名] Ajugasterone D
 [CAS No.] 80651-74-7
 [化合物分類] ステロイド (Neutral cholestane steroid). (C27)
 [構造式]



[基原] *Ajuga nipponensis*

-----文献-----

Li, W. et al., Huaxue Xuebao, 1981, 39, 735; CA, 97, 145120b

§ 4,18-Epoxy-1,6,12,19-tetrahydroxy-13-cleroden-15,16-olide; (ent-1 α ,4 β ,6 β ,12R)-form, 6,19-Di-Ac

[化学名・別名] Ajugamarin C1
 [CAS No.] 121449-64-7
 [化合物分類] テルペノイド (Clerodane diterpenoid)
 [構造式]
 [分子式] $C_{24}H_{34}O_8$
 [分子量] 466.527
 [正確な分子量] 466.220285
 [基原] *Ajuga nipponensis*
 [性状] 無定型の塊
 [比旋光度]: $[\alpha]_D^{30} +5.5$ (c, 2.3 in $CHCl_3$)



-----文献-----

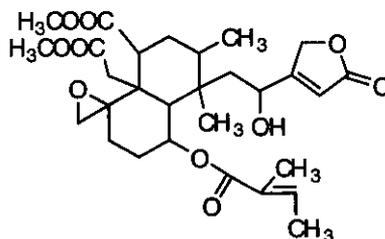
Shimomura, H. et al., Chem. Pharm. Bull., 1983, 31, 2192; 1989, 37, 354; 988; 996, (分離, H-NMR, C13-NMR, 結晶構造)

Shen, X. et al., Phytochemistry, 1993, 33, 887; 34, 1091, (Ajugamacrins, Ajugapantin A)

Amano, T. et al., Biosci., Biotechnol., Biochem., 1997, 61, 1518, (Ajugatakasin)

§ 4,18-Epoxy-1,6,12,19-tetrahydroxy-13-cleroden-15,16-olide; (ent-1 α ,4 β ,6 β ,12R)-form, 1-Tigloyl, 6,19-di-Ac

[化学名・別名] Ajugamarin A1. Ajugamarin
 [CAS No.] 78798-40-0
 [化合物分類] テルペノイド (Clerodane diterpenoid)
 [構造式]
 [分子式] $C_{29}H_{40}O_{10}$
 [分子量] 548.629
 [正確な分子量] 548.26215
 [基原] *Ajuga nipponensis* の葉



[性状] 針状結晶 (CCl₄)
[融点] Mp 93-95 °C
[比旋光度]: $[\alpha]_D^{25} -20$ (c, 0.4 in CCl₄)
[UV]: [neutral] $\lambda_{max} 212$ (ϵ 20000) (95% EtOH)

-----文献-----

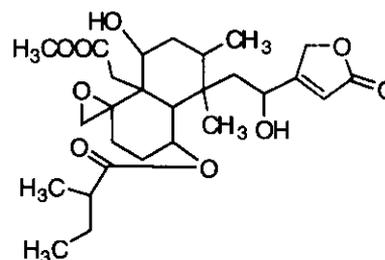
Shimomura, H. et al., Chem. Pharm. Bull., 1983, 31, 2192; 1989, 37, 354; 988; 996, (分離, H-NMR, C13-NMR, 結晶構造)

Shen, X. et al., Phytochemistry, 1993, 33, 887; 34, 1091, (Ajugamacrins, Ajugapantin A)

Amano, T. et al., Biosci., Biotechnol., Biochem., 1997, 61, 1518, (Ajugatakasin)

§ 4,18-Epoxy-1,6,12,19-tetrahydroxy-13-cleroden-15,16-olide; (*ent*-1 α ,4 β ,6 β ,12*R*)-form, 1-(2*S*-Methylbutanoyl), 19-Ac

[化学名・別名] Ajugamarin B3
[CAS No.] 121449-66-9
[化合物分類] テルペノイド (Clerodane diterpenoid)
[構造式]
[分子式] C₂₇H₄₀O₉
[分子量] 508.608
[正確な分子量] 508.267235
[基原] *Ajuga nipponensis*
[性状] 無定型の塊
[比旋光度]: $[\alpha]_D^{22} +22$ (c, 0.9 in CHCl₃)



-----文献-----

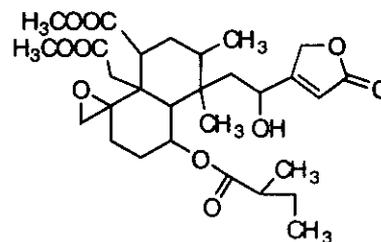
Shimomura, H. et al., Chem. Pharm. Bull., 1983, 31, 2192; 1989, 37, 354; 988; 996, (分離, H-NMR, C13-NMR, 結晶構造)

Shen, X. et al., Phytochemistry, 1993, 33, 887; 34, 1091, (Ajugamacrins, Ajugapantin A)

Amano, T. et al., Biosci., Biotechnol., Biochem., 1997, 61, 1518, (Ajugatakasin)

§ 4,18-Epoxy-1,6,12,19-tetrahydroxy-13-cleroden-15,16-olide; (*ent*-1 α ,4 β ,6 β ,12*R*)-form, 1-(2*S*-Methylbutanoyl), 6,19-di-Ac

[化学名・別名] Ajugamarin B1. Dihydroajugamarin
[CAS No.] 85447-28-5
[化合物分類] テルペノイド (Clerodane diterpenoid)
[構造式]
[分子式] C₂₉H₄₂O₁₀
[分子量] 550.645
[正確な分子量] 550.2778
[基原] *Ajuga nipponensis*
[性状] 無定型の塊



-----文献-----

Shimomura, H. et al., Chem. Pharm. Bull., 1983, 31, 2192; 1989, 37, 354; 988; 996, (分離, H-NMR, C13-NMR, 結晶構造)

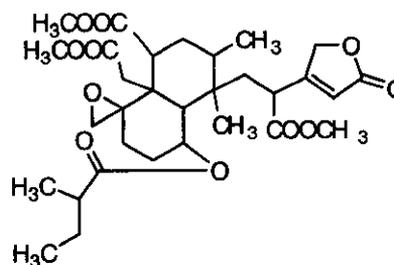
Shen, X. et al., Phytochemistry, 1993, 33, 887; 34, 1091, (Ajugamacrins, Ajugapantin A)

Amano, T. et al., Biosci., Biotechnol., Biochem., 1997, 61, 1518, (Ajugatakasin)

§ 4,18-Epoxy-1,6,12,19-tetrahydroxy-13-cleroden-15,16-olide; (*ent*-1 α ,4 β ,6 β ,12*R*)-form, 1-(2*S*-Methylbutanoyl), tri-Ac

[化学名・別名] Ajugamarin B2

[CAS No.] 121449-65-8
 [化合物分類] テルペノイド (Clrodane diterpenoid)
 [構造式]
 [分子式] $C_{31}H_{44}O_{11}$
 [分子量] 592.682
 [正確な分子量] 592.288365
 [基原] *Ajuga nipponensis*
 [性状] 結晶 (EtOH)
 [融点] Mp 154-155 °C
 [比旋光度]: $[\alpha]_D^{20} -25$ (c, 0.8 in $CHCl_3$)

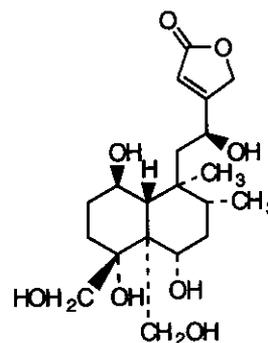


-----文献-----

Shimomura, H. et al., Chem. Pharm. Bull., 1983, 31, 2192; 1989, 37, 354; 988; 996, (分離, H-NMR, C13-NMR, 結晶構造)
 Shen, X. et al., Phytochemistry, 1993, 33, 887; 34, 1091, (Ajugamacrins, Ajugapantoin A)
 Amano, T. et al., Biosci., Biotechnol., Biochem., 1997, 61, 1518, (Ajugatakasin)

§ 1,4,6,12,18,19-Hexahydroxy-13-cleroden-15,16-olide
 [構造式]

[分子式] $C_{20}H_{32}O_8$
 [分子量] 400.468
 [正確な分子量] 400.20972
 [基原] *Ajuga nipponensis*



-----文献-----

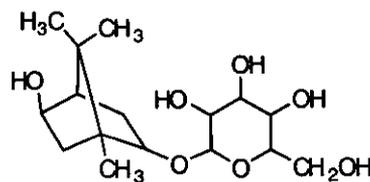
Shimomura, H. et al., Chem. Pharm. Bull., 1989, 37, 354, (分離, H-NMR, C13-NMR, Mas)

*****シユクシヤ (Shukusha) *****

§ § ショウガ科シユクシヤ (*Amomum xanthioides* Wallich) の種子, 成熟果実。

§ 2,5-Bornanediol; (1R,2S,5R)-form, 2-O-β-D-Glucopyranoside

[化学名・別名] Amomumside
 [CAS No.] 117615-23-3
 [化合物分類] テルペノイド (Camphane monoterpene)
 [構造式]
 [分子式] $C_{16}H_{28}O_7$
 [分子量] 332.393
 [正確な分子量] 332.183505
 [基原] *Amomum xanthioides*, *Berchemia racemosa*
 [性状] 無定型の粉末
 [比旋光度]: $[\alpha]_D^{20} -12.6$ (c, 0.6 in MeOH)



-----文献-----

Marquet, A. et al., Bull. Soc. Chim. Fr., 1967, 128, (合成法)
 Allen, M.S. et al., Can. J. Chem., 1979, 57, 733, (合成法)
 Mahmood, U. et al., Phytochemistry, 1983, 22, 774, (分離)
 Gunawardana, Y.A.G.P. et al., J. Nat. Prod., 1988, 51, 142, (分離, C13-NMR, H-NMR)
 Inoshiri, S. et al., Phytochemistry, 1988, 27, 2869, (分離, H-NMR, C13-NMR)
 Ahmed, A.A. et al., Phytochemistry, 1991, 30, 1207, (分離)
 Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1595, (配糖体)

§ § ヒノキ科セイヨウネズ (*Juniperus communis* L.) の果実。

§ 8,11,13-Abietatrien-12-ol; 6,7-Didehydro

[化学名・別名] 6,8,11,13-Abietatetraen-12-ol. Δ^6 -Dehydroferruginol. 6,7-Didehydroferruginol

[化合物分類] テルペノイド (Abietane diterpenoid)

[構造式]

[分子式] $C_{20}H_{28}O$

[分子量] 284.441

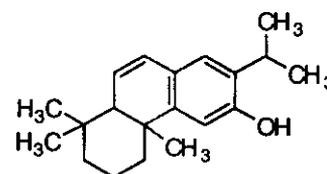
[正確な分子量] 284.214015

[基原] 次の植物の木部から分離: *Juniperus communis*, *Podocarpus*

dacrydioides, *Salvia apiana*

[性状] 淡黄色の塊

[比旋光度]: $[\alpha]_D^{20}$ -60 (EtOH)



-----文献-----

Briggs, L.H. et al., *Tetrahedron*, 1959, 7, 270, (Dehydroferruginol)

Gonzaacutetez, A.G. et al., *Phytochemistry*, 1992, 31, 1691, (6,7-Didehydroferruginol)

Su, W.-C. et al., *Phytochemistry*, 1994, 35, 1279, (6,7-Didehydroferruginol methyl ether, C13-NMR)

§ 4-Acetyl-1,4-dimethyl-1-cyclohexene

[化学名・別名] 1-(1,4-Dimethyl-3-cyclohexenyl) ethanone

[CAS No.] 43219-68-7

[化合物分類] テルペノイド (Other cyclohexane monoterpene)

[構造式]

[分子式] $C_{10}H_{16}O$

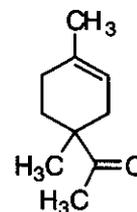
[分子量] 152.236

[正確な分子量] 152.120115

[基原] *Juniperus communis* のオイル

[性状] オイル

[比旋光度]: $[\alpha]_D^{20}$ +2.1 (c, 1 in CCl_4)



-----文献-----

Thomas, A.F., *Helv. Chim. Acta*, 1973, 56, 1800, (分離)

Kreiser, W. et al., *Helv. Chim. Acta*, 1974, 57, 164, (合成法)

Vig, O.P. et al., *Indian J. Chem., Sect. B*, 1976, 14, 932, (合成法)

§ 4(15),10(14)-Cadinadiene

[化学名・別名] Decahydro-1,6-bis(methylene)-4-(1-methylethyl)naphthalene (CAS 名).

Decahydro-4-isopropyl-1,6-dimethylenenaphthalene. ϵ -Cadinene

[CAS No.] 25548-04-3

[関連 CAS No.] 1080-67-7, 27542-04-7

[化合物分類] 脂肪族化合物 (Simple heteroalicyclics (2 × O))

[構造式]

[分子式] $C_{15}H_{24}$

[分子量] 204.355

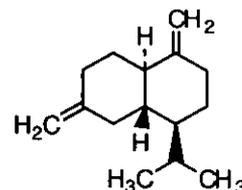
[正確な分子量] 204.1878

[基原] *Mentha arvensis*, *Juniperus communis*

[性状] オイル

[沸点] Bp_2 99-100 °C

[比旋光度]: $[\alpha]_D^{22}$ +50.7 (c, 1.5 in $CHCl_3$)



Absolute configuration

-----文献-----

Burk, L.A. et al., *Tetrahedron*, 1976, 32, 2083, (成書)

Koster, F.-H. et al., *Annalen*, 1986, 78, (合成法, C13-NMR)

Hagiwara, H. et al., *J.C.S. Perkin 1*, 1993, 2173, (合成法)

§ 4-Cadinen-10-ol; 10 α -form

[化学名・別名] α -Cadinol

[CAS No.] 481-34-5

[化合物分類] 脂肪族化合物 (Simple heteroalicyclics (2 × O))

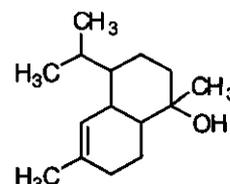
[構造式]

[基原] *Chamaecyparis lawsoniana* and *Juniperus communis*. また, *Chamaecyparis obtusa*, *Chamaecyparis pisifera*, *Juniperus horizontalis*, *Juniperus scopulorum*, *Athrotaxis* spp., *Neocallitropsis araucaroides*

[性状] 結晶

[融点] Mp 74.5-75 °C

[比旋光度]: $[\alpha]_D^{25}$ -47 (-38.5)



-----文献-----

Nagasampagi, B.A. et al., Tet. Lett., 1968, 1913, (分離)

Caine, D. et al., Tet. Lett., 1977, 3107, (合成法)

Borg-Karlson, A.-K. et al., Tetrahedron, 1981, 37, 425, (stereochem)

Bottini, A.T. et al., J. Nat. Prod., 1987, 50, 732, (C13-NMR)

Dupreacute, S. et al., Phytochemistry, 1991, 30, 1211, (α -Cadinol methyl ether)

Claeson, P. et al., Planta Med., 1991, 57, 352, (T-Cadinol, H-NMR, C13-NMR)

Labbeacate, C. et al., Phytochemistry, 1993, 34, 441, (T-Cadinol, H-NMR, C13-NMR)

§ Campholenic alcohol

[化学名・別名] 2,2,3-Trimethyl-3-cyclopentene-1-ethanol. 4-(2-Hydroxyethyl)-1,5,5-trimethylcyclopentene

[CAS No.] 1901-38-8

[化合物分類] テルペノイド (Other cyclopentane monoterpene)

[構造式]

[分子式] C₁₀H₁₈O

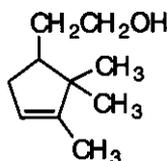
[分子量] 154.252

[正確な分子量] 154.135765

[基原] *Juniperus communis*

[性状] オイル

[比旋光度]: $[\alpha]_D^{25}$ -1.5 (c, 8 in CCl₄)



-----文献-----

Thomas, A.F., Helv. Chim. Acta, 1972, 55, 815

§ Campholenic alcohol; Ac

[化合物分類] テルペノイド (Other cyclopentane monoterpene)

[構造式]

[分子式] C₁₂H₂₀O₂

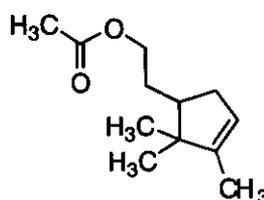
[分子量] 196.289

[正確な分子量] 196.14633

[基原] *Juniperus communis*

[性状] オイル

[比旋光度]: $[\alpha]_D^{25}$ -1 (c, 8 in CCl₄)



-----文献-----

Thomas, A.F., Helv. Chim. Acta, 1972, 55, 815

§ Campholenic alcohol; Aldehyde

[化学名・別名] 2,2,3-Trimethyl-3-cyclopenten-1-ylacetaldehyde. Campholenic aldehyde

[CAS No.] 4501-58-0

[化合物分類] テルペノイド (Other cyclopentane monoterpene)

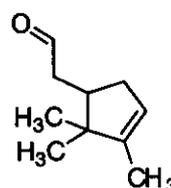
[構造式]

[分子式] C₁₀H₁₆O

[分子量] 152.236

[正確な分子量] 152.120115

[基原] *Juniperus communis*



[性状] オイル
[沸点] Bp_{10} 77 °C
[比旋光度]: $[\alpha]_D^{20}$ -3.1 (CCl₄)

-----文献-----

Thomas, A.F., *Helv. Chim. Acta*, 1972, 55, 815

§ **Campholenic alcohol; Aldehyde, 3,4-epoxide**

[化学名・別名] 1,2,2-Trimethyl-6-oxabicyclo[3.1.0]hexane-3-acetaldehyde (CAS 名). Epoxycampholenic aldehyde

[CAS No.] 36789-60-3

[化合物分類] テルペノイド (Other cyclopentane monoterpeneoid)

[構造式]

[分子式] C₁₀H₁₆O₂

[分子量] 168.235

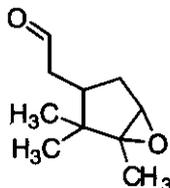
[正確な分子量] 168.11503

[基原] *Juniperus communis*

[性状] オイル

[沸点] Bp_{10} 101-102 °C

[比旋光度]: $[\alpha]_D^{20}$ -0.83 (CHCl₃)



-----文献-----

Thomas, A.F., *Helv. Chim. Acta*, 1972, 55, 815

§ **14,15-Dihydroxy-8(17),13(16)-labdadien-19-oic acid; (14S)-form**

[化合物分類] テルペノイド (Labdane diterpenoid)

[構造式]

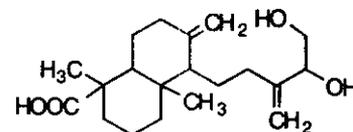
[基原] *Juniperus communis*

[性状] オイル (as Me ester)

[比旋光度]: $[\alpha]_D$ +43 (c, 1.6 in CHCl₃) (Me ester)

-----文献-----

de Pascual Teresa, J. et al., *Phytochemistry*, 1980, 19, 1153



§ **4(15)-Eudesmen-6-ol; (5 α,6 α,7 β,10 β)-form**

[化学名・別名] Junenol

[CAS No.] 472-07-1

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

[構造式]

[基原] juniper berry (*Juniperus communis*), black dammar resin

[性状] 結晶 (petrol or by subl.)

[融点] Mp 62.5-63 °C

[沸点] Bp_1 121-122 °C

[比旋光度]: $[\alpha]_D$ +52 (c, 3.35 in CHCl₃)

-----文献-----

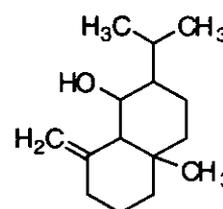
Shaligram, A.H. et al., *Tetrahedron*, 1962, 18, 969, (分離)

Hinge, V.K. et al., *Tetrahedron*, 1965, 21, 3197, (分離)

Thomas, A.F. et al., *Tetrahedron*, 1976, 32, 2261, (分離, 構造決定)

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

Warmers, U. et al., *Phytochemistry*, 1999, 52, 1519, (7-Epijunenol)



§ **Geijjerone**

[化学名・別名] 4-Ethenyl-4-methyl-3-(1-methylethenyl)cyclohexanone (CAS 名).

3-Isopropenyl-4-methyl-4-vinylcyclohexanone

[CAS No.] 41411-01-2

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

[構造式]

[分子式] $C_{12}H_{18}O$

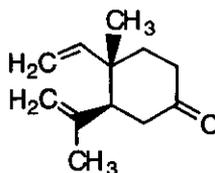
[分子量] 178.274

[正確な分子量] 178.135765

[基原] *Juniperus communis*

[沸点] $B_{p.1}$ 81-86 °C

[比旋光度]: $[\alpha]_D^{20}$ -27.8 (CCl₄)



-----文献-----

Vig, O.P. et al., Indian J. Chem., Sect. B, 1976, 14, 564

Kato, M. et al., J.C.S. Perkin 1, 1979, 2740, (合成法)

Kim, D. et al., J.O.C., 1987, 52, 4633, (合成法)

Wakamatsu, T. et al., Heterocycles, 1987, 26, 1203, (合成法)

§ 5,10(14)-Germacradiene-1,4-diol; (1 β , 4 β OH, 5E)-form

[CAS No.] 63181-39-5

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

[構造式]

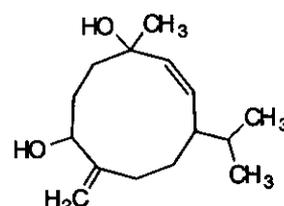
[基原] 次の植物から分離: *Senecio adenophyllus*, *Juniperus communis* subsp.

hemisphaerica

[性状] 結晶 (hexane)

[融点] M_p 84-86 °C

[比旋光度]: $[\alpha]_D^{24}$ -13 (c, 1.3 in CHCl₃). $[\alpha]_D^{25}$ -147.9 (c, 0.3 in CHCl₃)



-----文献-----

Wratten, S.J. et al., J.O.C., 1977, 42, 3343, (分離)

Izac, R.R. et al., Tetrahedron, 1982, 38, 301, (分離, acetate)

Kitagawa, I. et al., Chem. Pharm. Bull., 1987, 35, 124, (Nephthediol, Nephtheoxydiol)

Jakupovic, J. et al., Phytochemistry, 1987, 26, 761, (分離)

Dupreacate, S. et al., Phytochemistry, 1991, 30, 1211, (分離, H-NMR)

San Feliciano, A. et al., J. Nat. Prod., 1995, 58, 1059, (分離, H-NMR, C13-NMR, 合成法)

§ 5,10(14)-Germacradiene-1,4-diol; (1 α , 4 β OH, 5E)-form

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

[構造式]

[基原] *Juniperus communis* subsp. *hemisphaerica*

-----文献-----

Wratten, S.J. et al., J.O.C., 1977, 42, 3343, (分離)

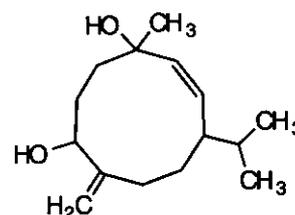
Izac, R.R. et al., Tetrahedron, 1982, 38, 301, (分離, acetate)

Kitagawa, I. et al., Chem. Pharm. Bull., 1987, 35, 124, (Nephthediol, Nephtheoxydiol)

Jakupovic, J. et al., Phytochemistry, 1987, 26, 761, (分離)

Dupreacate, S. et al., Phytochemistry, 1991, 30, 1211, (分離, H-NMR)

San Feliciano, A. et al., J. Nat. Prod., 1995, 58, 1059, (分離, H-NMR, C13-NMR, 合成法)

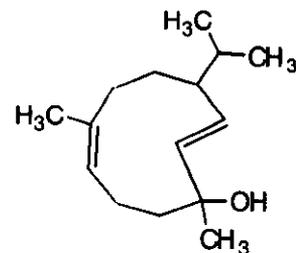


§ 1(10),5-Germacradien-4-ol; (1(10)E, 4 β , 5E)-form

[CAS No.] 74841-87-5

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

[構造式]



[基原] *Pseudobrickellia brasiliensis*, *Juniperus communis* subsp. *hemisphaerica*

[性状] オイル

[比旋光度]: $[\alpha]_D^{24} -109$ (c, 0.02 in CHCl_3)

-----文献-----

Izac, R.R. et al., *Tetrahedron*, 1982, 38, 301, (分離)

Bohlmann, F. et al., *Phytochemistry*, 1984, 23, 1798, (分離)

Kitagawa, I. et al., *Chem. Pharm. Bull.*, 1987, 35, 124

Schmaus, G. et al., *Planta Med.*, 1989, 55, 482, (分離, H-NMR, C13-NMR)

Bergström, G. et al., *Acta Chem. Scand.*, 1995, 48, 187, (分離)

San Feliciano, A. et al., *J. Nat. Prod.*, 1995, 58, 1059, (分離, H-NMR, C13-NMR)

§ 12-Hydroxy-8,11,13-abietatriene-6,7-dione; 5 α -form

[化学名・別名] Prexanthoperol. Hypargenin C

[CAS No.] 119817-27-5

[化合物分類] テルペノイド (Abietane diterpenoid)

[構造式]

[分子式] $\text{C}_{20}\text{H}_{26}\text{O}_3$

[分子量] 314.424

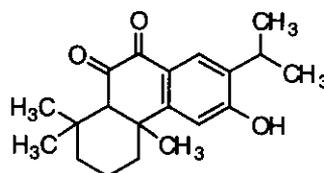
[正確な分子量] 314.188195

[基原] *Juniperus communis* の微量成分と、また *Salvia hypargeia* から得られる

[性状] 黄色結晶もしくは橙色の無定型の塊

[融点] Mp 207-210 °C

[UV]: [neutral] λ_{max} 218 (ϵ 3150); 320 (ϵ 12500); 333 (ϵ 15800); 403 (ϵ 5000) (MeOH)



-----文献-----

Brendenberg, J.B. et al., *Acta Chem. Scand.*, 1956, 10, 1511, (分離)

Nasipuri, D. et al., *J.C.S.*, 1962, 4248, (合成法)

Kondo, Y. et al., *Chem. Pharm. Bull.*, 1963, 11, 678, (構造決定)

Ulubelen, A. et al., *J. Nat. Prod.*, 1988, 51, 1178, (分離, H-NMR, C13-NMR)

Ghosal, M. et al., *Indian J. Chem., Sect. B*, 1992, 31, 524, (合成法)

§ 12-Hydroxy-8,11,13-abietatriene-6,7-dione; 5 β -form

[化学名・別名] Xanthoperol

[CAS No.] 564-23-8

[化合物分類] テルペノイド (Abietane diterpenoid)

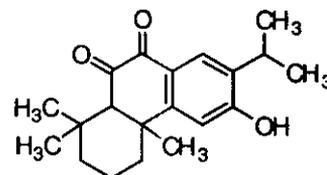
[構造式]

[基原] *Juniperus communis* とその他の木部, 例えば, *Podocarpus dactyloides*, *Cryptomeria japonica*

[性状] 黄色結晶 (C_6H_6)

[融点] Mp 255-270 °C で分解

[比旋光度]: $[\alpha]_D^{20} +132.5$ (c, 1.2 in EtOH)



-----文献-----

Brendenberg, J.B. et al., *Acta Chem. Scand.*, 1956, 10, 1511, (分離)

Nasipuri, D. et al., *J.C.S.*, 1962, 4248, (合成法)

Kondo, Y. et al., *Chem. Pharm. Bull.*, 1963, 11, 678, (構造決定)

Ulubelen, A. et al., *J. Nat. Prod.*, 1988, 51, 1178, (分離, H-NMR, C13-NMR)

Ghosal, M. et al., *Indian J. Chem., Sect. B*, 1992, 31, 524, (合成法)

§ 12-Hydroxy-8,11,13-abietatrien-7-one

[化学名・別名] Sugiol. Isomicropinic acid. 7-Oxoferruginol

[CAS No.] 511-05-7

[化合物分類] テルペノイド (Abietane diterpenoid)

[構造式]

[分子式] $C_{20}H_{28}O_2$

[分子量] 300.44

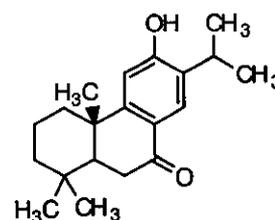
[正確な分子量] 300.20893

[基原] *Cryptomeria japonica*, *Dacrydium cupressinum*, *Juniperus communis*, *Salvia miltiorrhiza*

[性状] 結晶 (AcOH)

[融点] Mp 295-297 °C

[比旋光度]: $[\alpha]_D^{20} +22.6$ (c, 1.2 in dioxan)



-----文献-----

Kupchan, S.M. et al., J.O.C., 1969, 34, 3912, (分離)

Cambie, R.C. et al., Aust. J. Chem., 1971, 24, 217, (分離)

Meyer, W.L. et al., J.O.C., 1975, 40, 3686, (合成法, 成書)

Matsumoto, T. et al., Bull. Chem. Soc. Jpn., 1977, 50, 1575, (成書)

Chang, H.M. et al., J.O.C., 1990, 55, 3537, (分離, H-NMR, C13-NMR)

Ulubelen, A. et al., Planta Med., 1990, 56, 82, (Trilobinol)

Das, S. et al., Tet. Lett., 1994, 35, 4027, (合成法)

Kuo, Y.H. et al., Phytochemistry, 1996, 42, 779, (sugiol methyl ether)

Gao, J. et al., Phytochemistry, 1997, 44, 759, (Sugiol, C13-NMR)

§ 7-Hydroxy-8(14),15-isopimaradien-18-oic acid; 7 α -form

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

[構造式]

[基原] *Salvia microphylla*, *Juniperus communis*

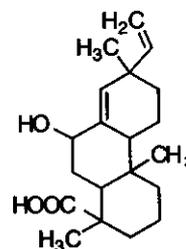
[性状] オイル (as Me ester)

[比旋光度]: $[\alpha]_D -41$ (c, 0.84 in $CHCl_3$) (Me ester)

-----文献-----

De Pasacual, J. et al., Phytochemistry, 1980, 19, 1153, (分離)

Esquivel, B. et al., Planta Med., 1989, 55, 62, (分離, H-NMR, C13-NMR)



§ 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 の心材に存在する. 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] pK_{a1} 6.72 (25 °C, I 2.0)

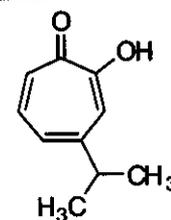
[傷害・毒性] 50%致死量 (LD₅₀) (マウス, 腹腔内投与) 85 mg/kg

[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)

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhauser



Verlag, Basel, 1972, no. 573, (生育)

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.

参考文献

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.

参考文献

JMCMAR Journal of Medicinal Chemistry. (American Chemical Soc., Distribution Office Dept. 223, POB 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.

参考文献

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.

参考文献

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).

参考文献

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 : 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

FCTOD7 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

[化学名・別名] 7 α -Hydroxy-8(14),15-isopimaradien-18-oic acid. 7 α -Hydroxysandaracopimaric acid

[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*

[性状] オイル (as Me ester)

[比旋光度]: $[\alpha]_D -41$ (c, 0.8 in CHCl₃) (Me ester)

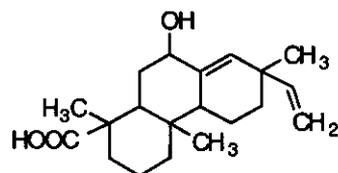
-----文献-----

de Pascual Teresa, J. et al., *Phytochemistry*, 1980, 19, 1153, (7-hydroxysandaracopimaric acid)

de Kimpe, N. et al., *J.O.C.*, 1982, 47, 3628, (分離, 結晶構造)

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-ketone

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

[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*

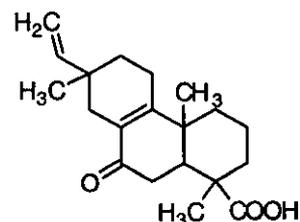
[性状] オイル (as Me ester)

[比旋光度]: $[\alpha]_D +77.6$ (c, 0.8 in CHCl₃)

-----文献-----

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

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



§ Junionone

[化学名・別名] 4-(2,2-Dimethylcyclobutyl)-3-buten-2-one

[CAS No.] 51847-79-1

[化合物分類]テルペノイド (Cyclobutane monoterpene)

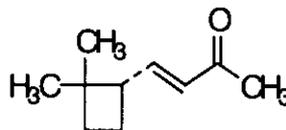
[構造式]

[分子式] C₁₀H₁₆O

[分子量] 152.236

[正確な分子量] 152.120115

[基原] *Juniperus communis* の果実オイル



-----文献-----

Thomas, A.F., Chem. Comm., 1973, 746

Gaoni, Y., Tet. Lett., 1982, 23, 5219, (合成法)

Gaoni, Y. et al., J.O.C., 1985, 50, 2948, (合成法)

Ghosh, A. et al., Tetrahedron, 1990, 46, 3077, (合成法)

§ 8(17)-Labdene-15,19-diol; (13S)-form, Dialdehyde

[化学名・別名] 8(17)-Labdene-15,19-dial. Junicedral

[CAS No.] 70901-87-0

[化合物分類]テルペノイド (Labdane diterpenoid)

[構造式]

[分子式] C₂₀H₃₂O₂

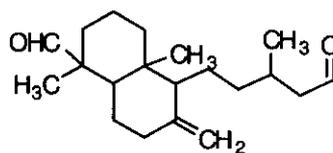
[分子量] 304.472

[正確な分子量] 304.24023

[基原] 次の植物から分離: *Juniperus communis*

[性状] オイル

[比旋光度]: [α]_D +16.1 (c, 0.99 in CHCl₃)



-----文献-----

Bruns, K., Tetrahedron, 1968, 24, 3417

Haeuser, J. et al., Tetrahedron, 1970, 16, 3461

De Pascual Teresa, J. et al., An. Quim., 1974, 70, 1015; 1977, 73, 568, (Junicedral)

Calderacuteon, J.J. et al., Phytochemistry, 1987, 26, 2639

Kuo, Y.-H. et al., Chem. Pharm. Bull., 1996, 44, 1242, (*Juniperus formosana* deriv)

Su, W.-C. et al., Phytochemistry, 1996, 41, 255, (Junicedric acid, C13-NMR)

§ 4-Muurolen-10-ol; (1α,6α,7α,10β)-form

[化学名・別名] Cedrelanol. Brown-algae cadinol. Pilgerol

[CAS No.] 5937-11-1

[化合物分類] 脂肪族化合物 (Simple heteroalicyclics (2 × O))

[構造式]

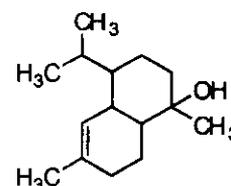
[基原] *Pinus albicaulis*, *Pinus armandii*, *Juniperus communis*, *Pilgerodendron*

uniferum. また, *Cedrela odorata*, *Chamaecyparis lawsoniana*, *Athrotaxis selaginoides*,

Cryptomeria japonica, *Dictyopteris divaricata*, およびその他 (some earlier identifications prob. erroneous in view of uncertainty over struct.)

[融点] Mp 139-140 °C

[比旋光度]: [α]_D²⁰ -102 (c, 3.2 in EtOH)



-----文献-----

Cheng, Y.S. et al., Chem. Comm., 1967, 565, (分離)

Nagasampagi, B.A. et al., Tet. Lett., 1968, 1913, (合成法)

Vig, O.P. et al., Indian J. Chem., Sect. B, 1979, 17, 552, (合成法)

Borg-Karlson, A.-K. et al., Tetrahedron, 1981, 37, 425, (構造決定, 構造)

Rodriguez-Avial Franke, L.R. et al., Tetrahedron, 1984, 40, 3491, (合成法)

Tkachev, A.V. et al., Khim. Prir. Soedin., 1990, 26, 635; Chem. Nat. Compd. (Engl. Transl.), 1990, 26, 539, (H-NMR, C13-NMR)

Nagashima, F. et al., Phytochemistry, 1994, 37, 1323, (*ent*-T-Muurolool)

§ 3',4',5,6,7-Pentahydroxyflavone; 6-O-β-D-Xylopyranoside

[CAS No.] 65876-67-7

[化合物分類] フラボノイド (Flavones; 5 × O-置換基)

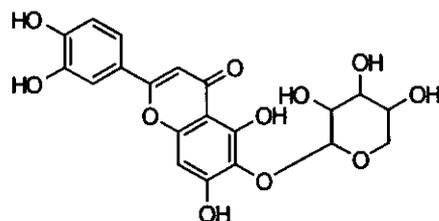
[構造式]

[分子式] $C_{20}H_{18}O_{11}$

[分子量] 434.356

[正確な分子量] 434.084915

[基原] 次の植物から分離: *Juniperus communis*



-----文献-----

- Harborne, J.B. et al., *Phytochemistry*, 1971, 10, 367, (分離)
Seshadri, J.R. et al., *Indian J. Chem.*, 1973, 11, 338, (分離)
Greger, H. et al., *Phytochemistry*, 1973, 12, 1693, (分離)
Mathuram, S. et al., *Phytochemistry*, 1976, 15, 838, (3',7-di-Me ether glycoside)
Nair, A.G.R. et al., *Phytochemistry*, 1976, 15, 839, (6-glucuronoside)
Nair, A.G.R., *Indian J. Chem., Sect. B*, 1979, 18, 188, (6-glucoside)
Inuma, M. et al., *Chem. Pharm. Bull.*, 1980, 28, 708, (C13-NMR, 誘導體)
Jain, N. et al., *J. Chem. Res., Synop.*, 1990, 396, (3'-rhamnoside 6-glucoside)
Chau, J.P. et al., *Phytochemistry*, 1996, 41, 941, (6-rhamnoside)

§ 3,4',5,7-Tetrahydroxyflavan; (2R,3R)-form

[化学名・別名] (-)-Epiatzelechin

[CAS No.] 24808-04-6

[化合物分類] フラボノイド (Flavan-3-ol)

[構造式]

[基原] *afzelia hardwood, Larix sibirica, Actinidia chinensis, Juniperus communis, Cassia javanica*

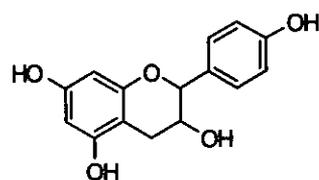
[性状] 針状結晶 (EtOH 溶液)

[融点] Mp 240-243 °C で分解 (312 °C)

[比旋光度]: $[\alpha]_D^{19} -58.9$ (c, 3 in EtOH). $[\alpha]_D -4$ (c, 1 in Me₂CO)

-----文献-----

- Sethi, V.K. et al., *Phytochemistry*, 1984, 23, 2402, (Epiatzelechin 5-glucoside)



§ 4',5,6,7-Tetrahydroxyflavone; 6-O-β-D-Xylopyranoside

[CAS No.] 65876-68-8

[化合物分類] フラボノイド (Flavones; 4 × O-置換基)

[構造式]

[分子式] $C_{20}H_{18}O_{10}$

[分子量] 418.356

[正確な分子量] 418.09

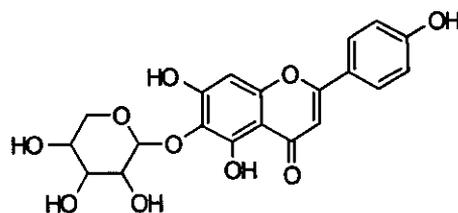
[基原] 次の植物から分離: *Juniperus communis*

-----文献-----

- Sastri, V.D. et al., *Proc. - Indian Acad. Sci., Sect. A*, 1946, 23, 262, (分離)
Bandyukova, V.A. et al., *Khim. Prir. Soedin.*, 1969, 5, 324; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, 5, 274, (5-O-glucuronide)
Zaitsev, V.G. et al., *Khim. Prir. Soedin.*, 1969, 5, 504; 598; 1974, 10, 92; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, 5, 423; 516, (Sorbarin, Flavosorbin, Sorbifolin)
Ulubelen, A. et al., *J. Nat. Prod.*, 1981, 44, 294, (6-O-glucoside)
Prakach, S. et al., *Phytochemistry*, 1982, 17, 2992, (分離)
Markham, K.R. et al., *Phytochemistry*, 1983, 22, 316, (分離, 構造決定)
The Flavonoids: *Advances in Research since 1980*, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Ahmad, N.J.M. et al., *J. Chem. Res., Synop.*, 1991, 218, (6-rhamnosylgalactoside)
Krishnaswamy, N.R. et al., *Indian J. Chem., Sect. B*, 1995, 34, 750, (7-Me 6-glucoside)

§ 4',5,6,7-Tetrahydroxyflavone; 4',5,6-Tri-Me ether, 7-O-β-D-glucopyranoside

[CAS No.] 17680-85-2



[化合物分類]フラボノイド (Flavones; 4 × O-置換基)

[構造式]

[分子式] C₂₄H₂₆O₁₁

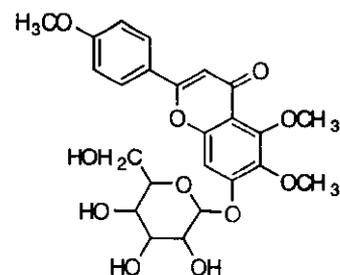
[分子量] 490.463

[正確な分子量] 490.147515

[基原] *Juniperus communis*

[性状] 針状結晶 (MeOH)

[融点] Mp 172-175 °C (semisynthetic)



-----文献-----

Sastri, V.D. et al., Proc. - Indian Acad. Sci., Sect. A, 1946, 23, 262, (分離)

Boikova, A., Khim. Prir. Soedin., 1969, 5, 596; Chem. Nat. Compd. (Engl. Transl.), 1969, 5, 513, (7-O-glucuronide)

Harborne, J.B. et al., Z. Naturforsch., C, 1984, 39, 18, (7-glucoside)

Washington, J.S. et al., J. Indian Chem. Soc., 1986, 63, 226, (7-glucosylrhamnoside)

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

Kraut, L. et al., Phytochemistry, 1993, 34, 211; 1999, 52, 749, (7-HMG glucoside)

Petrovic, S.D. et al., Phytochemistry, 1999, 50, 293, (7-xylosylglucoside)

§ 1,7,7-Trimethyltricyclo[2.2.1.0^{2,4}]heptane (CAS 名)

[化学名・別名] Tricyclene. Cyclene

[CAS No.] 508-32-7

[化合物分類]テルペノイド (Tricyclic monoterpene)

[構造式]

[分子式] C₁₀H₁₆

[分子量] 136.236

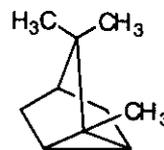
[正確な分子量] 136.1252

[基原] Found in turpentine and その他の精油, 例えば, *Juniperus communis*, *Ferula galbaniflua*, *Picea* spp.

[性状] 結晶 (EtOH)

[融点] Mp 67-68 °C

[沸点] Bp 152-153 °C



-----文献-----

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, 1, 56C, (NMR)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, 3, 57D, (IR)

Lipp, P., Ber., 1920, 53, 779, (合成法) Komppa, G., Ber., 1929, 62, 1366, (合成法)

Thomas, A.F. et al., Helv. Chim. Acta, 1964, 47, 475, (Mas)

Bardyshev, I.I. et al., Khim. Prir. Soedin., 1968, 4, 191; Chem. Nat. Compd. (Engl. Transl.), 1968, 4, 165, (生育, IR)

*****シヨウガ (Ginger) *****

§ § シヨウガ科シヨウガ (*Zingiber officinale* Roscoe) の根茎。

§ 1,10-Bisaboladien-3-ol

[化学名・別名] Zingiberenol

[CAS No.] 58334-55-7

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

[構造式]

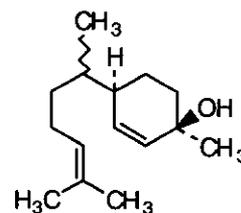
[分子式] C₁₅H₂₆O

[分子量] 222.37

[正確な分子量] 222.198365

[基原] *Zingiber officinale*, ガスクロによって分離

[性状] オイル



-----文献-----

Terhune, S.J. et al., Can. J. Chem., 1975, 53, 3285, (分離)

Paquette, L.A. et al., Tet. Lett., 1982, 23, 131, (合成法)

§ 1,3(15),10-Bisabolatriene

[化学名・別名] 3-(1,5-Dimethyl-4-hexenyl)-6-methylenecyclohexene (CAS 名). β -Sesquiphellandrene

[CAS No.] 20307-83-9

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

[構造式]

[分子式] $C_{15}H_{24}$

[分子量] 204.355

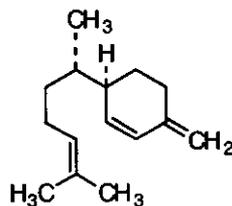
[正確な分子量] 204.1878

[基原] ショウガ (*Zingiber officinale*) のオイル

[性状] オイル

[沸点] Bp, 90 °C

[比旋光度]: $[\alpha]_D^{20}$ -3.99 (neat)



-----文献-----

Connell, D.W. et al., Aust. J. Chem., 1966, 19, 283, (β -Sesquiphellandrene)

Bohlmann, F. et al., Phytochemistry, 1979, 18, 677, (12-Oxo- β -sesquiphellandrene)

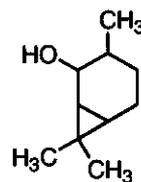
§ 2-Caranol; (1R*,2S*,3S*,6S*)-form

[CAS No.] 118395-91-8

[化合物分類] テルペノイド (Carane monoterpene)

[構造式]

[基原] *Chrysanthemum indicum*, *Zingiber officinale*. 次に示す物質の成分: Sheng Jiang



-----文献-----

Acharya, S.P. et al., J.A.C.S., 1967, 89, 1925-1932, (合成法, 絶対構造)

Kuczynski, H. et al., Tet. Lett., 1967, 2371-2376, (合成法)

Chen, Y. et al., CA, 1993, 119, 34075h, (分離)

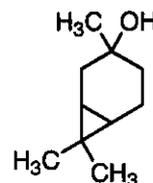
§ 3-Caranol; (1R*,3R*,6S*)-form

[CAS No.] 38748-97-9

[化合物分類] テルペノイド (Carane monoterpene)

[構造式]

[基原] *Lavandula stoechas*, *Zingiber officinale*. 次に示す物質の成分: Sheng Jiang



-----文献-----

Gollnick, K. et al., Tetrahedron, 1966, 22, 133-137, (合成法)

Gollnick, K. et al., Annalen, 1969, 721, 133-153, (合成法, 絶対構造)

Kokkalou, E., Planta Med., 1988, 54, 58-59, (分離)

Misra, A.N. et al., Tetrahedron, 1988, 44, 6941-6946, (合成法)

§ 4-(3,4-Dihydroxyphenyl)-2-butanone; 3-Me ether

[化学名・別名] 4-(4-Hydroxy-3-methoxyphenyl)-2-butanone. Vanillylacetone. Zingerone. [0] Paradol

[CAS No.] 122-48-5

[化合物分類] 単環芳香族 (Simple phenol)

[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] ショウガ (*Zingiber officinale*) の刺激の素だと考えられている

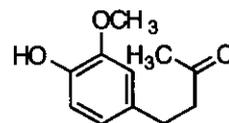
[用途] 人工果実臭, ジンジャービール, ジンジャーエール等の風味原料に用いられる。

[性状] 結晶 (petrol)

[融点] Mp 41 °C

[傷害・毒性] 皮膚刺激. 50%致死量 (LD₅₀) (ラット, 経口) 2580 mg/kg

[化学物質毒性データ総覧 (RTECS) 登録番号] EL8900000



-----文献-----

Arctander, S., Perfume and Flavour Chemistry, 1969, no. 3101, (Zingerone)