

Hikino, H. et al., Chem. Pharm. Bull., 1967, 15, 1065; 1968, 16, 827, (分離, 構造決定, 絶対構造)
St. Pyrek, J. et al., Pol. J. Chem. (Rocz. Chem.), 1976, 50, 1931

§ Curcumanolide A

[CAS No.] 97550-04-4

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

[構造式]

[分子式] $C_{15}H_{22}O_2$

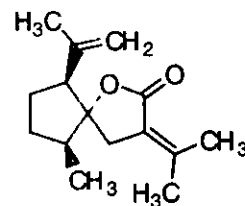
[分子量] 234.338

[正確な分子量] 234.16198

[基原] the crude drug zedoary (*Curcuma zedoaria*) and of *Curcuma heyneana*

[性状] オイル

[比旋光度]: $[\alpha]_D -33$ (c, 1.2 in $CHCl_3$)



-----文献-----

Shiobara, Y. et al., Phytochemistry, 1985, 24, 2629

Shiobara, Y. et al., Tet. Lett., 1985, 26, 913, (IR, H-NMR, C13-NMR, Mass, 構造決定)

Firman, K. et al., Phytochemistry, 1988, 27, 3887, (分離)

Fujita, T. et al., J.O.C., 1997, 62, 3824, (合成法)

§ Curcumanolide A; 1-Epimer

[化学名・別名] Curcumanolide B

[CAS No.] 97452-55-6

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

[構造式]

[分子式] $C_{15}H_{22}O_2$

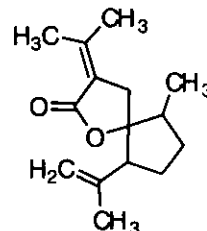
[分子量] 234.338

[正確な分子量] 234.16198

[基原] *Curcuma zedoaria*, *Curcuma heyneana*

[性状] オイル

[比旋光度]: $[\alpha]_D +21.2$ (c, 1.4 in $CHCl_3$)



-----文献-----

Shiobara, Y. et al., Phytochemistry, 1985, 24, 2629

Shiobara, Y. et al., Tet. Lett., 1985, 26, 913, (IR, H-NMR, C13-NMR, Mass, 構造決定)

Firman, K. et al., Phytochemistry, 1988, 27, 3887, (分離)

Fujita, T. et al., J.O.C., 1997, 62, 3824, (合成法)

§ Curcumenone

[CAS No.] 100347-96-4

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

[構造式]

[分子式] $C_{15}H_{22}O_2$

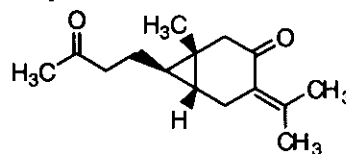
[分子量] 234.338

[正確な分子量] 234.16198

[基原] the crude drug zedoary (*Curcuma zedoaria*)

[性状] オイル

[比旋光度]: $[\alpha]_D -12.7$ (c, 1.1 in MeOH)



-----文献-----

Shiobara, Y. et al., Phytochemistry, 1985, 24, 2629, (Curcumenone)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1998, 46, 1186, (Dihydrocurcumenone)

§ Curcumin

[化学名・別名] 1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione (CAS 名).

Diferuloylmethane. Curcuma yellow. E 100

[CAS No.] 458-37-7

[関連 CAS No.] 24939-16-0, 33171-05-0

[化合物分類] PM6450, PS8300, 単環芳香族 (Diarylalkyl) 薬物: 抗菌性剤 (Antibacterial agent), 薬物: 抗カビ薬 (Antifungal agent), 薬物: 抗炎症薬 (Antiinflammatory agent),

[構造式]

[分子式] C₂₁H₂₀O₆

[分子量] 368.385

[正確な分子量] 368.12599

[基原] 次の植物から分離: *Curcuma zedoaria* (ウコン), その他の *Curcuma* spp., またその他の属

[用途] 抗炎症薬. 強い細菌およびカビ起因生症状への作用.

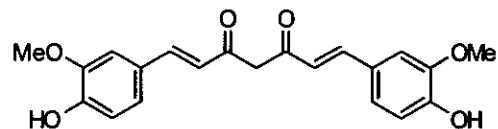
細胞毒薬

[性状] 橙色のプリズム結晶

[融点] Mp 183 °C

[Log P 計算値] Log P 2.05 (計算値)

[化学物質毒性データ総覧 (RTEC) 登録番号] MI5230000



-----文献-----

Jentzsch, K. et al., *Sci. Pharm.*, 1968, 36, 251; *CA*, 70, 90793h, (分離)

Sastry, B.S., *Res. Ind.*, 1970, 15, 258; *CA*, 75, 75063e, (分離)

Kuroyagi, M. et al., *Yakugaku Zasshi*, 1970, 90, 1467; *CA*, 74, 61612a, (分離)

Wahlstrom, B. et al., *Acta Pharmacol. Toxicol.*, 1978, 43, 86, (代謝)

Holder, G.M. et al., *Xenobiotica*, 1978, 8, 761, (代謝)

Ravindranath, V. et al., *Phytochemistry*, 1980, 19, 2031, (Dihydrocurcumin)

Tønnesen, H.H. et al., *Acta Chem. Scand., Ser. B*, 1982, 36, 475, (結晶構造, 成書)

Cheng, K.L. et al., *Handbook of Organic Analytical Reagents*, CRC Press, Boca Raton, 1982, 511, (用途)

Ammon, H.P.T. et al., *Planta Med.*, 1991, 57, 1, (レビュー, 薬理)

Jitoe, A. et al., *J. Agric. Food Chem.*, 1992, 40, 1337, (生育)

Khar, A. et al., *FEBS Lett.*, 1999, 445, 165, (antitumour prop)

RTECS (化学物質毒性データ)

生体影響物質 : 催腫瘍物質. 変異原物質. 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>> 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 : >2 gm/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参考文献

PLMEAA *Planta Medica*. (Georg Thieme Verlag, Postfach 732, D-7000 Stuttgart 1, Fed. Rep. Ger.)

V.1- 1953- [Vol.,頁,年(19-)] 64,353,1998

<<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 : >2 gm/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参考文献

JPPMAB *Journal of Pharmacy and Pharmacology*. (Pharmaceutical Soc. of Great Britain, 1 Lambeth High St., London SE1 7JN, UK) V.1- 1949- [Vol.,頁,年(19-)] 25,447,1973

<<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 : 1500 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

IJMRAQ *Indian Journal of Medical Research*. (Indian Council of Medical Research, Ansari Nagar, New Delhi 110 029, India) V.1- 1913- [Vol.,頁,年(19-)] 64,601,1976

変異原性に関するデータ

<<試験方法>> 小核試験.

試験系 : ヒトの胚
投与量・期間 : 73600 ug/L

参考文献

SNSHBT Senshokutai. Chromosome. (Sensyokutai Gakkai, Kaokusai Kirisutokyo Daigaku, Mitaka, Tokyo-to, Japan) No.1- 1946- Adopted new numbering in 1976. [Vol.,頁,年(19-)] (20),574,1980

<<試験方法>> DNA 阻害.

試験系 : ヒト HeLa 細胞.

投与量・期間 : 1 umol/L

参考文献

CRNGDP Carcinogenesis (London). (Oxford Univ. Press, Pinkhill House, Southfield Road, Eynsham, Oxford OX8 1JJ, UK) V.1- 1980- [Vol.,頁,年(19-)] 18,83,1997

<<試験方法>> 変異原試験-通常の試験法.

試験系 : ヒト HeLa 細胞.

投与量・期間 : 500 nmol/L

参考文献

CRNGDP Carcinogenesis (London). (Oxford Univ. Press, Pinkhill House, Southfield Road, Eynsham, Oxford OX8 1JJ, UK) V.1- 1980- [Vol.,頁,年(19-)] 18,83,1997

<<試験方法>> 細胞遺伝学分析試験

試験系 : ヒトの胚

投与量・期間 : 36800 ug/L

参考文献

SNSHBT Senshokutai. Chromosome. (Sensyokutai Gakkai, Kaokusai Kirisutokyo Daigaku, Mitaka, Tokyo-to, Japan) No.1- 1946- Adopted new numbering in 1976. [Vol.,頁,年(19-)] (20),574,1980

<<試験方法>> 細胞遺伝学分析試験

試験系 : げっ歯類-ラット骨髄

投与量・期間 : 7980 mg/kg/38 週間(連続的投与)

参考文献

CYTBAI Cytobios. (Faculty Press, 88 Regent St., Cambridge, UK) V.1- 1969- [Vol.,頁,年(19-)] 62,111,1990

<<試験方法>> 姉妹染色分体交換試験

試験系 : げっ歯類-マウス骨髄

投与量・期間 : 25 mg/kg

参考文献

CYTBAI Cytobios. (Faculty Press, 88 Regent St., Cambridge, UK) V.1- 1969- [Vol.,頁,年(19-)] 62,111,1990

<<試験方法>> 小核試験.

試験系 : ヒトの肺.

投与量・期間 : 73600 ug/L

参考文献

SNSHBT Senshokutai. Chromosome. (Sensyokutai Gakkai, Kaokusai Kirisutokyo Daigaku, Mitaka, Tokyo-to, Japan) No.1- 1946- Adopted new numbering in 1976. [Vol.,頁,年(19-)] (20),574,1980

<<試験方法>> 細胞遺伝学分析試験

試験系 : げっ歯類-ハムスター肺

投与量・期間 : 20 mg/L

参考文献

GMCRCDC Gann Monograph on Cancer Research. (Plenum Pub. Corp., 233 Spring St., New York, NY 10013) No. 11- 1971- [Vol.,頁,年(19-)] 27,95,1981

§ Curcumin; Demethoxy

[化学名・別名] 1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione (CAS 名).

p-Hydroxycinnamoylferuloylmethane. Demethoxycurcumin

[CAS No.] 22608-11-3

[化合物分類] 単環芳香族 (Diarylalkyl)

[構造式]

[分子式] $C_{20}H_{18}O_5$

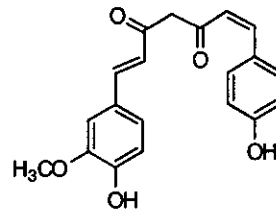
[分子量] 338.359

[正確な分子量] 338.115425

[基原] 次の植物から分離: *Curcuma zedoaria*, *Curcuma longa*, *Curcuma domestica*, *Curcuma xanthorrhiza*

[性状] 橙-黄色の粉末

[融点] Mp 168 °C



-----文献-----

Ammon, H.P.T. et al., *Planta Med.*, 1991, 57, 1, (レビュー, 薬理)

Jitoe, A. et al., *J. Agric. Food Chem.*, 1992, 40, 1337, (生育)

Masuda, T. et al., *Phytochemistry*, 1992, 31, 3645, (5'-Methoxycurcumin)

Nakayama, R. et al., *Phytochemistry*, 1993, 33, 501, (O-de-Me)

§ Curcumin; Bis-demethoxy

[化学名・別名] 1,7-Bis(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione (CAS 名).

p,p'-Dihydroxydicinnamoylmethane. Bisdemethoxycurcumin

[CAS No.] 22608-12-4

[化合物分類] 単環芳香族 (Diarylalkyl)

[構造式]

[分子式] $C_{19}H_{16}O_4$

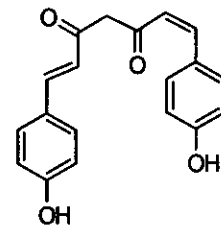
[分子量] 308.333

[正確な分子量] 308.10486

[基原] 次の植物から分離: *Curcuma zedoaria*, *Curcuma longa*, *Curcuma domestica*, *Curcuma aromatica*. Absent in some *Curcuma* spp.

[性状] 黄色の板状結晶 + H₂O (EtOH)

[融点] Mp 224 °C



-----文献-----

Masuda, T. et al., *Phytochemistry*, 1992, 31, 3645, (5'-Methoxycurcumin)

Nakayama, R. et al., *Phytochemistry*, 1993, 33, 501, (O-de-Me)

Syu, W.-J. et al., *J. Nat. Prod.*, 1998, 61, 1531, (分離, 合成法)

Khar, A. et al., *FEBS Lett.*, 1999, 445, 165, (antitumour prop)

§ Curcumol

[化学名・別名] 5,8-Epoxy-10(14)-guaian-8-ol

[CAS No.] 4871-97-0

[化合物分類] 薬物: 抗腫瘍薬 (Antineoplastic agent), テルペノイド (Simple guaianes sesquiterpenoid)

[構造式]

[分子式] $C_{15}H_{24}O_2$

[分子量] 236.353

[正確な分子量] 236.17763

[基原] *Curcuma wenyujin*, *Curcuma zedoaria*

[用途] 抗腫瘍作用を示す

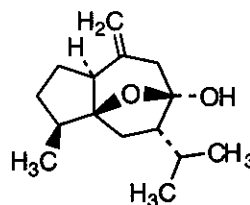
[性状] 結晶

[融点] Mp 141-142 °C

[比旋光度]: $[\alpha]_D^{25} -32.26$ (c, 2.127 in CHCl₃)

[溶解性] BERDY SOL: ヘキサンに難溶

[Log P 計算値] Log P 3.4 (未確認値) (計算値)



-----文献-----

Hikino, H. et al., *Chem. Pharm. Bull.*, 1966, 14, 1241, (分離, 構造決定)

Inayama, S. et al., *Chem. Pharm. Bull.*, 1984, 32, 3783, (結晶構造, 絶対構造)

Harimaya, K. et al., *Chem. Pharm. Bull.*, 1991, 39, 843, (分離, H-NMR, 結晶構造)

§ Curzeone; (-)-form

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

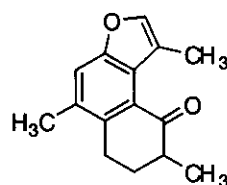
[構造式]

[基原] *Curcuma zedoaria*

[性状] 結晶

[融点] Mp 72-74 °C (66-67 °C)

[比旋光度]: $[\alpha]_D^{26} +61.5 (+24)$



-----文献-----

Shiobara, Y. et al., *Phytochemistry*, 1986, 25, 1351

Yang, C., *Chin. Trad. Herbal Drugs*, 1998, 29, 154, (絶対構造)

§ Curzerenone

[化学名・別名] Zedoarone

[CAS No.] 20493-56-5

[関連 CAS No.] 19956-58-2

[化合物分類] 薬物: 抗腫瘍薬 (Antineoplastic agent), テルペノイド (Elemene 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] *Curcuma zedoaria*

[用途] 抗腫瘍作用を示す.

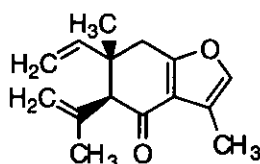
[性状] オイル

[比旋光度]: $[\alpha]_D 0$

[溶解性] BERDY SOL: 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 3.85 (計算値)

[UV]: [neutral] λ_{max} 272 (log ϵ 3.44) (EtOH) [neutral] λ_{max} 276 (ϵ 5623) (EtOH) [neutral] λ_{max} 264 (ϵ 3550) (hexane)



-----文献-----

Fukushima, S. et al., *Yakugaku Zasshi*, 1968, 88, 792; 1970, 90, 863, (分離, 薬理)

Hikino, H. et al., *J.C.S. Perkin 1*, 1975, 478, (分離, 構造決定)

Miyashita, M. et al., *J.O.C.*, 1984, 49, 3728, (合成法, 成書)

§ Curzerenone; 5-Epimer

[化学名・別名] 5-Epicurzerenone. 5-*epi*-Curzerenone

[CAS No.] 20085-85-2

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

[構造式]

[分子式] $C_{15}H_{18}O_2$

[分子量] 230.306

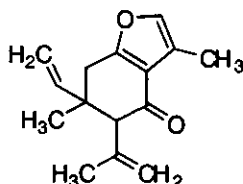
[正確な分子量] 230.13068

[基原] *Curcuma zedoaria*

[性状] オイル

[比旋光度]: $[\alpha]_D 0$

[UV]: [neutral] λ_{max} 220 (log ϵ 3.92); 270 (log ϵ 3.44) (EtOH)



-----文献-----

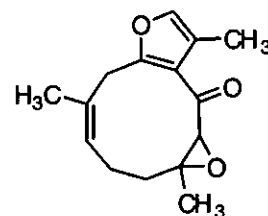
Fukushima, S. et al., *Yakugaku Zasshi*, 1968, 88, 792; 1970, 90, 863, (分離, 薬理)

Hikino, H. et al., *J.C.S. Perkin 1*, 1975, 478, (分離, 構造決定)

Miyashita, M. et al., *J.O.C.*, 1984, 49, 3728, (合成法, 成書)

§ 4,5:8,12-Diepoxy-1(10),7,11-germacatrien-6-one; (1(10)*E*,4 β ,5 β)-form

[化学名・別名] Zederone
[CAS No.] 7727-79-9
[化合物分類] テルペノイド (12,8-Germacranolide and furanogermacrane sesquiterpenoid)
[構造式]
[基原] *Curcuma zedoaria*
[性状] 結晶 (EtOAc)
[融点] Mp 153.5-154 °C
[比旋光度]: $[\alpha]_D^{25} +265.8$ (c, 0.5 in CHCl₃)

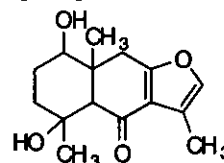


-----文献-----

Hikino, H. et al., Chem. Pharm. Bull., 1968, 16, 1081, (分離, 構造決定)
Shibuya, H. et al., Chem. Pharm. Bull., 1987, 35, 924, (絶対構造, 結晶構造)

§ 1,4-Dihydroxyfuraneremophilan-6-one; (1 β,4 α)-form

[化学名・別名] Curcolonol
[CAS No.] 217817-09-9
[化合物分類] テルペノイド (Eremophilanolide and furanoeremophilane sesquiterpenoid)
[構造式]
[基原] *Curcuma zedoaria*
[性状] 結晶 (Me₂CO)
[融点] Mp 183-184 °C
[比旋光度]: $[\alpha]_D^{25} 0$ (c, 2 in EtOH)

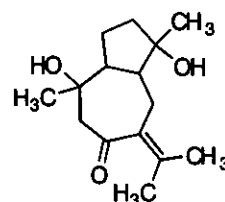


-----文献-----

Syu, W.-J. et al., J. Nat. Prod., 1998, 61, 1531, (分離, H-NMR, C13-NMR)

§ 4,10-Dihydroxy-7(11)-guaian-8-one; (1 α,4 β,5 β,10 β)-form

[化学名・別名] Zedoarondiol
[CAS No.] 98644-24-7
[化合物分類] テルペノイド (Simple guaiane sesquiterpenoid)
[構造式]
[基原] *Curcuma zedoaria*, *Curcuma aromatica*
[性状] 針状結晶 (CHCl₃)
[融点] Mp 133-134 °C
[比旋光度]: $[\alpha]_D^{25} -44$ (c, 1.0 in MeOH)

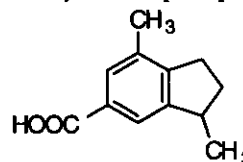


-----文献-----

Kouno, I. et al., Phytochemistry, 1985, 24, 1845, (分離)
Takano, I. et al., Phytochemistry, 1995, 40, 1197, (H-NMR, C13-NMR)

§ 3,7-Dimethyl-5-indanecarboxylic acid; (R)-form

[CAS No.] 217802-61-4
[化合物分類] 多環芳香族 (Indene), テルペノイド (Miscellaneous bicyclic sesquiterpenoid)
[構造式]
[基原] *Curcuma zedoaria*
[性状] 針状結晶 (hexane)
[融点] Mp 153-155 °C
[比旋光度]: $[\alpha]_D^{25} +18$ (c, 1 in C₆H₆)



-----文献-----

Syu, W.-J. et al., J. Nat. Prod., 1998, 61, 1531, (分離, IR, H-NMR, C13-NMR, Mas)

§ 4,5-Epoxy-1(10),7(11)-germacradien-8-one; (1(10)*E*,4 β,5 α)-form

[化学名・別名] Germacrone 4,5-epoxide

[CAS No.] 92691-35-5

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

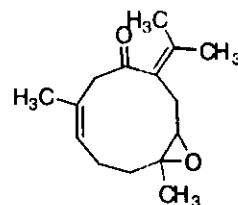
[構造式]

[基原] *Curcuma zedoaria* の精油. また *Smyrnum creticum* から得られる

[性状] プリズム結晶 (hexane)

[融点] Mp 59-60 °C

[比旋光度]: $[\alpha]_D^{25} +399$ (c, 1.05 in CHCl₃)



-----文献-----

Yoshihara, M. et al., Chem. Pharm. Bull., 1984, 32, 2059; 1986, 34, 434, (分離, 結晶構造)

§ 8,12-Epoxy-1(10),4,7,11-germacratetraene; (1(10)*E*,4*E*)-form

[化学名・別名] Furanodiene. Isofuranodiene

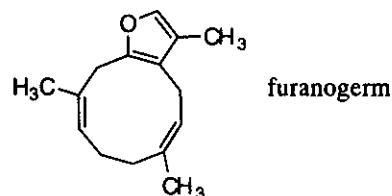
[化合物分類] テルペノイド (12,8-Germacranolide and acrane sesquiterpenoid)

[構造式]

[基原] *Curcuma zedoaria*, *Stenocylax michelii*

[性状] 結晶

[融点] Mp 66 °C



-----文献-----

Hikino, H. et al., Chem. Pharm. Bull., 1970, 18, 752, (分離, 構造決定)

Rücker, G. et al., Phytochemistry, 1971, 10, 221, (分離)

§ 8,12-Epoxy-1(10),4,7,11-germacratetraen-6-one; (1(10)*E*,4*E*)-form

[化学名・別名] Furanodienone

[CAS No.] 24268-41-5

[化合物分類] テルペノイド (12,8-Germacranolide and furanogermacrane sesquiterpenoid)

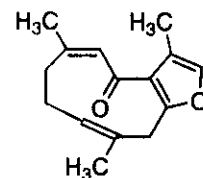
[構造式]

[基原] *Curcuma zedoaria*

[性状] 結晶

[融点] Mp 89.5-90.5 °C

[UV]: [neutral] λ_{max} 241 (log ϵ 2.98); 248 (log ϵ 3.95) (EtOH)



-----文献-----

Hikino, H. et al., J.C.S. Perkin 1, 1975, 478, (Furanodienone, Isofuranodienone)

Brieskorn, E.H. et al., Phytochemistry, 1983, 22, 1270

§ 8,12-Epoxy-1(10),4,7,11-germacratetraen-6-one; (1(10)*E*,4*Z*)-form

[化学名・別名] Isofuranodienone

[CAS No.] 24268-42-6

[化合物分類] テルペノイド (12,8-Germacranolide and furanogermacrane sesquiterpenoid)

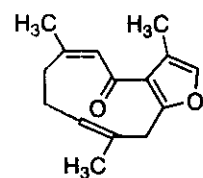
[構造式]

[基原] *Curcuma zedoaria*

[性状] 結晶 (petrol)

[融点] Mp 70-71 °C

[UV]: [neutral] λ_{max} 223 (log ϵ 4.17); 248 (log ϵ 3.95) (EtOH)



-----文献-----

Hikino, H. et al., J.C.S. Perkin 1, 1975, 478, (Furanodienone, Isofuranodienone)

Brieskorn, E.H. et al., Phytochemistry, 1983, 22, 1270

§ 8,12-Epoxy-1(10),7,11-germacratrien-5-one; (1(10)E,4 α H)-form

[化学名・別名] Furanogermenone

[CAS No.] 81678-18-4

[化合物分類] テルペノイド (12,8-Germacranolide and furanogermacrane sesquiterpenoid)

[構造式]

[基原] *Curcuma zedoaria*

[性状] 結晶

[融点] Mp 46.5-47.5 °C

[比旋光度]: $[\alpha]_D^{22} +135$ (CHCl₃)

[化学物質毒性データ総覧(RTEC)登録番号] LU3420000

-----文献-----

Shibuya, H. et al., *Heterocycles*, 1982, 17, 215

Shibuya, H. et al., *Yakugaku Zasshi*, 1986, 106, 212

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 : 590 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

YKKZAJ *Yakugaku Zasshi*. *Journal of Pharmacy*. (Nippon Yakugakkai, 2-12-15 Shibuya, Shibuya-ku, Tokyo 150, Japan) No.1- 1881- [Vol.,頁,年(19-)] 102,221,1982

§ 5,8-Epoxy-7(11),9-guaiadien-8-ol; (1 α,4 β,5 β,8 β)-form

[化学名・別名] Curcumenol

[CAS No.] 19431-84-6

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

[構造式]

[基原] *Curcuma zedoaria*, *Curcuma longa*

[性状] 結晶 (EtOAc)

[融点] Mp 118.5-119.5 °C

[比旋光度]: $[\alpha]_D +397$ (c, 5.1 in CHCl₃)

-----文献-----

Hikino, H. et al., *Chem. Pharm. Bull.*, 1968, 16, 39; 1969, 17, 959

Shiobara, Y. et al., *Phytochemistry*, 1985, 24, 2629, (分離, 構造決定)

Shibuya, H. et al., *Yakugaku Zasshi*, 1986, 212, 216, (分離)

Firman, K. et al., *Phytochemistry*, 1988, 27, 3887, (Oxycurcumenol)

Bats, J.W. et al., *Acta Cryst. C*, 1999, 55, 1595, (絶対構造, 成書, Isocurcumenol)

§ 5,8-Epoxy-7(11),9-guaiadien-8-ol; (1 α,4 β,5 β,8 β)-form, Δ¹⁰⁽¹⁴⁾-Isomer

[化学名・別名] Isocurcumenol, 5,8-Epoxy-7(11),10(14)-guaiadien-8-ol

[CAS No.] 24063-71-6

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

[構造式]

[分子式] C₁₅H₂₂O₂

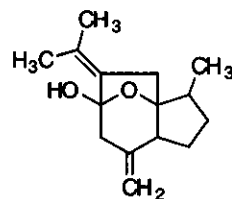
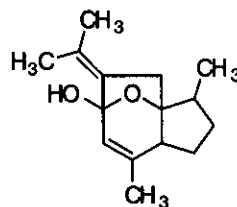
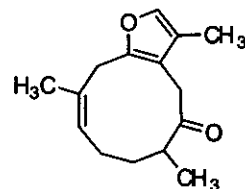
[分子量] 234.338

[正確な分子量] 234.16198

[基原] *Curcuma zedoaria*, *Curcuma kwangsiensis*, *Curcuma heyneana*, *Curcuma aeruginosa*, *Curcuma cochinchinensis*, *Curcuma harmandii*, *Curcuma phaeocaulis*

[性状] 結晶 (EtOAc)

[融点] Mp 139-141 °C



[比旋光度]: $[\alpha]_D +34$ (c, 1.0 in CHCl_3)

-----文献-----

Bats, J.W. et al., Acta Cryst. C, 1999, 55, 1595, (絶対構造, 成書, Isocurcumenol)

§ 1(10)-Germacrene-5,8-dione; (1(10)*E*,4 α *H*,7 β *H*)-form

[化学名・別名] Curdione

[CAS No.] 13657-68-6

[化合物分類] 薬物: 抗腫瘍薬 (Antineoplastic agent), テルペノイド (Simple germacrene sesquiterpenoid)

[構造式]

[基原] *Curcuma aeruginosa*, *Curcuma zedoaria*, *Curcuma wenyujin*

[性状] 結晶

[融点] Mp 61-62 °C

[比旋光度]: $[\alpha]_D^{25} +26$ (c, 1.00 in CHCl_3)

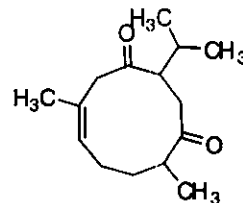
[溶解性] BERDY SOL: ヘキサンに難溶

[Log P 計算値] Log P 3.16 (計算値)

[その他のデータ] 薬理的活性な異性体

[傷害・毒性] 50%致死量 (LD_{50}) (マウス, 腹腔内投与) 414 mg/kg; BERDY HAZD : 50%致死量 (LD_{50}) (マウス, 腹腔内投与) 414 mg/kg

[化学物質毒性データ総覧 (RTEC) 登録番号] LY3960000



-----文献-----

Hikino, H. et al., Chem. Pharm. Bull., 1967, 15, 1390; 1972, 20, 987, (分離, 構造決定)

Inayama, S. et al., Chem. Pharm. Bull., 1985, 33, 1323; 2179, (絶対構造, 結晶構造)

Shibuya, H. et al., Yakugaku Zasshi, 1986, 106, 212, (分離, Dehydrocurdione)

Harimaya, K. et al., Chem. Pharm. Bull., 1991, 39, 843, (分離, 結晶構造, Neocurdione)

Panddji, C. et al., Phytochemistry, 1993, 34, 415, (分離)

***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>> LD_{50} 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 : 414 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

85PEAG "Zhongliu Yanjiu" Cancer Review, Yu, R., et al., eds., Shanghai Science/Technology Publisher, Peop. Rep. China, 1994 [Vol.,頁,年(19-)],178,1994

§ 1(10)-Germacrene-5,8-dione; (1(10)*E*,4 α *H*,7 β *H*)-form, 7,11-Didehydro

[化学名・別名] 1(10),7(11)-Germacradiene-5,8-dione. Dehydrocurdione

[CAS No.] 38230-32-9

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

[構造式]

[分子式] $\text{C}_{15}\text{H}_{20}\text{O}_2$

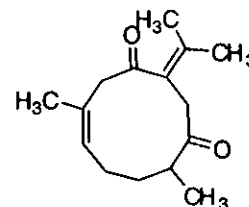
[分子量] 234.338

[正確な分子量] 234.16198

[基原] *Curcuma zedoaria*

[性状] オイル

[比旋光度]: $[\alpha]_D +67.9$ (c, 0.5 in CHCl_3)



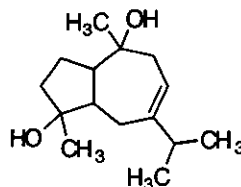
-----文献-----

Shibuya, H. et al., Yakugaku Zasshi, 1986, 106, 212, (分離, Dehydrocurdione)

Panddji, C. et al., Phytochemistry, 1993, 34, 415, (分離)

§ 7-Guaiene-4,10-diol

[化学名・別名] Curcumadiol
[CAS No.] 31946-48-2
[化合物分類] テルペノイド (Simple guaiane sesquiterpenoid)
[構造式]
[分子式] $C_{15}H_{26}O_2$
[分子量] 238.369
[正確な分子量] 238.19328
[基原] *Curcuma zedoaria*
[性状] 結晶 (EtOAc)
[融点] Mp 145-145.5 °C
[比旋光度]: $[\alpha]_D -11.6$ (c, 1.7 in EtOH)

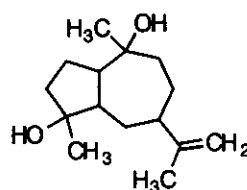


-----文献-----

Hinkino, H. et al., Chem. Pharm. Bull., 1971, 19, 93

§ 11-Guaiene-4,10-diol; (1 β ,4 β ,5 β ,10 β)-form

[化学名・別名] Guaidiol
[CAS No.] 217817-10-2
[化合物分類] テルペノイド (Simple guaiane sesquiterpenoid)
[構造式]
[基原] *Curcuma zedoaria*
[性状] 結晶 (C_6H_6 /hexane)
[融点] Mp 134-136 °C
[比旋光度]: $[\alpha]_D^{25} +30$ (c, 1 in EtOH)

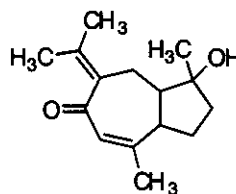


-----文献-----

Syu, W.-J. et al., J. Nat. Prod., 1998, 61, 1531-1534, (分離, H-NMR, C13-NMR, 結晶構造)

§ 4-Hydroxy-7(11),9-guaiadien-8-one; (1 α ,4 β ,5 β)-form

[化学名・別名] Procurcumenol
[CAS No.] 21698-40-8
[化合物分類] テルペノイド (Simple guaiane sesquiterpenoid)
[構造式]
[基原] *Curcuma zedoaria* と *Curcuma longa* の乾燥根茎
[性状] オイル
[比旋光度]: $[\alpha]_D +140.9$ (c, 10.5 in $CHCl_3$)
[その他のデータ] 構造は 1986 年に改正された



-----文献-----

Hikino, H. et al., Chem. Pharm. Bull., 1968, 16, 1605; 1977, 25, 6, (分離)

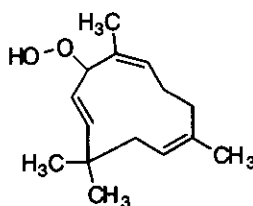
Yoshihara, M. et al., Chem. Pharm. Bull., 1986, 34, 434, (構造決定)

Kuroyanagi, M. et al., Chem. Pharm. Bull., 1990, 38, 55, (Epi-procurcumenol)

Ohshiro, M. et al., Phytochemistry, 1990, 29, 2201, (分離, H-NMR, C13-NMR)

§ 2,6,9-Humulatrien-8-ol; (2E,6E,8 ξ ,9E)-form, Hydroperoxide

[化学名・別名] 8-Hydroperoxy-2,6,9-humulatriene. Humulene-8-hydroperoxide
[CAS No.] 228565-88-6
[化合物分類] テルペノイド (Humulane sesquiterpenoid)
[構造式]
[分子式] $C_{15}H_{24}O_2$
[分子量] 236.353
[正確な分子量] 236.17763
[基原] *Curcuma zedoaria*



-----文献-----

Chabra, B.R. et al., Indian J. Chem., 1975, 13, 222, (Zerumbone oxide)

Dai, J.-R. et al., Nat. Prod. Lett., 1997, 10, 115-118, (Zerumbone, H-NMR, C13-NMR)

Phan, M.G. et al., CA, 1998, 131, 71211d, (hydroperoxide)

Kitayama, T. et al., J.O.C., 1999, 64, 2667-2672, (分離, 成書)

§ 4-Hydroxy-7(11),9-guaiadien-8-one; (1 α ,4 β ,5 β)-form

[化学名・別名] Procurcumenol

[CAS No.] 21698-40-8

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

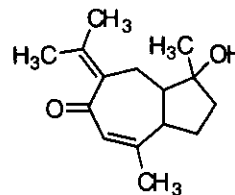
[構造式]

[基原] 次の植物の乾燥根茎; *Curcuma zedoaria*, *Curcuma longa*

[性状] オイル

[比旋光度]: $[\alpha]_D^{25} +140.9$ (c, 10.5 in CHCl_3)

[その他のデータ] 構造式は 1986 年に改正された



-----文献-----

Hikino, H. et al., Chem. Pharm. Bull., 1968, 16, 1605-1607; 1977, 25, 6, (分離)

Yoshihara, M. et al., Chem. Pharm. Bull., 1986, 34, 434, (構造)

Kuroyanagi, M. et al., Chem. Pharm. Bull., 1990, 38, 55, (Epi-procurcumenol)

Ohshiro, M. et al., Phytochemistry, 1990, 29, 2201, (分離, H-NMR, C13-NMR)

§ 4-Hydroxy-7(11),10(14)-guaiadien-8-one; (1 α ,4 β ,5 β)-form

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

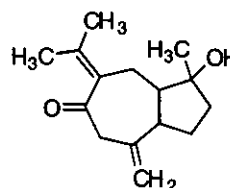
[構造式]

[基原] *Curcuma zedoaria* のオイルの微量成分

[性状] 針状結晶 (Et₂O/hexane)

[融点] Mp 96-98 °C

[比旋光度]: $[\alpha]_D^{18} -44$ (CHCl_3)



-----文献-----

Yoshihara, M. et al., Chem. Pharm. Bull., 1986, 34, 434, (結晶構造)

Kuroyanagi, M. et al., Chem. Pharm. Bull., 1990, 38, 55, (Isoprocurcumenol)

§ Isogermacrene

[化学名・別名] Isofuranogermacrene. Curzerene

[CAS No.] 17910-09-7

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

[構造式]

[分子式] C₁₅H₂₀O

[分子量] 216.322

[正確な分子量] 216.151415

[基原] *Lindera strychnifolia* の根から分離されたもの。また, *Curcuma zedoaria* から分離され, present to some extent in nearly all *Curcuma* spp.

[性状] オイル

[比旋光度]: $[\alpha]_D^{20} -0.7$ (c, 0.87 in CHCl_3)

[UV]: [neutral] λ_{max} 210 (log ϵ 3.8) (EtOH)

[その他のデータ] おそらく非天然物

-----文献-----

Ishii, H. et al., Tetrahedron, 1968, 24, 625, (分離)

Hikino, H. et al., Chem. Pharm. Bull., 1970, 18, 752, (分離, 絶対構造)

Lu, Y.-C. et al., CA, 1981, 94, 7575r, (Neocurzerene)

Miyashita, M. et al., Chem. Lett., 1981, 593, (合成法)

§ Pyrocurzerenone

[化学名・別名] 6,7-Dihydro-1,5,8-trimethylnaphtho[2,1-b]-furan (CAS 名)

[CAS No.] 20013-75-6

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

[構造式]

[分子式] $C_{15}H_{16}O$

[分子量] 212.291

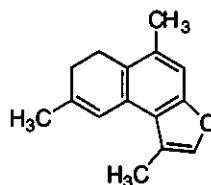
[正確な分子量] 212.120115

[基原] *Curcuma zedoaria* の根茎

[性状] 結晶 (petrol)

[融点] Mp 76.5-77.5 °C

[UV]: [neutral] λ_{max} 233 (log ϵ 4.75); 239 (log ϵ 4.72); 249 (log ϵ 4.62); 283 (log ϵ 4.4); 293 (log ϵ 4.4) (EtOH)



-----文献-----

Viswanatha, V. et al., J.C.S. Perkin 1, 1974, 450, (合成法)

Hikino, H. et al., J.C.S. Perkin 1, 1975, 478, (分離, 構造決定)

Takemoto, T. et al., Chem. Pharm. Bull., 1976, 24, 531, (誘導體)

Miyashita, M. et al., J.O.C., 1984, 49, 3728, (合成法)

§ Zedoarol

[CAS No.] 103994-22-5

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

[構造式]

[分子式] $C_{15}H_{16}O_3$

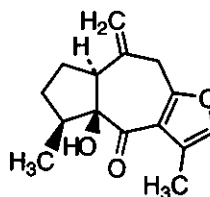
[分子量] 246.305

[正確な分子量] 246.125595

[基原] *Curcuma zedoaria*

[性状] オイル

[比旋光度]: $[\alpha]_D^{28} +11.6$ (c, 2.0 in $CHCl_3$)



-----文献-----

Shiobara, Y. et al., Phytochemistry, 1986, 25, 1351-1353

*****セネガ (Senega) *****

§ § ヒメハギ科セネガ (*Polygala senega* L.) の根。

§ 1,5-Anhydroglucitol; D-form

[CAS No.] 154-58-5

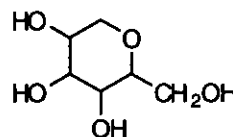
[化合物分類] 炭水化物 (Hexitol), 炭水化物 (1,5-Anhydrosugar)

[構造式]

[基原] Occurs in *Polygala tenuifolia*, *Polygala vulgaris*, *Polygala amara*, *Polygala senega* and in human cerebrospinal fluid

[融点] Mp 142-143 °C

[比旋光度]: $[\alpha]_D^{20} +42.3$ (c, 0.84 in H_2O)



-----文献-----

Powers, J.L. et al., J. Am. Pharm. Assoc., 1940, 29, 209, (Acertannin)

Wiggins, L.F., Adv. Carbohydr. Chem., 1950, 5, 191, (レビュー)

Pitkanen, E., Clin. Chim. Acta, 1973, 48, 159, (生育)

Bock, K. et al., Phytochemistry, 1980, 19, 2033, (Aceritannin)

Song, C et al., Huaxue Xuebao, 1982, 40, 1142; CA, 98, 86267a, (Ginnalin)

Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515, (Aceritannin, Acergallotannin)

Boeyens, J.C.A. et al., Phytochemistry, 1983, 22, 1959, (conform, 結晶構造)

Hatano, T. et al., Chem. Pharm. Bull., 1990, 38, 1902, (Acergallotannin)

Ikeya, Y. et al., Chem. Pharm. Bull., 1991, 39, 2600, (Tenuifoliside D)

Elvebak, L.E. et al., Carbohydr. Res., 1995, 274, 85, (誘導體)

§ Polygalic acid

[化学名・別名] 2 β ,3 β -Dihydroxy-27-nor-13-oleanene-23,28-dioic acid. Senegenic acid

[CAS No.] 1260-04-4

[化合物分類] テルペノイド (Nor-, seco- and abeooleanane triterpenoid)

[構造式]

[分子式] C₂₉H₄₄O₆

[分子量] 488.663

[正確な分子量] 488.31379

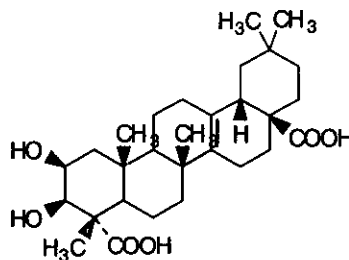
[基原] *Polygala senega*

[性状] 結晶 (EtOH)

[融点] Mp 299-301 °C

[比旋光度]: $[\alpha]_D^{23} +18$ (EtOH)

[その他のデータ] おそらく非天然物



-----文献-----

Dugan, J.J. et al., Tet. Lett., 1964, 2567, (分離)

Pelletier, S.W. et al., Tet. Lett., 1964, 3065, (分離)

§ Senegenin

[化学名・別名] Tenuifolic acid

[CAS No.] 2469-34-3

[化合物分類] テルペノイド (Nor-, seco- and abeooleanane triterpenoid)

[構造式]

[分子式] C₃₀H₄₅ClO₆

[分子量] 537.135

[正確な分子量] 536.290467

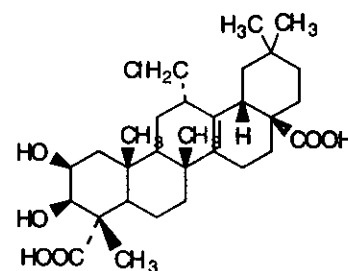
[基原] *Polygala senega*. Derived from Presenegenin by treatment with HCl. また *Polygala tenuifolia*, *Bredemeyera floribunda* から得られる

[性状] 結晶 (EtOH 溶液)

[融点] Mp 290-292 °C

[比旋光度]: $[\alpha]_D +19$ (c, 0.74 in EtOH)

[化学物質毒性データ総覧 (RTEC) 登録番号] RC8815000



-----文献-----

Shamma, M. et al., Chem. Ind. (London), 1960, 1272, (H-NMR)

Tschesche, R. et al., Naturwissenschaften, 1965, 52, 303

Pelletier, S.W. et al., Chem. Comm., 1966, 727, (構造決定)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, SBY000

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>> 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-マウス

投与量・期間 : 1 gm/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない。

参照文献

HBAMAK "Abdernalden's Handbuch der Biologischen Arbeitsmethoden." (Leipzig, Ger. Dem. Rep.)

[Vol.,頁,年(19-)] 4,1289,1935

<<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 : 3 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

85GDA2 "CRC Handbook of Antibiotic Compounds," Vols.1- , Berdy, J., Boca Raton, FL, CRC Press, 1980- [Vol.,頁,年(19-)] 8(2),259,1982

<<試験方法>> 認知されている最小致死量(LDL₀)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 : 30 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

HBAMAK "Abdernalden's Handbuch der Biologischen Arbeitsmethoden." (Leipzig, Ger. Dem. Rep.)

[Vol.,頁,年(19-)]4,1289,1935

<<試験方法>> 認知されている最小致死量(LDL₀)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 : 45 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

HBAMAK "Abdernalden's Handbuch der Biologischen Arbeitsmethoden." (Leipzig, Ger. Dem. Rep.)

[Vol.,頁,年(19-)]4,1289,1935

§ Senegose D

[CAS No.] 151466-63-6

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₅₇H₇₂O₃₃

[分子量] 1285.176

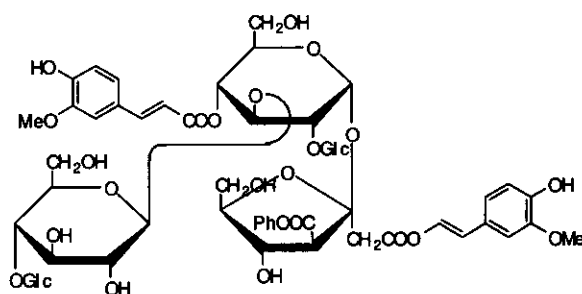
[正確な分子量] 1284.395595

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)の根

[性状] 無定型の粉末・二水和物

[比旋光度]: $[\alpha]_D^{25}$ -6.9 (c, 1 in MeOH)

[UV]: [neutral] λ_{max} 220 (ϵ 28180); 233 (ϵ 29510); 284 (sh) (ϵ 17780); 299 (sh) (ϵ 24550); 325 (ϵ 33880) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6^β-Ac

[化学名・別名] Senegose C

[CAS No.] 151466-62-5

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₅₉H₇₄O₃₄

[分子量] 1327.213

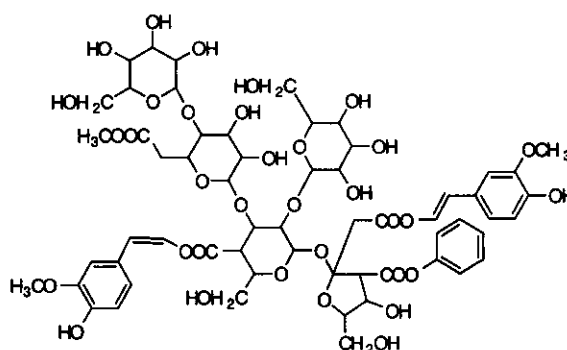
[正確な分子量] 1326.40616

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末・二水和物

[比旋光度]: $[\alpha]_D^{25}$ -16 (c, 1.3 in MeOH)

[UV]: [neutral] λ_{max} 219 (ϵ 33110); 233 (ϵ 33880); 284 (sh) (ϵ 20420); 297 (sh) (ϵ 26910); 327 (ϵ 40740) (MeOH)



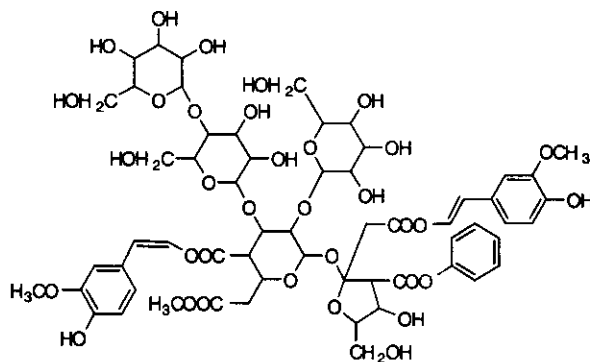
-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6^c-Ac

[化学名・別名] Senegose B
[CAS No.] 151466-61-4
[化合物分類] 炭水化物 (Oligosaccharide)
[構造式]

[分子式] C₅₉H₇₄O₃₄
[分子量] 1327.213
[正確な分子量] 1326.40616
[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)
[性状] 無定形の粉末・一水和物
[比旋光度]: $[\alpha]_D^{23}$ -10.2 (c, 1.2 in MeOH)
[UV]: [neutral] λ_{\max} 220 (ϵ 38020); 233 (ϵ 38020); 284 (sh) (ϵ 24550); 299 (sh) (ϵ 30200); 327 (ϵ 43650) (MeOH)



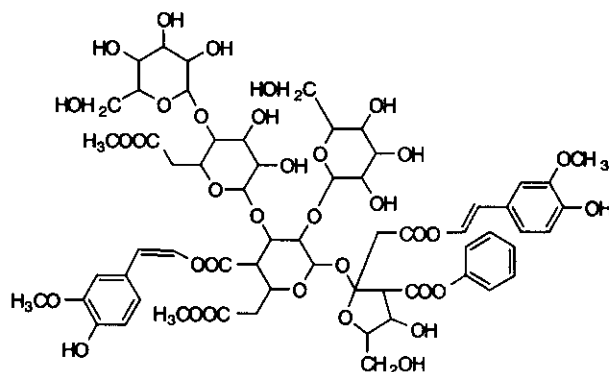
-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6^b,6^c-Di-Ac

[化学名・別名] Senegose A
[CAS No.] 151466-60-3
[化合物分類] 炭水化物 (Oligosaccharide)
[構造式]

[分子式] C₆₁H₇₆O₃₅
[分子量] 1369.25
[正確な分子量] 1368.416725
[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)
[性状] 無定形の粉末 + 4·1/2H₂O
[比旋光度]: $[\alpha]_D^{23}$ -9.9 (c, 1.2 in MeOH)
[UV]: [neutral] λ_{\max} 220 (ϵ 33110); 233 (ϵ 33110); 284 (sh) (ϵ 20420); 299 (sh) (ϵ 26300); 328 (ϵ 38900) (MeOH)



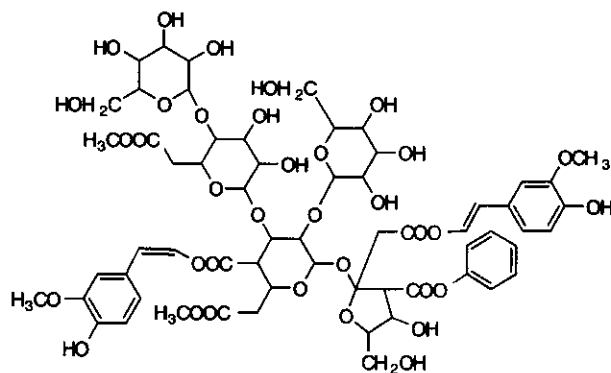
-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6^b,6^c-Di-Ac, 2'-Z-isomer

[化学名・別名] Senegose E
[CAS No.] 151530-27-7
[化合物分類] 炭水化物 (Oligosaccharide)
[構造式]

[分子式] C₆₁H₇₆O₃₅
[分子量] 1369.25
[正確な分子量] 1368.416725
[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)
[性状] 無定形の粉末・三水和物
[比旋光度]: $[\alpha]_D^{23}$ +64.5 (c, 0.6 in MeOH)
[UV]: [neutral] λ_{\max} 220 (ϵ 35480); 232 (ϵ 35480); 284 (sh) (ϵ 19500); 301 (sh) (ϵ 25700); 327 (ϵ 36310) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 4^a-Deglucosyl, 6^a-Ac

[化学名・別名] Senegose G

[CAS No.] 156031-87-7

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₅₅H₆₄O₂₉

[分子量] 1165.071

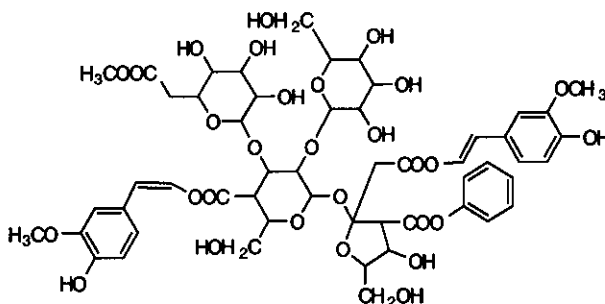
[正確な分子量] 1164.353335

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末・三水和物

[比旋光度]: [α]_D +1.2 (c, 1.2 in MeOH)

[UV]: [neutral] λ_{max} 220 (ε 29510); 233 (ε 30200); 285 (sh) (ε 17380); 299 (sh) (ε 22910); 327 (ε 34670) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 4^a-Deglucosyl, 6^c-Ac

[化学名・別名] Senegose H

[CAS No.] 156031-88-8

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₅₅H₆₄O₂₉

[分子量] 1165.071

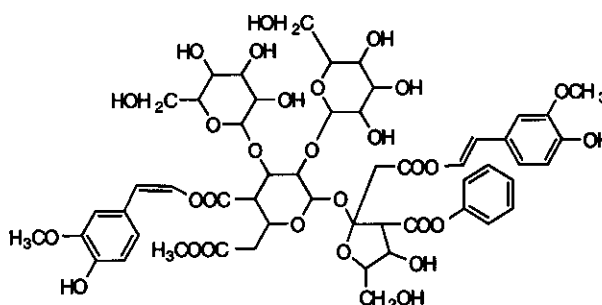
[正確な分子量] 1164.353335

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末 + 2・1/2H₂O

[比旋光度]: [α]_D -3 (c, 0.66 in MeOH)

[UV]: [neutral] λ_{max} 219 (ε 38020); 233 (ε 38020); 286 (sh) (ε 22390); 301 (sh) (ε 29510); 328 (ε 43650) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 4^a-Deglucosyl, 6^a,6^c-di-Ac

[化学名・別名] Senegose F

[CAS No.] 156031-89-9

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₅₅H₆₄O₃₀

[分子量] 1207.108

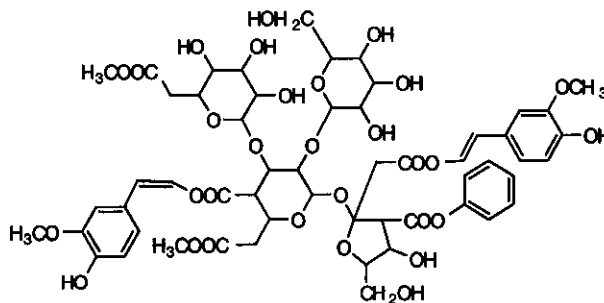
[正確な分子量] 1206.3639

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末・三水和物

[比旋光度]: [α]_D²² -11.5 (c, 1.2 in MeOH)

[UV]: [neutral] λ_{max} 219 (ε 38020); 233 (ε 38020); 285 (sh) (ε 22910); 299 (sh) (ε 28840); 327 (ε 43650) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 2^c-Deglucosyl, 6^b,6^c-Di-Ac

[化学名・別名] Senegose I

[CAS No.] 156031-86-6

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₅₅H₆₆O₃₀

[分子量] 1207.108

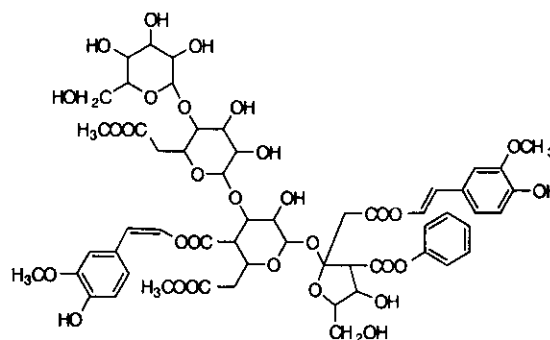
[正確な分子量] 1206.3639

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末 + 2·1/2H₂O

[比旋光度]: [α]_D²² -29.1 (c, 0.8 in MeOH)

[UV]: [neutral] λ_{max} 220 (ε 35480); 234 (ε 35480); 287 (sh) (ε 21880); 300 (sh) (ε 26910); 328 (ε 40740) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6''-Demethoxy, 6^c-Ac

[化学名・別名] Senegose K

[CAS No.] 156250-47-4

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₅₈H₇₂O₃₃

[分子量] 1297.187

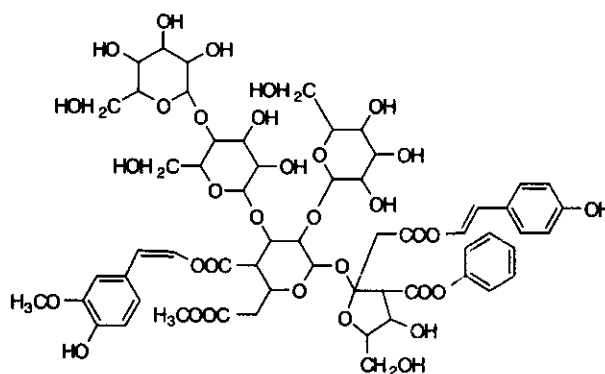
[正確な分子量] 1296.39595

[基原] *Polygala senega* (ヒメハギ科)

[性状] 無定型の粉末・三水合物

[比旋光度]: [α]_D²⁵ -2.6 (c, 1 in MeOH)

[UV]: [neutral] λ_{max} 223 (ε 26910); 231 (ε 28840); 287 (sh) (ε 20890); 302 (sh) (ε 28180); 319 (ε 33880) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6'-Demethoxy, 6^c-Ac

[化学名・別名] Senegose M

[CAS No.] 156250-49-6

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₅₈H₇₂O₃₃

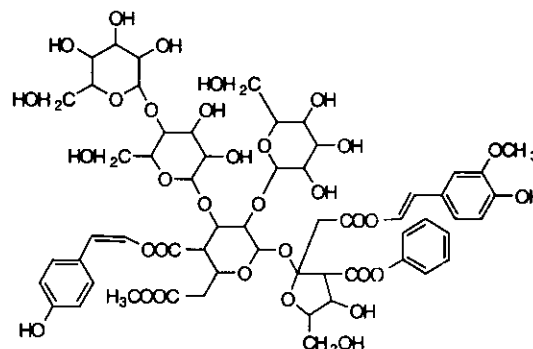
[分子量] 1297.187

[正確な分子量] 1296.39595

[基原] *Polygala senega* (ヒメハギ科)

[比旋光度]: [α]_D²⁵ +4.4 (c, 0.6 in MeOH)

[UV]: [neutral] λ_{max} 223 (ε 32360); 232 (ε 34670); 287 (sh) (ε 22910); 302 (sh) (ε 29510); 320 (ε 36310) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6^a,6^c-di-Ac

[化学名・別名] Senegose L

[CAS No.] 156250-48-5

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₆₀H₇₄O₃₄

[分子量] 1339.224

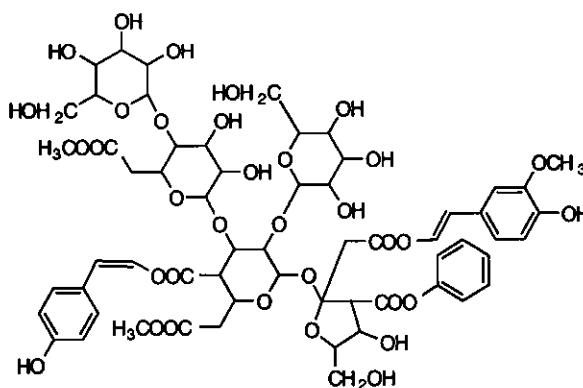
[正確な分子量] 1338.40616

[基原] *Polygala senega* (ヒメハギ科)

[性状] 無定形の粉末・四水和物

[比旋光度]: [α]_D²⁵ -6.3 (c, 1 in MeOH)

[UV]: [neutral] λ_{max} 222 (ε 22910); 232 (ε 25120); 286 (sh) (ε 16980); 302 (sh) (ε 23440) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6^a-Demethoxy, 6^a,6^c-di-Ac

[化学名・別名] Senegose J

[CAS No.] 156250-46-3

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₆₀H₇₄O₃₄

[分子量] 1339.224

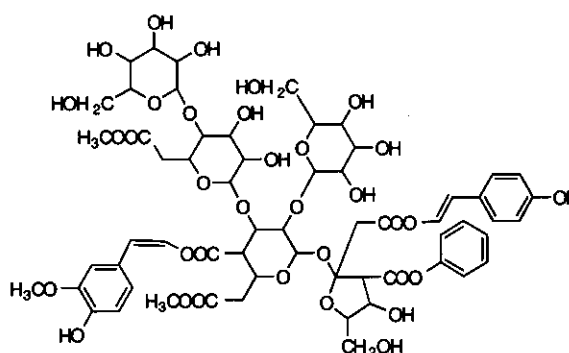
[正確な分子量] 1338.40616

[基原] *Polygala senega* (ヒメハギ科)

[性状] 無定形の粉末・四水和物

[比旋光度]: [α]_D²⁵ -6.6 (c, 1.1 in MeOH)

[UV]: [neutral] λ_{max} 224 (ε 27540); 231 (ε 30200); 288 (sh) (ε 22910); 303 (sh) (ε 30900); 320 (ε 38020) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6^a-Demethoxy, 6^a,6^c-di-Ac, 2'-Z-isomer

[化学名・別名] Senegose N

[CAS No.] 156317-48-5

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₆₀H₇₄O₃₄

[分子量] 1339.224

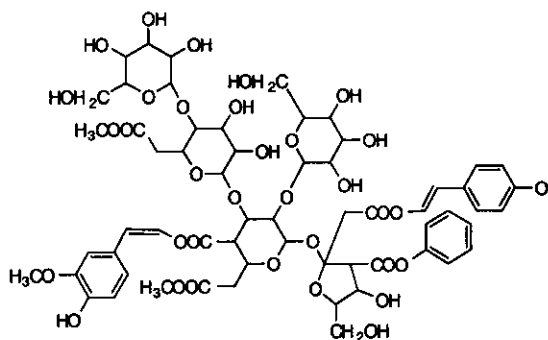
[正確な分子量] 1338.40616

[基原] *Polygala senega* (ヒメハギ科)

[性状] 無定形の粉末・五水和物

[比旋光度]: [α]_D²⁵ +39.6 (c, 0.8 in MeOH)

[UV]: [neutral] λ_{max} 224 (ε 23990); 230 (ε 25120); 286 (sh) (ε 18620); 302 (sh) (ε 25120); 318 (ε 30200) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6^a,6^c-di-Ac, 2''Z-isomer

[化学名・別名] Senegose O

[CAS No.] 156317-49-6

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C₆₀H₇₄O₃₄

[分子量] 1339.224

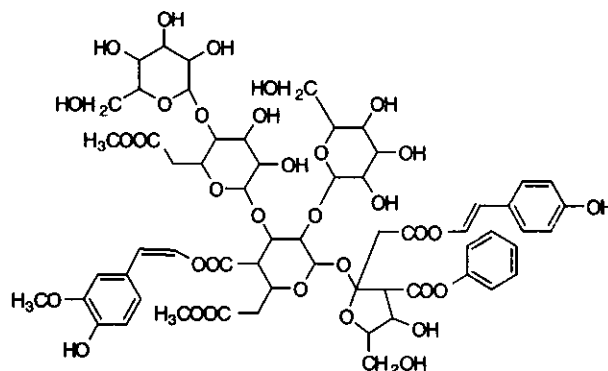
[正確な分子量] 1338.40616

[基原] *Polygala senega* (ヒメハギ科)

[性状] 無定型の粉末・四水和物

[比旋光度]: [α]_D²⁵ -13.1 (c, 0.7 in MeOH)

[UV]: [neutral] λ_{max} 220 (ε 2690); 230 (ε 2630); 286 (sh) (ε 1740); 301 (sh) (ε 2240); 320 (ε 2630) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-form

[化学名・別名] Presenegenin

[CAS No.] 2163-40-8

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

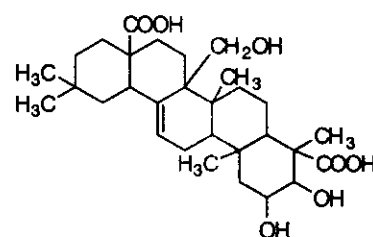
[構造式]

[基原] 次の植物から得られるサポゲニン: *Polygala senega*, *Carpobrotia glabrescens*, その他

[性状] 結晶 (EtOH 溶液)

[融点] Mp 310-311 °C

[比旋光度]: [α]_D +91 (c, 1.2 in MeOH)



-----文献-----

Shimizu, Y. et al., J.A.C.S., 1966, 88, 1544, (構造決定)

Yosioka, I. et al., Tet. Lett., 1966, 6303, (分離)

Pelletier, S.W. et al., Tetrahedron, 1971, 27, 4417

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)

Brieskorn, C.H. et al., Arch. Pharm. (Weinheim, Ger.), 1975, 308, 824, (誘導體)

Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

Miyase, T. et al., Chem. Pharm. Bull., 1995, 43, 466, (Reinoside)

Zhang, D. et al., Chem. Pharm. Bull., 1996, 44, 173; 810; 2092, (Polygalasaponin)

Pereira, B.M.R. et al., Fitoterapia, 1996, 67, 323, (Bredemeyeroside C)

Daros, M. do R. et al., Planta Med., 1996, 62, 523, (Bredemeyeroside B)

Zhang, D. et al., Phytochemistry, 1998, 47, 459, (Polygalasaponins XLIII-XLVI)

Desbegravene, S. et al., J. Nat. Prod., 1999, 62, 923, (Polygala amarella saponin)

Wu, Z. et al., Yunnan Zhiwu Yanjiu, 1999, 21, 357; CA, 132, 205416f, (Arillatanoside)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-form, 3-O-β-D-Glucopyranoside

[化学名・別名] Tenuifolin

[CAS No.] 20183-47-5

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

[構造式]

[分子式] C₃₆H₅₆O₁₂

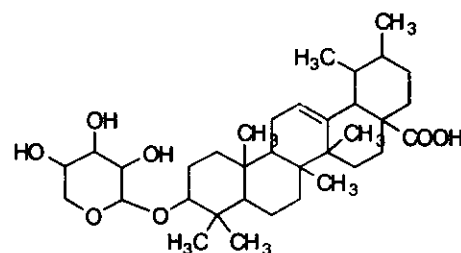
[分子量] 680.831

[正確な分子量] 680.37718

[基原] *Polygala tenuifolia*, *Polygala senega* and *Pygeum africanum*

[性状] 結晶 (EtOH)

[融点] Mp 298-300 °C



[比旋光度]: $[\alpha]_D +49$ (c, 0.8 in EtOH)

-----文献-----

- Yosioka, I. et al., Tet. Lett., 1966, 6303, (分離)
Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)
Brieskorn, C.H. et al., Arch. Pharm. (Weinheim, Ger.), 1975, 308, 824, (誘導體)
Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)
Miyase, T. et al., Chem. Pharm. Bull., 1995, 43, 466, (Reinoside)
Zhang, D. et al., Chem. Pharm. Bull., 1996, 44, 173; 810; 2092, (Polygalasaponin)
Pereira, B.M.R. et al., Fitoterapia, 1996, 67, 323, (Bredemeyeroside C)
Daros, M. do R. et al., Planta Med., 1996, 62, 523, (Bredemeyeroside B)
Zhang, D. et al., Phytochemistry, 1998, 47, 459, (Polygalasaponins XLIII-XLVI)
Desbegravene, S. et al., J. Nat. Prod., 1999, 62, 923, (Polygala amarella saponin)
Wu, Z. et al., Yunnan Zhiwu Yanjiu, 1999, 21, 357; CA, 132, 205416f, (Arillatanoside)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2 β ,3 β)-form, 3-O- β -D-Glucopyranoside, 28-O-
[β -D-galactopyranosyl-(1 \rightarrow 4)- β -D-xylopyranosyl-(1 \rightarrow 4)- α -L-rhamnopyranosyl-(1 \rightarrow 2)-
[4-methoxy-*E*-cinnamoyl-(\rightarrow 4)- β -D-fucopyranosyl]] ester

[化学名・別名] *E*-Senegasaponin B

[CAS No.] 162870-58-8

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

[構造式]

[分子式] $C_{69}H_{102}O_{31}$

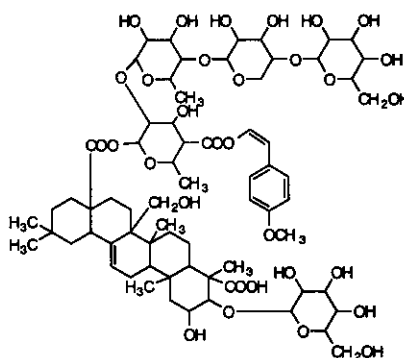
[分子量] 1427.546

[正確な分子量] 1426.640515

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 251-254 °C



-----文献-----

- Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2 β ,3 β)-form, 3-O- β -D-Glucopyranoside, 28-O-
[β -D-galactopyranosyl-(1 \rightarrow 4)- β -D-xylopyranosyl-(1 \rightarrow 4)- α -L-rhamnopyranosyl-(1 \rightarrow 2)-
[4-methoxy-*Z*-cinnamoyl-(\rightarrow 4)- β -D-fucopyranosyl]] ester

[化学名・別名] *Z*-Senegasaponin B

[CAS No.] 162613-71-0

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

[構造式]

[分子式] $C_{69}H_{102}O_{31}$

[分子量] 1427.546

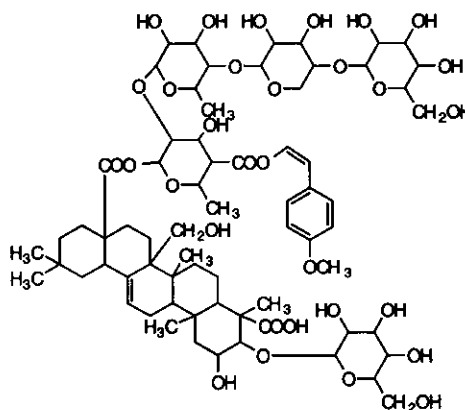
[正確な分子量] 1426.640515

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 252-255 °C

[比旋光度]: $[\alpha]_D -13.2$ (MeOH)



-----文献-----

- Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2 β ,3 β)-form, 3-O- β -D-Glucopyranoside, 28-O-
[β -D-galactopyranosyl-(1 \rightarrow 4)- β -D-xylopyranosyl-(1 \rightarrow 4)- α -L-rhamnopyranosyl-(1 \rightarrow 2)-
[3,4-dimethoxycinnamoyl-(\rightarrow 4)- α -L-fucopyranosyl]] ester

[化学名・別名] Senegin II

[CAS No.] 34366-31-9