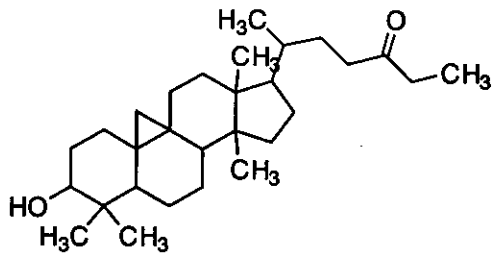
Cho, H.J. et al., Phytochemistry, 1992, 31, 3893, (生育)
Tabata, M. et al., J. Nat. Prod., 1993, 56, 165, (分離, 用途)
Cho, H.J. et al., Phytochemistry, 1993, 33, 1407, (生合成)
Kosela, S. et al., Phytochemistry, 1995, 38, 691, (Bryononic acid, H-NMR, C13-NMR, 結晶構造)

§ 3-Hydroxy-27-norcycloartan-24-one; 3 β-form
[CAS No.] 17984-23-5
[化合物分類] テルペノイド (Cycloartane triterpenoids)
[構造式]

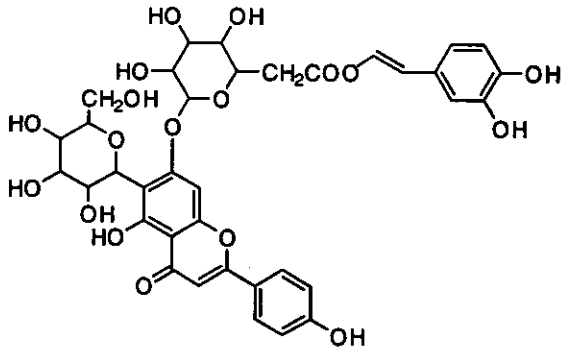


[分子式] $C_{29}H_{46}O_2$
[分子量] 428.697
[基原] *Bryonia dioica*

---文 献---

Akihisa, T. et al., Phytochemistry, 1998, 49, 1757-1760, (分離, H-NMR, C13-NMR)

§ Isovitexin; 7-*O*-[3,4-Dihydroxycinnamoyl-(→ 6)-β-D-glucopyranoside]
[化学名・別名] 6'''-*O*-Caffeoylsaponarin
[化合物分類] フラボノイド (Flavones; 3 × O-置換基)
[構造式]



[分子式] $C_{36}H_{36}O_{18}$
[分子量] 756.67
[基原] *Bryonia dioica*
[性状] 結晶 (MeOH 溶液)
[融点] Mp 251-254 ℃

---文 献---

Hoerhammer, L. et al., Tet. Lett., 1965, 1707, (H-NMR, 構造決定, Saponarin)
Krauze-Baranowska, M. et al., Phytochemistry, 1995, 39, 727, (6'''-Caffeoylsaponarin)

§ 2-Methylaminoacetic acid
[化学名・別名] *N*-Methylglycine (CAS 名). Sarcosine
[CAS No.] 107-97-1
[関連 CAS No.] 4316-73-8, 10051-96-4
[化合物分類] アミノ酸とペプチド (Non-protein α-aminoacids)
[構造式] $MeNHCH_2COOH$
[分子式] $C_3H_7NO_2$
[分子量] 89.094
[基原] Residue present in actinomycins. フリーの状態でいくつかのカビや高等植物から分離される. 例えば, *Bryonia dioica* の根
[性状] 結晶 (EtOH)
[融点] Mp 212-213 ℃で分解
[PKa 値] pK_{a1} 2.3; pK_{a2} 10.14
[化学物質毒性データ総覧 (RTECS) 登録番号] VQ2897000
[販売元] Aldrich:13177-6; Fluka:84529; Sigma:S9881

---文 献---

Webert, J.-M. et al., J. Het. Chem., 1983, 20, 49, (合成法, H-NMR, ester)
Mostad, A. et al., Acta Chem. Scand., 1989, 43, 1004, (結晶構造)
Sax, N.I., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold, 1979, 822; 868

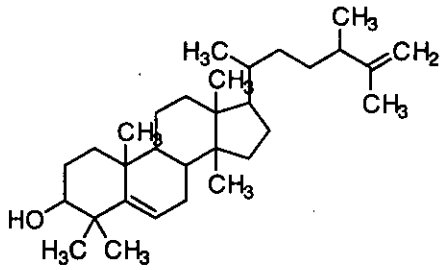
***RTECS (化学物質毒性データ) ***

生体影響物質 : 変異原性物質.

米国に於ける状況

EPA GENETOX PROGRAM 1988, Negative: N crassa-aneuploidy
EPA TSCA Section 8(b) CHEMICAL INVENTORY

§ 24-Methyltirucalla-5,25-dien-3-ol; (3 β,24*S*)-form
[CAS No.]178275-70-2
[化合物分類]テルペノイド(Tirucallane/euphane triterpenoids)
[構造式]

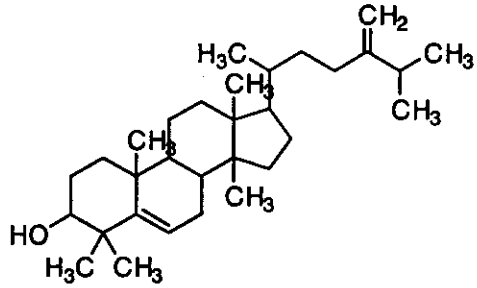


[分子式]$C_{31}H_{52}O$
[分子量]440.751
[基原]*Bryonia dioica*

---文 献---

Akihisa, T. et al., J.C.S. Perkin 1, 1996, 2379-2384, (分離, H-NMR, Mass, C13-NMR)

§ 24-Methyltirucalla-5,25-dien-3-ol; (3 β,24*S*)-form, 24,24^1-Didehydro, 25,26-dihydro
[化学名・別名]24-Methylenetirucall-5-en-3-ol
[CAS No.]178275-69-9
[化合物分類]テルペノイド(Tirucallane/euphane triterpenoids)
[構造式]

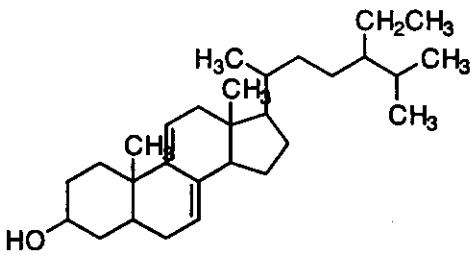


分子式]$C_{31}H_{52}O$
[分子量]440.751
[基原]*Bryonia dioica*
[性状]結晶
[融点]Mp 165-167 ℃

---文 献---

Akihisa, T. et al., J.C.S. Perkin 1, 1996, 2379-2384, (分離, H-NMR, Mass, C13-NMR)

§ Stigmasta-7,9(11)-dien-3-ol; (3 β,5 α,24*R*)-form
[CAS No.]59957-40-3
[化合物分類]ステロイド(Stigmastane steroids). (C29).
[構造式]

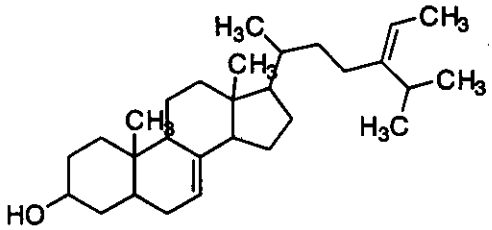


[分子式]$C_{29}H_{48}O$
[分子量]412.698
[基原]*Bryonia dioica*

---文 献---

Akihisa, T. et al., Chem. Pharm. Bull., 1996, 44, 1202-1207, (分離, H-NMR, Mass)

§ Stigmasta-7,24(28)-dien-3-ol; (3 β,5 α,24(28)*E*)-form
[化合物分類]ステロイド(Stigmastane steroids). (C29).
[構造式]

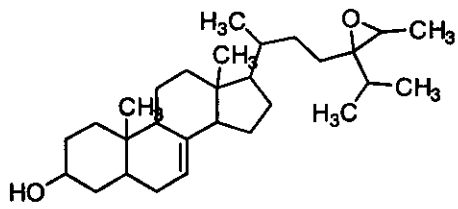


[分子式]$C_{29}H_{48}O$
[分子量]412.698
[基原]*Bryonia dioica*

---文 献---

Idler, D.R. et al., J.A.C.S., 1953, 75, 1712, (分離)
Frost, D.J. et al., Tet. Lett., 1968, 3779, (構造決定)
Lin, H.-K. et al., Phytochemistry, 1972, 11, 2319, (分離)
Akihisa, T. et al., Chem. Pharm. Bull., 1996, 44, 1202, (分離, H-NMR, Mass)

§ Stigmasta-7,24(28)-dien-3-ol; (3 β,5 α,24(28)*E*)-form, 24*R*,28*R*-Epoxide
[化学名・別名]24,28-Epoxystigmast-7-en-3-ol.
24,28-Epoxyisoavenasterol
[CAS No.]260390-78-1
[化合物分類]ステロイド(Stigmastane steroids). (C29).
[構造式]



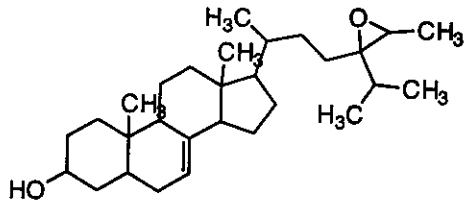
[分子式]$C_{29}H_{48}O_2$
[分子量]428.697

[基原]*Bryonia dioica*

---文 献---

Idler, D.R. et al., J.A.C.S., 1953, 75, 1712, (分離)
Frost, D.J. et al., Tet. Lett., 1968, 3779, (構造決定)
Lin, H.-K. et al., Phytochemistry, 1972, 11, 2319, (分離)
Akihisa, T. et al., Chem. Pharm. Bull., 1996, 44, 1202, (分離, H-NMR, Mass)

§ Stigmasta-7,24(28)-dien-3-ol; (3 β,5 α,24(28)*E*)-form, 24*S*,28*S*-Epoxide
[CAS No.]260390-79-2
[化合物分類]ステロイド(Stigmastane steroids). (C29).
[構造式]

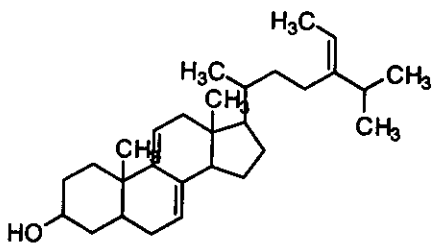


[分子量]428.697
[基原]*Bryonia dioica*

---文 献---

Idler, D.R. et al., J.A.C.S., 1953, 75, 1712, (分離)
Frost, D.J. et al., Tet. Lett., 1968, 3779, (構造決定)
Lin, H.-K. et al., Phytochemistry, 1972, 11, 2319, (分離)
Akihisa, T. et al., Chem. Pharm. Bull., 1996, 44, 1202, (分離, H-NMR, Mass)

§ Stigmasta-7,9(11),24(28)-trien-3-ol; (3 β,5 α,24(28)*E*)-form
[CAS No.]178455-06-6
[化合物分類]ステロイド(Stigmastane steroids). (C29).
[構造式]

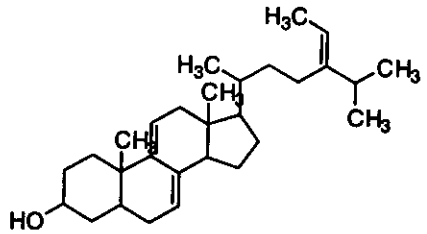


[分子式]$C_{29}H_{46}O$
[分子量]410.682
[基原]*Bryonia dioica*

---文 献---

Akihisa, T. et al., Chem. Pharm. Bull., 1996, 44, 1202-1207, (分離, H-NMR, Mass)

§ Stigmasta-7,22,24(28)-trien-3-ol; (3 β,5 α,22*E*,24(28)*Z*)-form
[CAS No.]178275-60-0
[化合物分類]ステロイド(Stigmastane steroids). (C29).
[構造式]

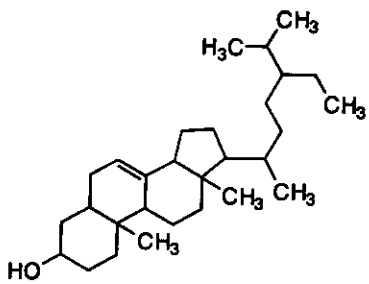


[分子式]$C_{29}H_{46}O$
[分子量]410.682
[基原]*Bryonia dioica*

---文 献---

Akihisa, T. et al., Chem. Pharm. Bull., 1996, 44, 1202-1207, (分離, H-NMR, C13-NMR, Mass)

§ Stigmast-7-en-3-ol; (3 β,5 α,24*R*)-form
[化学名・別名]Schottenol. 22-Dihydrochondrillasterol. 22,23-Dihydro-α-spinasterol
[CAS No.]521-03-9
[化合物分類]ステロイド(Stigmastane steroids). (C29).
[構造式]

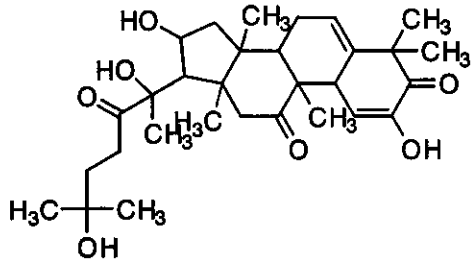


[分子式]$C_{29}H_{50}O$
[分子量]414.713
[基原]*Cucumis sativus*. また, *Lophocereus schottii*, *Bupleurum falcatum*, *Bryonia dioica*, その他
[性状]結晶(MeOH)
[融点]Mp 151-151.5 ℃
[比旋光度]:$[\alpha]_D^{30}$ +9.1 (c, 0.95 in $CHCl_3$)
[その他のデータ]Prob. indentical with β-Spinasterol

---文 献---

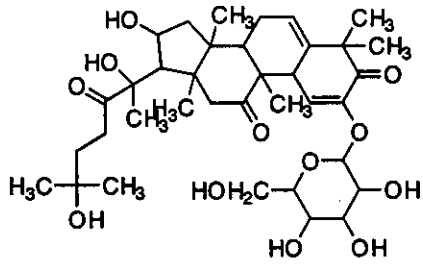
Terauchi, H. et al., Chem. Pharm. Bull., 1970, 18, 213, (分離, 構造決定)
Lin, H.-K. et al., Phytochemistry, 1972, 11, 2319, (分離)
Ulubelen, A. et al., Planta Med., 1976, 30, 221, (分離)
Siefert, K. et al., Pharmazie, 1977, 32, 125, (分離)

§ 2,16,20,25-Tetrahydroxycucurbita-1,5,23-triene-3,11,22-trione; (16 α,20*R*,23*E*)-form, 23,24-Dihydro
[化学名・別名] 2,16,20,25-Tetrahydroxycucurbita-1,5-diene-3,11,22-trione. 16,20,25-Trihydroxycucurbit-5-ene-2,3,11,22-tetrone. Cucurbitacin L
[CAS No.] 1110-02-7
[化合物分類] テルペノイド (Cucurbitane triterpenoids)
[構造式]
[分子式] $C_{30}H_{44}O_7$
[分子量] 516.673
[基原] *Citrullus ecirrhosus*, *Citrullus colocynthis*, *Gratiola officinalis*, *Bryonia dioica*
[性状] 結晶+ 1/2H_2O (MeOH 溶液)
[融点] Mp 122-127 ℃
[比旋光度]: $[\alpha]_D^{28}$ –41 (EtOH)
UV: [neutral] λ_{max} 270 (8050) (EtOH) (Berdy)



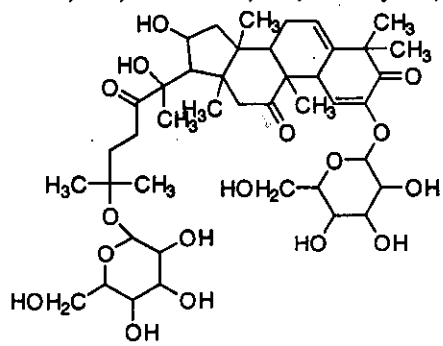
文 献
Nielsen, J.K. et al., Phytochemistry, 1977, 16, 1519-1522, (Cucurbitacin E, Cucurbtacin I)
Yamada, Y. et al., Phytochemistry, 1978, 17, 1798, (Cucurbitacin E, Cucurbitacin I, Cucurbitacin L)

§ 2,16,20,25-Tetrahydroxycucurbita-1,5,23-triene-3,11,22-trione; (16 α,20*R*,23*E*)-form, 23,24-Dihydro, 2-*O*-β-D-glucopyranoside
[化学名・別名] Bryoamaride
[CAS No.] 61105-51-9
[化合物分類] テルペノイド (Cucurbitane triterpenoids)
[構造式]
[分子式] $C_{36}H_{54}O_{12}$
[分子量] 678.815
[基原] *Bryonia dioicam*, *Citrullus colocynthis*
[融点] Mp 228-235 ℃
[比旋光度]: $[\alpha]_D^{20}$ –85.7 (c, 0.82 in EtOH)



文 献
Nielsen, J.K. et al., Phytochemistry, 1977, 16, 1519-1522, (Cucurbitacin E, Cucurbtacin I)
Yamada, Y. et al., Phytochemistry, 1978, 17, 1798, (Cucurbitacin E, Cucurbitacin I, Cucurbitacin L)
Oobayashi, K. et al., Phytochemistry, 1992, 31, 943-946, (Brydioside A)

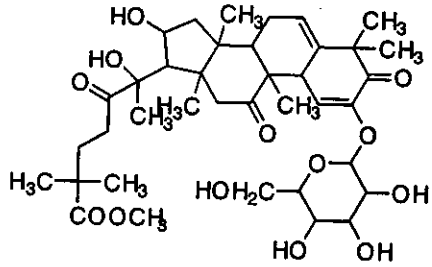
§ 2,16,20,25-Tetrahydroxycucurbita-1,5,23-triene-3,11,22-trione; (16 α,20*R*,23*E*)-form, 23,24-Dihydro, 2,25-di-*O*-β-D-glucopyranoside
[化学名・別名] Brydioside A
[CAS No.] 142674-88-2
[化合物分類] テルペノイド (Cucurbitane triterpenoids)
[構造式]
[分子式] $C_{42}H_{64}O_{17}$
[分子量] 840.957
[基原] *Bryonia dioica*
[性状] 結晶
[融点] Mp 180-181.5 ℃
[比旋光度]: $[\alpha]_D$ –28.6 (c, 0.8 in MeOH)



文 献
Oobayashi, K. et al., Phytochemistry, 1992, 31, 943-946, (Brydioside A)

§ 2,16,20,25-Tetrahydroxycucurbita-1,5,23-triene-3,11,22-trione; (16 α,20*R*,23*E*)-form, 23,24-Dihydro, 25-Ac, 2-*O*-β-D-glucopyranoside
[化学名・別名] 25-*O*-Acetylbryoamaride

[CAS No.]61014-18-4
[化合物分類]テルペノイド(Cucurbitane triterpenoids)
[構造式]

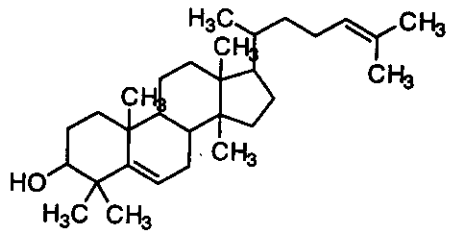


[分子式]$C_{36}H_{56}O_{13}$
[分子量]720.853
[基原]*Bryonia dioica*
[比旋光度]:[α]$_D^{20}$ −34.3 (c, 1.04 in $CHCl_3$)

----------文献----------

Nielsen, J.K. et al., Phytochemistry, 1977, 16, 1519-1522, (Cucurbitacin E, Cucurbtacin I)
Yamada, Y. et al., Phytochemistry, 1978, 17, 1798, (Cucurbitacin E, Cucurbitacin I, Cucurbitacin L)
Oobayashi, K. et al., Phytochemistry, 1992, 31, 943-946, (Brydioside A)

§ Tirucalla-5,24-dien-3-ol; 3 β-form
[CAS No.]178455-08-8
[化合物分類]テルペノイド(Tirucallane/euphane triterpenoids)
[構造式]

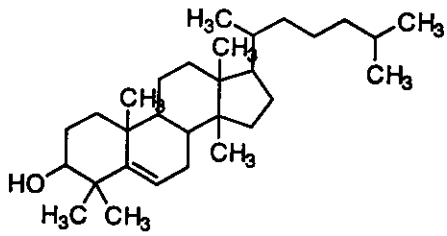


[分子式]C30H50O
[分子量]426.724
[基原]*Bryonia dioica*

----------文献----------

Akihisa, T. et al., J.C.S. Perkin 1, 1996, 2379-2384, (分離, H-NMR, C13-NMR)

§ Tirucalla-5,24-dien-3-ol; 3 β-form, 24,25-Dihydro
[化学名・別名]Tirucall-5-en-3-ol
[CAS No.]178275-68-8
[化合物分類]テルペノイド(Tirucallane/euphane triterpenoids)
[構造式]



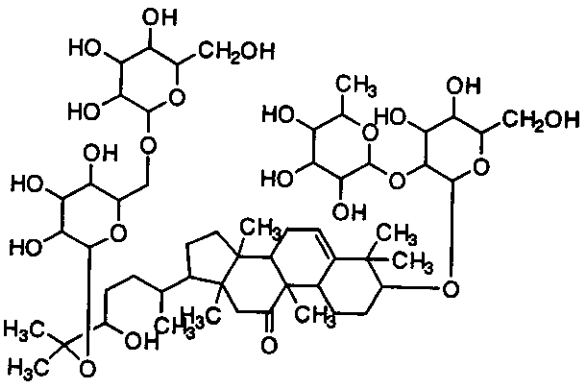
[分子式]$C_{30}H_{52}O$
[分子量]428.74
[基原]*Bryonia dioica*

----------文献----------

Akihisa, T. et al., J.C.S. Perkin 1, 1996, 2379-2384, (分離, H-NMR, C13-NMR)

§ 3,24,25-Trihydroxycucurbit-5-en-11-one; (3 β,24 ξ)-form, 3-*O*-[α-L-Rhamnopyranosyl(1 → 2)-β-D-glucopyranoside], 25-*O*-[β-D-glucopyranosyl(1 → 6)-β-D-glucopyranoside]
[化学名・別名]Bryonoside
[CAS No.]83725-21-7
[化合物分類]テルペノイド(Cucurbitane triterpenoids)

[構造式]



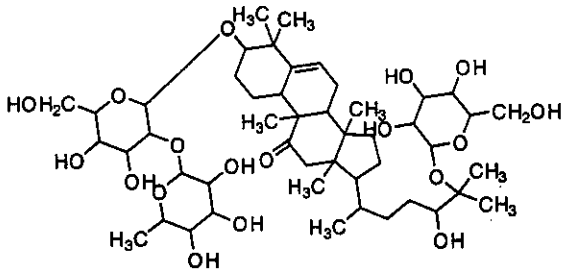
[分子式]$C_{54}H_{90}O_{23}$
[分子量]1107.291
[基原]*Bryonia dioica*
[性状]粉末 (propanol)
[融点]Mp 207-213 ℃
[比旋光度]:[α]$_D$ +26.1 (c, 1.04 in MeOH)
[その他のデータ]構造式は1992年に改正された

----------文献----------

Tunmann, P. et al., Arch. Pharm. (Weinheim, Ger.), 1966, 299, 596, (Bryodulcoside)
Oobayashi, K. et al., Phytochemistry, 1992, 31, 943, (Bryonoside, Brydiosides)

§ 3,24,25-Trihydroxycucurbit-5-en-11-one; (3 β,24 ξ)-form, 3-*O*-α-L-Rhamnopyranosyl(1 → 2)-β-D-glucopyranosyl, 25-*O*-β-D-glucopyranosyl
[化学名・別名]Bryoside

[CAS No.]83775-20-6
[化合物分類]テルペノイド(Cucurbitane triterpenoids)
[構造式]

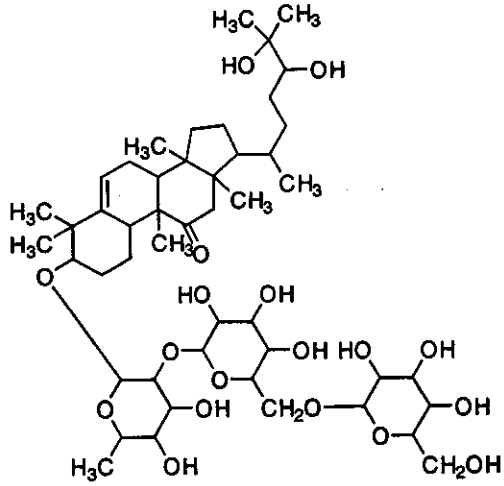


[分子式]$C_{48}H_{80}O_{18}$
[分子量]945.149
[基原]*Bryonia dioica*
[性状]粉末 (2-propanol)
[融点]Mp 179-183 ℃
[比旋光度]:[α]$_D$ +30.9 (c, 0.86 in MeOH)

----------文 献----------

Oobayashi, K. et al., Phytochemistry, 1992, 31, 943, (Bryonoside, Brydiosides)

§ 3,24,25-Trihydroxycucurbit-5-en-11-one; (3 β,24 ξ)-form, 3-*O*-[β-D-Glucopyranosyl(1 → 6)-β-D-glucopyranosyl(1 → 2)-6-deoxy-D-guloside]
[化学名・別名]Bryodulcoside
[CAS No.]11028-18-5
[化合物分類]テルペノイド(Cucurbitane triterpenoids)
[構造式]

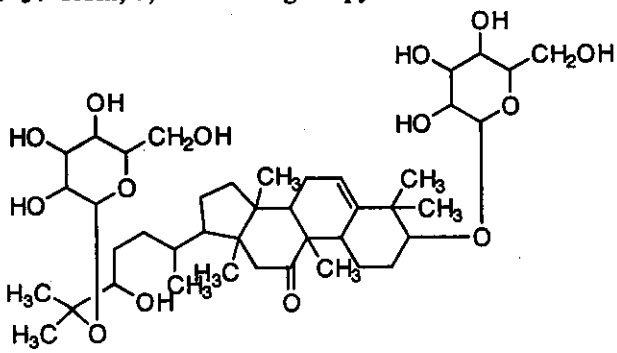


[分子式]$C_{48}H_{80}O_{18}$
[分子量]945.149
[基原]次の植物の根から分離: *Bryonia dioica*
[性状]結晶
[融点]Mp 203-205 ℃
[比旋光度]:[α]$_D^{20}$ +36.2 (c, 7.9 in H_2O)

----------文 献----------

Tunmann, P. et al., Arch. Pharm. (Weinheim, Ger.), 1966, 299, 596, (Bryodulcoside)

§ 3,24,25-Trihydroxycucurbit-5-en-11-one; (3 β,24 ξ)-form, 3,25-Di-*O*-D-glucopyranoside
[化学名・別名]Brydioside B
[CAS No.]142674-89-3
[化合物分類]テルペノイド
(Cucurbitane triterpenoids)
[構造式]

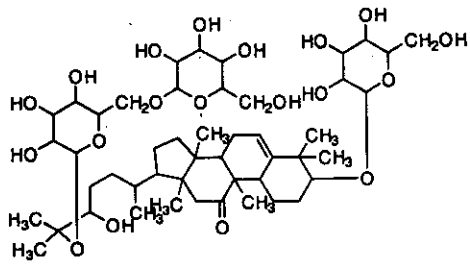


[分子式]$C_{42}H_{70}O_{14}$
[分子量]799.007
[基原]*Bryonia dioica*
[性状]結晶
[融点]Mp 164-165 ℃
[比旋光度]:[α]$_D$ +60.1 (c, 2.8 in MeOH)

----------文 献----------

Oobayashi, K. et al., Phytochemistry, 1992, 31, 943, (Bryonoside, Brydiosides)

§ 3,24,25-Trihydroxycucurbit-5-en-11-one; (3 β,24 ξ)-form, 3-*O*-β-D-Glucopyranoside, 25-*O*-[β-D-glucopyranosyl-(1 → 6)-β-D-glucopyranoside]
[化学名・別名]Brydioside C
[CAS No.]142705-64-4
[化合物分類]テルペノイド(Cucurbitane triterpenoids)
[構造式]



[分子式]$C_{48}H_{80}O_{19}$
[分子量]961.149
[基原]*Bryonia dioica*
[性状]結晶

[融点]Mp 267-268 ℃
[比旋光度]:[α]$_D$ +50.6 (c, 1.7 in MeOH)

----------文 献----------

Oobayashi, K. et al., Phytochemistry, 1992, 31, 943, (Bryonoside, Brydiosides)

§ ***Bryonia dioica*** **Trypsin inhibitor II**
[化学名・別名]BDTI II
[化合物分類]アミノ酸とペプチド(Linear polypeptides)
[構造式]

[一般的性質] Struct. of reduced form shown

H-Arg-Gly-Cys-Pro-Arg-Ile-Leu-Met-Arg-Cys-Lys-Arg-Asp-Ser-Asp-Cys-Leu-Ala-Gly-Cys-Val-Cys-Gln-Lys-Asn-Gly-Tyr-Cys-Gly-OH

[基原]*Bryonia dioica* の種子
[用途]Trypsin inhibitor

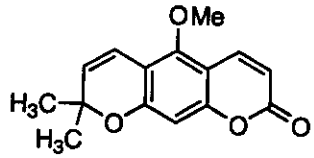
----------文 献----------

Otlewski, J. et al., Hoppe Seyler's Z. Physiol. Chem., 1987, 368, 1505-1507, (分離, 構造決定)

**********プリックリーアッシュ (Prickly ash) **********

§§ミカン科アメリカサンショウ(***Zanthoxylum americanum*** **Miller)の樹皮。**

§ **Xanthoxyletin**
[化学名・別名]5-Methoxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:5,4-*b*']dipyran-2-one (CAS 名). Xanthoxylin N. Xanthoxyloin
[CAS No.]84-99-1
[化合物分類]ベンゾピラノイド(Pyranocoumarins), 薬物: 抗痙攣薬(Anticonvulsants), ベンゾピラノイド(5,7-Dioxygenated coumarins)
[構造式]



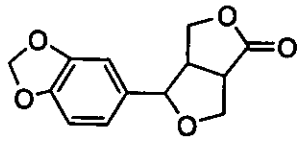
[分子式]$C_{15}H_{14}O_4$
[分子量]258.273
[基原]次の植物から分離: *Zanthoxylum americanum*, *Melicope ternata*, *Halfordia scleroxyla*, *Afraegle paniculata*, *Eriostemon trachyphyllus*, *Chloroxylon swietenia*
[用途]抗痙攣薬
[性状]結晶(petrol)
[融点]Mp 133 ℃
[Log P 計算値]Log P 3.04 (計算値)

----------文 献----------

Vrkov, J. et al., Phytochemistry, 1972, 11, 2647, (分離)
Mujumdar, R.B. et al., Indian J. Chem., Sect. B, 1977, 15, 200, (分離)
Gray, A.J. et al., J.C.S. Perkin 2, 1978, 391, (H-NMR)
Murray, R.D.H. et al., Tetrahedron, 1984, 40, 3129, (合成法, 成書)
Fukai, T. et al., Heterocycles, 1994, 38, 1089, (Kanzonol Q)

§§ミカン科ティンバー(***Zanthoxylum alatum*** **Roxburgh)の樹皮。**

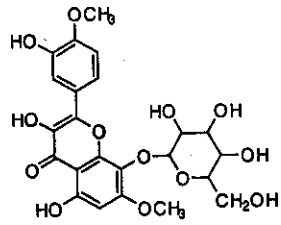
§ **Acuminatolide; 4-Epimer**
[化学名・別名]Pluviatide
[化合物分類]リグナン化合物(Norlignans), リグナン化合物(Simple furofuranoid lignans)
[構造式]



[基原]*Zanthoxylum alatum*, *Zanthoxylum pluviatile*
[性状]プリズム結晶 ($CHCl_3$/MeOH)
[融点]Mp 173-174 ℃
[その他のデータ]非天然物.

----------文 献----------

Corrie, J.E.T. et al., Aust. J. Chem., 1970, 23, 133, (分離)
Dashpande, V.H. et al., Indian J. Chem., Sect. B, 1977, 15, 95, (分離)
Jakupovic, J. et al., Phytochemistry, 1987, 26, 803, (分離, 構造決定)

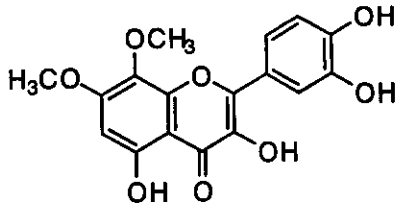


§ 3,3',4',5,7,8-Hexahydroxyflavone; 4',7-Di-Me ether, 8-*O*-β-D-glucopyranoside
[化学名・別名]Tambuletin
[CAS No.]32427-55-7
[化合物分類]フラボノイド(Flavonols; 6 × O-置換基)
[構造式]
[分子式]$C_{23}H_{24}O_{13}$
[分子量]508.435
[基原]次の植物から分離: *Zanthoxylum acanthopodium*, *Zanthoxylum alatum*, *Achillea depressa*
[性状]黄色の結晶(EtOAc)
[融点]Mp 272-274 ℃ (268-270 ℃)

----------文 献----------

Nair, A.G.R. et al., Phytochemistry, 1982, 21, 483, (Tambuletin)

§ 3,3',4',5,7,8-Hexahydroxyflavone; 7,8-Di-Me ether
[化学名・別名]3,3',4',5-Tetrahydroxy-7,8-dimethoxyflavone. Zanthoxylflavone
[CAS No.]102487-38-7
[化合物分類]フラボノイド(Flavonols; 6 × O-置換基)
[構造式]

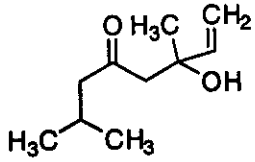


[分子式]$C_{17}H_{14}O_8$
[分子量]346.293
[基原]*Calycadenia ciliosa*, *Zanthoxylum alatum*
[性状]金色の結晶(MeOH)
[融点]Mp 156-157 ℃

----------文 献----------

Ramidi, R. et al., Pharmazie, 1999, 54, 781-782, (Zanthoxylflavone)

§ 6-Hydroxy-2,6-dimethyl-7-octen-4-one; (+)-form
[CAS No.]23007-34-3
[化合物分類]テルペノイド(Acyclic monoterpenoids)
[構造式]

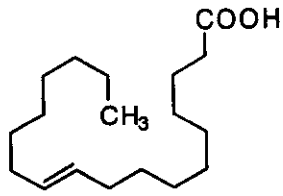


[基原]次の植物から分離: *Cinnamomum camphora* の精油, *Citrus junos*, *Zanthoxylum alatum*
[性状]液体
[沸点]Bp_4 72-74 ℃
[比旋光度]:$[\alpha]_D^{15}$ +4.8 (c, 3 in CCl_4)

----------文 献----------

Yoshida, T. et al., Agric. Biol. Chem., 1969, 33, 343, (分離, H-NMR, 構造決定)
Kitahara, T. et al., Agric. Biol. Chem., 1980, 44, 897, (分離, 合成法)
Ahmad, A. et al., Fitoterapia, 1988, 59, 413, (分離)

§ 10-Octadecenoic acid; (Z)-form
[CAS No.]2442-70-8
[化合物分類]脂肪族化合物(Unbranched alkenic carboxylic acids and lactones)
[構造式]

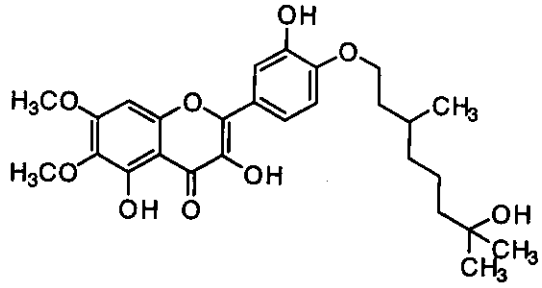


[分子式]$C_{18}H_{34}O_2$
[分子量]282.465
[基原]Found in partially hydrogenated fats as a glyceride. *Zanthoxylum alatum* の種子オイルから分離される
[融点]Mp 22.2-22.8 ℃

----------文 献----------

Swern, D. et al., J. Am. Oil Chem. Soc., 1955, 32, 539, (結晶構造)
Venkatachalam, S.R. et al., Indian J. Chem., Sect. B, 1996, 35, 515, (分離, Mass)

§ 3,3',4',5-Tetrahydroxy-6,7-dimethoxyflavone; 4'-*O*-(7 ξ-Hydroxy-3 ξ,7-dimethyloctyl)



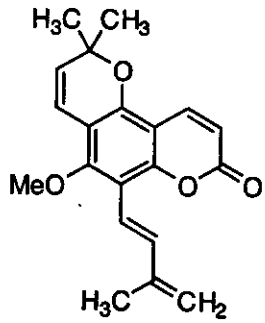
[化学名・別名]Geranioloxyalatumflavone
[CAS No.]252351-60-3
[化合物分類]フラボノイド(Flavonols; 6 × O-置換基)
[構造式]
[分子式]$C_{27}H_{34}O_9$
[分子量]502.56
[基原]*Zanthoxylum alatum* の種子
[性状]淡黄色の結晶(MeOH)
[融点]Mp 190-191 ℃
UV: [neutral] λ_{max} 205 ; 220 ; 272 ; 330 (MeOH)
[その他のデータ]Misleading synonym

----------文 献----------

Ramidi, R. et al., Pharmazie, 1999, 54, 781-782, (Geranioloxyalatumflavone)

§§ ミカン科ケイセンライ(*Zanthoxylum avicennae* de Candolle)の樹皮。

§ Avicennin

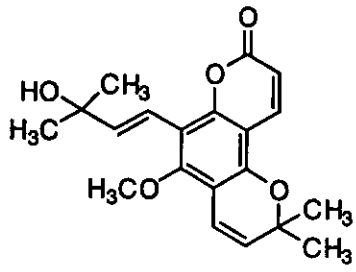


[CAS No.]53258-71-2
[化合物分類]ベンゾピラノイド(7-Oxygenated coumarins with miscellaneous 置換基), ベンゾピラノイド(Pyranocoumarins)
[構造式]
[分子式]$C_{20}H_{20}O_4$
[分子量]324.376
[基原]*Zanthoxylum avicennae*, *Eriostemon coccineum*
[性状]黄色のプリズム結晶
[融点]Mp 141-142 ℃

----------文 献----------

Arthur, H.R. et al., J.C.S., 1960, 4654; 1963, 3910, (分離, H-NMR)
Chow, P.W. et al., Aust. J. Chem., 1966, 19, 483, (分離)
Lai, T.F. et al., Acta Cryst. B, 1974, 30, 1570, (結晶構造)
Gray, A.I. et al., J.C.S. Perkin 1, 1975, 488, (構造決定)
Sarker, S.D. et al., Biochem. Syst. Ecol., 1994, 22, 641, (Z-isomer)

§ Avicennol; (*E*)-form

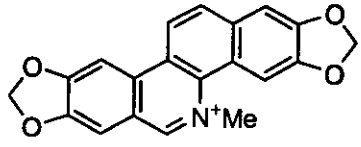


[CAS No.]56110-68-0
[化合物分類]ベンゾピラノイド(Pyranocoumarins), ベンゾピラノイド(5,7-Dioxygenated coumarins)
[構造式]
[分子式]$C_{20}H_{22}O_5$
[分子量]342.391
[基原]*Zanthoxylum avicennae* と *Zanthoxylum elephantiasis* の根皮
[性状]黄色の板状結晶(EtOAc/hexane)
[融点]Mp 124.5-125.5 ℃

----------文 献----------

Gray, A.I. et al., J.C.S. Perkin 1, 1975, 488, (構造決定)
Gray, A.I. et al., Phytochemistry, 1977, 16, 1017, (分離)
Rashid, M.A. et al., Phytochemistry, 1991, 30, 4033, (誘導体)

§ Avicine

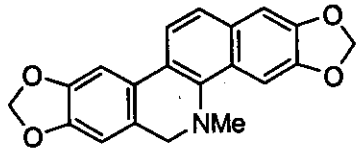


[化学名・別名]5-Methyl-1,3-benzodioxolo[5,6-*c*][1,3]dioxolo[4,5-*j*]phenanthridinium(1+) (CAS 名)
[CAS No.]24939-31-9
[化合物分類]アルカロイド化合物(Benzo[c]phenanthridine alkaloids)
[構造式]
[分子式]$C_{20}H_{14}NO_4^{(+)}$
[分子量]332.335

[基原]次の植物から得られるアルカロイド: *Zanthoxylum avicennae* の根皮, *Zanthoxylum inerme* (= *Fagara boninensis*) の樹皮(ミカン科)
[その他のデータ]Rather unstable; disproportionates into its dihydro- and oxy-derivs.

----------文 献----------

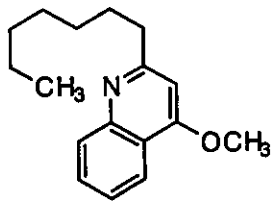
Arthur, H.R. et al., J.C.S., 1959, 4007, (分離)
Gopinath, K.W. et al., Tetrahedron, 1961, 14, 322, (合成法, UV, 誘導体)
Ishii, H. et al., Yakugaku Zasshi, 1972, 92, 118; 1976, 96, 1458; CA, 77, 16530y; 86, 136297k, (分離, H-NMR, 誘導体)

§ Dihydroavicine
[化学名・別名]5,6-Dihydro-5-methyl-1,3-benzodioxolo[5,6-*c*][1,3]dioxolo[4,5-*j*]phenanthridine(CAS 名)
[CAS No.]34490-82-9
[化合物分類]アルカロイド化合物(Benzo[c]phenanthridine alkaloids)
[構造式]


[分子式]$C_{20}H_{15}NO_4$
[分子量]333.343
[基原]次の植物から得られるアルカロイド: *Toddalia asiatica* の根, *Zanthoxylum avicennae* の根皮. Also prod. (together with oxyavicine) by disproportionation of Avicine, when the latter is liberated from its salts (ミカン科)
[性状]プリズム結晶 (EtOH or C_6H_6/Et_2O)
[融点]Mp 212-213 ℃

----------文 献----------

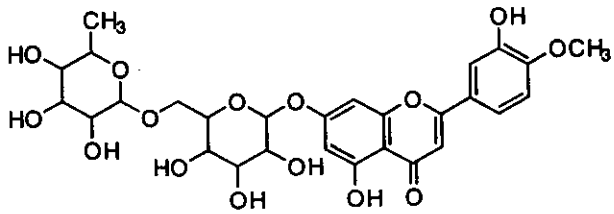
Fish, F. et al., Phytochemistry, 1975, 14, 841, (分離, Mass)
Ninomiya, I. et al., J.C.S. Perkin 1, 1975, 762, (合成法, IR, 誘導体)
Sharma, P.N. et al., Indian J. Chem., Sect. B, 1979, 17, 299, (分離, Mass)

§ 2-Heptyl-4-hydroxyquinoline; *OH*-form, Me ether
[化学名・別名]2-Heptyl-4-methoxyquinoline(CAS 名)
[CAS No.]80554-59-2
[化合物分類]アルカロイド化合物(Simple quinoline alkaloids)
[構造式]


[分子式]$C_{17}H_{23}NO$
[分子量]257.375
[基原]次の植物から得られるアルカロイド: *Zanthoxylum avicennae*
[融点]Mp 35-38 ℃

----------文 献----------

Hays, E.E. et al., J. Biol. Chem., 1945, 159, 725, (分離)
Cornforth, J.W. et al., Biochem. J., 1956, 63, 124; 130, (分離, 性質)
Wratten, S.J. et al., Antimicrob. Agents Chemother., 1977, 11, 411, (分離)
Budzikiewicz, H. et al., Monatsh. Chem., 1979, 110, 947, (分離, UV)
Kitamura, S. et al., J. Antibiot., 1986, 39, 1160, (分離, 構造決定, 性質)
Wu, W. et al., Zhongcaoyao, 1992, 23, 115; CA, 117, 76305h, (分離, Me ether)
Guilhon, G.M.S.P. et al., Phytochemistry, 1994, 37, 1193, (2-Heptyl-8-methoxy-1-methyl-4(1H)-quinolinone)

§ 3',5,7-Trihydroxy-4'-methoxyflavone; 7-*O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside]
[化学名・別名]Diosmetin 7-rutinoside. Diosmin, INN. Daflon. Ven-Detrex. Salinigricoflavonoloside. Barosmin
[CAS No.]520-27-4
[化合物分類]フラボノイド(Flavones; 4 × O-置換基), 薬物: 止血剤(Haemostatic agents)
[構造式]


[分子式]$C_{28}H_{32}O_{15}$
[分子量]608.552
[基原]次の植物から分離: *Zanthoxylum avicennae*, *Diosma crenulata*, その他, 最初はパセリから分離
[用途]Bioflavonoid used medicinally. 抗出血作用, venotonic
[性状]微細結晶・一水和物 (Py 溶液)

[融点]Mp 280 ℃で分解 (*in vacuo*)
[Log P 計算値]Log P -2.86 (未確認値) (計算値)
UV: [neutral] λ_{max} 255 ; 268 ; 345 (MeOH) (Berdy)
[販売元]Aldrich:24531-3; Sigma:D3525

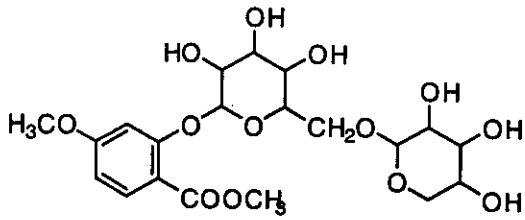
----------文 献----------

Rashid, M.A. et al., Fitoterapia, 1995, 66, 471, (Diosmin, H-NMR, C13-NMR)

*********プリムローズ (Primrose) *********

§§サクラソウ科セイヨウサクラソウ(*Primula officinalis* Jacquin)の花，根または全草。

§ 2,4-Dihydroxybenzoic acid; 4-Me ether, Me ester, 2-*O*-[β-D-xylopyranosyl(1 → 6)-β-D-glucopyranoside]

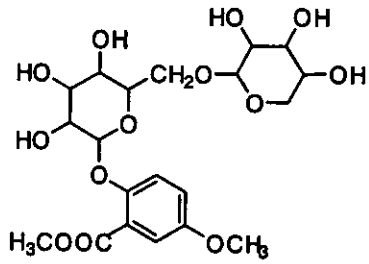


[化学名・別名]Primeverin. Primverin. Primveroside
[CAS No.]154-60-9
[化合物分類]単環芳香族(Simple benzoic acids and esters)
[構造式]
[分子式]$C_{20}H_{28}O_{13}$
[分子量]476.433
[基原]次の植物の根から分離: *Primula officinalis* とその他の *Primula* spp.
[性状]針状結晶(Me_2CO)
[融点]Mp 203-204 ℃
[比旋光度]:$[\alpha]_D^{20}$ -71.5 (H_2O)
[その他のデータ]For sugar residue see 6-*O*-β-D-Xylopyranosyl-D-glucose

----------文 献----------

Goris, A. et al., C. R. Hebd. Seances Acad. Sci., 1919, 169, 871; 975, (Primeverin)

§ 2,5-Dihydroxybenzoic acid; 5-Me ether, 2-*O*-[β-D-xylopyranosyl-(1 → 6)-β-D-glucopyranoside], Me ester

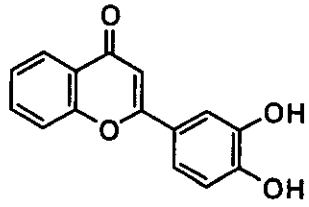


[化学名・別名]Primulaverin. Primulaveroside
[化合物分類]単環芳香族(Simple benzoic acids and esters)
[構造式]
[分子式]$C_{20}H_{28}O_{13}$
[分子量]476.433
[基原]次の植物の根から分離: *Primula officinalis*, *Primula acaulis*

----------文 献----------

Chaudhury, D.N. et al., J.C.S., 1948, 2220, (Primulaverin)
Meyer, K. et al., Science (Washington, D.C.), 1948, 108, 281, (薬理)

§ 3',4'-Dihydroxyflavone(旧 CAS 名)



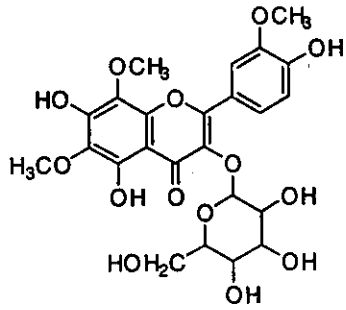
[化学名・別名]2-(3,4-Dihydroxyphenyl)-4*H*-1-benzopyran-4-one(CAS 名)
[CAS No.]4143-64-0
[化合物分類]フラボノイド(Flavones; 2 × O-置換基)
[構造式]
[分子式]$C_{15}H_{10}O_4$
[分子量]254.242
[基原]*Primula officinalis* の花に配糖体として見られる
[性状]淡黄色の結晶(EtOH)
[融点]Mp 243 ℃

----------文 献----------

Harborne, J.B., Phytochemistry, 1968, 7, 1215, (分離, 合成法)
Wollenweber, E., Biochem. Physiol. Pflanz., 1974, 166, 419, (分離)
Parvez, M. et al., Phytochemistry, 1990, 29, 2043, (分離, 合成法)

§ 3,3',4',5,6,7,8-Heptahydroxyflavone; 3',6,8-Tri-Me ether, 3-*O*-β-D-glucopyranoside

[化学名・別名]Limocitrol 3-glucoside
[CAS No.]77133-42-7
[化合物分類]フラボノイド(Flavonols; 7 × O-置換基)
[構造式]

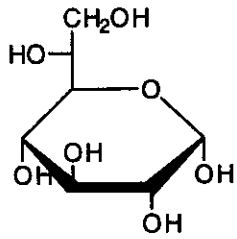


[分子式]$C_{24}H_{26}O_{14}$
[分子量]538.461
[基原]次の植物から分離: *Citrus limon*, *Primula officinalis*
[性状]黄色のプリズム結晶(H_2O)
[融点]Mp 163 ℃. Mp 203-204 ℃ (二相性)

----------文 献----------

Gentili, B. et al., Tetrahedron, 1964, 20, 2313, (Limocitrol, Isolimocitrol, 3-glucoside)
Gupta, V. et al., Indian J. Chem., Sect. B, 1989, 28, 282, (6,8-di-Me ether 3-arabinoside, Limocitrol 3-neohesperidoside)

§ **D-*glycero*-D-*gluco*-Heptose(CAS 名)**
[化学名・別名]D-*altro*-D-*gluco*-Heptose
[CAS No.]1949-75-3
[化合物分類]炭水化物(Higher aldoses)
[構造式]



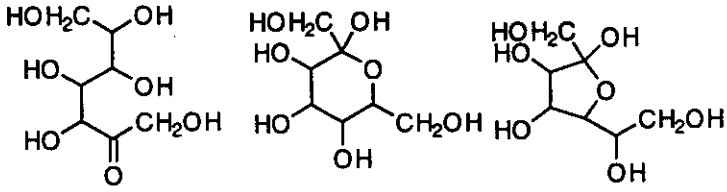
α-Pyranose-form

[分子式]$C_7H_{14}O_7$
[分子量]210.183
[基原]*Primula officinalis* の根
[性状]結晶(MeOH)
[融点]Mp 156-157 ℃
[比旋光度]:$[\alpha]_D^{20}$ +17 → +46 (c, 2.4 in H_2O)

----------文 献----------

Rosenfeld, D.A. et al., J.A.C.S., 1951, 73, 4907, (α-hexa-Ac)
Begbie, R. et al., Carbohydr. Res., 1966, 2, 272, (分離, β-hexa-Ac)

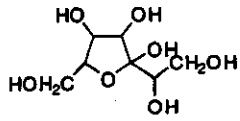
§ ***allo*-2-Heptulose; D-form**
[CAS No.]7101-28-2
[化合物分類]炭水化物(Higher ketoses)
[構造式]



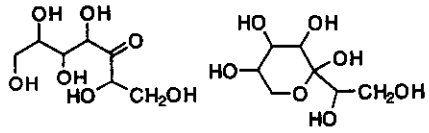
[分子式]$C_7H_{14}O_7$
[分子量]210.183
[基原]次の植物から分離: *Primula officinalis*
[融点]Mp 130-132 ℃
[比旋光度]:$[\alpha]_D^{20}$ +52.8 (c, 0.2 in H_2O)

----------文 献----------

Schaffer, R., J.O.C., 1964, 29, 1471, (合成法)
Begbie, R. et al., Carbohydr. Res., 1966, 2, 272, (分離)



§ ***altro*-3-Heptulose; D-form**
[CAS No.]13059-96-6
[化合物分類]AF2200, 炭水化物(Higher ketoses)
[構造式]



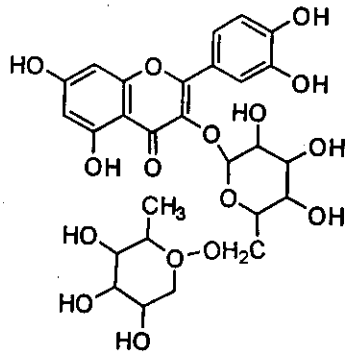
[分子式]$C_7H_{14}O_7$
[分子量]210.183
[基原]*Coriaria japonica*, *Coriaria nepalensis*, *Coriaria ruscifolia*, *Coriaria thymifolia*, *Coriaria intermedia*. また *Primula officinalis* の根
[融点]Mp 169-171 ℃
[比旋光度]:$[\alpha]_D^{27}$ +21.7 (H_2O)

----------文 献----------

Okuda, T. et al., Tetrahedron, 1968, 24, 6907, (分離, 構造決定, 合成法)
Taga, T. et al., Acta Cryst. B, 1970, 26, 991, (結晶構造)
Angyal, S.J. et al., Aust. J. Chem., 1976, 29, 1239, (C13-NMR)

Okuda, T. et al., Phytochemistry, 1977, 16, 600, (Mass)

§ **Hyperin; 6''-*O*-α-L-Rhamnopyranosyl**
[化学名・別名]Quercetin 3-robinobioside
[CAS No.]52525-35-6
[化合物分類]フラボノイド(Flavonols; 5 × O-置換基)
[構造式]

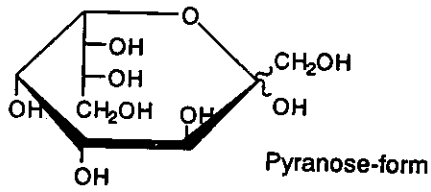


[分子式]$C_{27}H_{30}O_{16}$
[分子量]610.524
[基原]次の植物から分離: *Crataegus pinnatifida*, *Primula officinalis*, その他の植物属.

---文 献---

Sando, C.E., J. Biol. Chem., 1937, 113, 45, (分離)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1531, (生育)
Riess-Maurer, I. et al., Tetrahedron, 1982, 38, 1269, (Quercetin 3-rhamnoside)

§ **D-*erythro*-L-*galacto*-Nonulose**
[化合物分類]炭水化物(Higher ketoses)
[構造式]

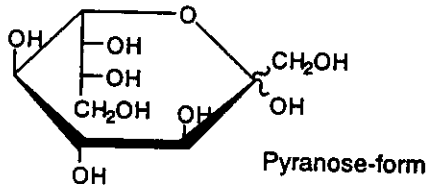


[分子式]$C_9H_{18}O_9$
[分子量]270.236
[基原]次の植物に存在する: アボガド, *Primula officinalis* とベンケイソウ科属の根
[比旋光度]:$[\alpha]_D^{20}$ -36.2 (c, 5.2 in MeOH 溶液)

---文 献---

Begbie, R. et al., Carbohydr. Res., 1966, 2, 272, (生育)
Sephton, H.H. et al., Carbohydr. Res., 1966, 2, 289, (合成法)

§ **D-*erythro*-L-*gluco*-Nonulose**
[化合物分類] 炭水化物(Higher ketoses)
[構造式]

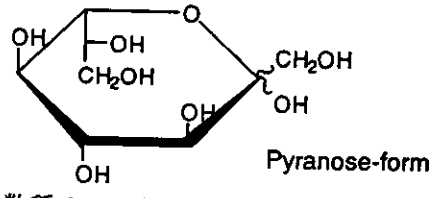


[分子式]$C_9H_{18}O_9$
[分子量]270.236
[基原]次の植物から分離: アボガド, *Primula officinalis* の乾燥根. また *Persea americana* の果実
[性状]シロップ
[比旋光度]:$[\alpha]_D^{20}$ -40 (c, 0.6 in H_2O)

---文 献---

Sephton, H.H. et al., J.O.C., 1963, 28, 2388, (分離)
Begbie, R. et al., Carbohydr. Res., 1966, 2, 272, (分離)
Sephton, H.H. et al., Carbohydr. Res., 1966, 2, 289, (合成法)

§ **D-*glycero*-L-*galacto*-Octulose**
[化合物分類]炭水化物(Higher ketoses)
[構造式]



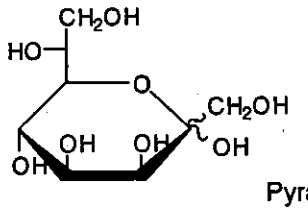
[分子式]$C_8H_{16}O_8$
[分子量]240.21
[基原]次の植物に存在する: 熟したアボガド, *Primula officinalis* と数種のベンケイソウ科植物の乾燥根
[比旋光度]:$[\alpha]_D^{20}$ -57 (c, 2 in H_2O)

---文 献---

Sephton, H.H. et al., J.O.C., 1963, 28, 1691, (生育, 合成法)
Sephton, H.H. et al., Carbohydr. Res., 1966, 2, 289, (生育, 合成法)
Schaffer, R., The Carbohydrates, Academic Press, 1972, 69, (レビュー)

§ **D-*glycero*-D-*manno*-Octulose**(旧 CAS 名)

[CAS No.]13111-79-0
[化合物分類]炭水化物(Higher ketoses)
[構造式]
[分子式]$C_6H_{16}O_8$
[分子量]240.21
[基原]次の植物に存在する: アボガド(*Persea gratissima*), *Sedum* spp., *Medicago sativa*, *Primula officinalis* の根, poppy (*Papaver somniferum*)等
[比旋光度]:[α]$_D^{20}$ +20 (c, 1.1 in MeOH)

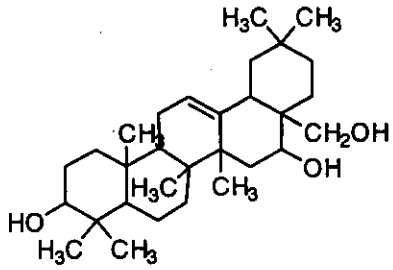


Pyranose-form

----------文 献----------

Charlson, A.J. et al., J.A.C.S., 1960, 82, 3428, (生育)
Haustveit, G. et al., Acta Chem. Scand., 1970, 24, 3059, (生育)

§ 12-Oleanene-3,16,28-triol; (3 β,16 α)-form
[化学名・別名]Primulagenin A. Armillarisgenin C. Schiwalligenin B_1
[CAS No.]465-95-2
[化合物分類]テルペノイド(Oleanane triterpenoids)
[構造式]
[分子式]$C_{30}H_{50}O_3$
[分子量]458.723
[基原]*Primula officinalis*, *Aegiceras corniculatum*, *Jacquinia* spp., その他の植物
[性状]結晶(CHCl$_3$/MeOH)
[融点]Mp 249.5-250 ℃
[比旋光度]:[α]$_D$ +58 (c, 0.7 in CHCl$_3$)
[その他のデータ]Identity of Primulagenin A and Armillarisgenin C not definitely confirmed



----------文 献----------

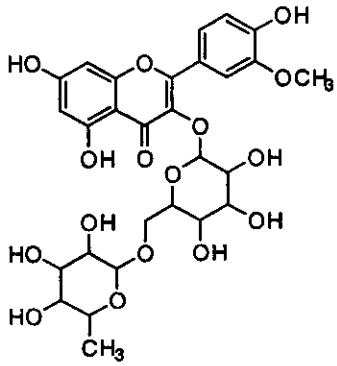
Tschesche, R. et al., Annalen, 1964, 674, 185-195, (Primulasaponin)
Zakharov, A.M. et al., Khim. Prir. Soedin., 1968, 4, 388-331; Chem. Nat. Compd. (Engl. Transl.), 1968, 4, 330, (Primulasaponin)

§ 3,4',5,7-Tetrahydroxyflavone; Di-*O*-α-L-rhamnopyranoside
[化学名・別名]Primulaflavonoside
[化合物分類]フラボノイド(Flavonoids 構造は一部又は全てが未知), フラボノイド(Flavonols; 4 × O-置換基)
[構造式]有効な構造式はない
[分子式]$C_{27}H_{30}O_{14}$
[分子量]578.526
[基原]次の植物の花から分離: *Primula officinalis*
[性状]Yellow microscopic needles (AcOH)
[融点]Mp 228 ℃
[比旋光度]:[α]$_D$ -20 (H$_2$O)

----------文 献----------

Paris, R.R., Ann. Pharm. Fr., 1959, 17, 331, (Primulaflavonoside)

§ 3,4',5,7-Tetrahydroxy-3'-methoxyflavone; 3-*O*-[α-L-Rhamnopyranosyl-(1→6)-β-D-galactopyranoside]
[化学名・別名]Keioside. Isorhamnetin 3-robinobioside
[CAS No.]107740-46-5
[化合物分類]フラボノイド(Flavonols; 5 × O-置換基)
[構造式]
[分子式]$C_{28}H_{32}O_{16}$
[分子量]624.551
[基原]次の植物から分離: *Campanula glomerata*, *Gomphrena martiana*, *Primula officinalis*, *Convallaria keiskei*, *Pyrus communis*, *Opuntia lindheimeri*
[性状]黄色の針状結晶 (EtOH 溶液)
[融点]Mp 183-186 ℃ (178-181 ℃)

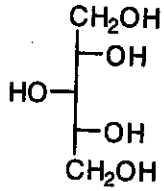


[比旋光度]:[α]$_D^{20}$ -21.4 (c, 0.84 in MeOH)
UV: [neutral] λ $_{max}$ 255 ; 267 ; 356 (MeOH) (Berdy) [base] λ $_{max}$ 273 ; 412 (MeO*H*-NAOH) (Berdy)

----------文 献----------

Heap, T., J.C.S., 1926, 2336-2344, (Isorhamnetin, 合成法)
Kuhn, R., Chem. Ber., 1948, 81, 363-367, (Isorhamnetin, 分離)

§ Xylitol (CAS 名)



[化学名・別名]Xylite. Xyliton. E967. Klinit. Kylit
[CAS No.]87-99-0
[その他の CAS No.]16277-71-7
[化合物分類]薬物: (Excipient), 炭水化物 (Pentitols)
[構造式]
[分子式]$C_5H_{12}O_5$
[分子量]152.147
[基原]マッシュルーム *Psalliota campestris*, *Primula officinalis* の根. Prod. industrially by redn. of Xylose obt. from wood cellulose
[用途]Nutritive sweetener. Sweetening agent used in sugar free sweets and chewing gums and pharmaceuticals
[性状]Two forms: metastable, rhombic cryst. and stable, monoclinic cryst.
[融点]Mp 61-61.5 ℃ (metastable). Mp 93-94.5 ℃ (stable)
[溶解性]BERDY SOL: ヘキサンに難溶
[その他のデータ]光学不活性 (*meso-*)
[傷害・毒性]50 %致死量 (LD_{50}) (マウス, 経口) 22000 mg/kg; 胃腸への逆作用効果 (大量投与時) ; BERDY HAZD : 50 %致死量 (LD_{50}) (マウス, 経口) 22000 mg/kg
[化学物質毒性データ総覧 (RTECS) 登録番号]ZF0800000
[販売元]Aldrich:85158-2; Fluka:95649; Supelco:4-6927

----------文 献----------

Xylitol, Int. Symp., (Ed. Counsell, J.N.), Applied Science Publishers, London, 1978, (専門書)

***RTECS (化学物質毒性データ) ***

生体影響物質 : 変異原性物質.

健康障害に関するデータ

急性毒性に関するデータ

<<試験方法>> LD50 試験 (50%致死量試験).
曝露経路 : 経口投与.
被験動物 : げっ歯類-ラット.
投与量・期間 : 16500 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

Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) 297,1990

<<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-ラット.
投与量・期間 : >25 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

Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) 297,1990

<<試験方法>> LD50 試験 (50%致死量試験).
曝露経路 : 静脈内投与.
被験動物 : げっ歯類-ラット.
投与量・期間 : 10800 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

Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) 297,1990

<<試験方法>> LD50 試験 (50%致死量試験).
曝露経路 : 筋肉内投与.
被験動物 : げっ歯類-ラット.
投与量・期間 : 15 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

Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) 297,1990

〈〈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：12500 mg/kg
毒性影響　　：〔行動〕全身麻痺.
〔胃腸〕胃の潰瘍または出血.
〔肝臓〕その他の変化.

参照文献

Gigiena i Sanitariya. For English translation, see HYSAAV. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) 36(2),25,1971

〈〈試験方法〉〉 認知されている最低致死量に関する試験

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：22100 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

Russian Pharmacology and Toxicology (English Translation). Translation of FATOAO. (Euromed Pub., 33, Woodlands Rd., Surbiton, Surrey, UK) 34,124,1971

〈〈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：18300 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

Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) 297,1990

〈〈試験方法〉〉 LD50 試験(50%致死量試験).

曝露経路　　：静脈内投与.
被験動物　　：げっ歯類-マウス.
投与量・期間：8500 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

Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) 352,1995

〈〈試験方法〉〉 LD50 試験(50%致死量試験).

曝露経路　　：筋肉内投与.
被験動物　　：げっ歯類-マウス.
投与量・期間：10200 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

Drugs in Japan (Ethical Drugs). (Yakugyo Jiho Co., Ltd., Tokyo, Japan) 297,1990

〈〈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-ウサギ.
投与量・期間：25 gm/kg
毒性影響　　：〔行動〕全身麻痺.
〔胃腸〕胃の潰瘍または出血.
〔肝臓〕その他の変化.

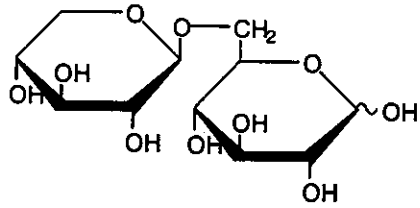
参照文献

Gigiena i Sanitariya. For English translation, see HYSAAV. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) 36(2),25,1971

〈〈試験方法〉〉 LD50 試験(50%致死量試験).

曝露経路　　：静脈内投与.
被験動物　　：げっ歯類-ウサギ.
投与量・期間：4 gm/kg
毒性影響　　：〔生化学〕[代謝 (中間)] その他

参照文献
Federation Proceedings, Federation of American Societies for Experimental Biology. (Bethesda, MD) 31,726,1972

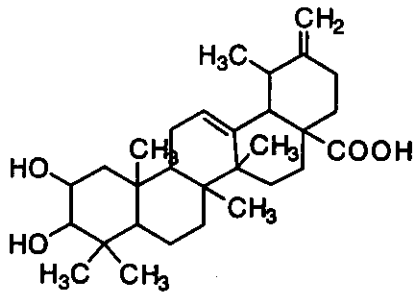
§ 6-*O*-β-D-Xylopyranosyl-D-glucose (CAS 名) (旧 CAS 名)
[化学名・別名]*O*-β-D-Xylopyranosyl-[1 → 6]-D-glucopyranose. Primeverose (CAS 名). Primverose
[CAS No.]26531-85-1
[化合物分類]炭水化物(Disaccharides)
[構造式]

[分子式]$C_{11}H_{20}O_{10}$
[分子量]312.273
[基原]a number of naturally occurring phenolic glycosides such as Primeverin and Primulaverin from *Primula officinalis*
[融点]Mp 194-197 ℃. Mp 210 ℃で分解
[比旋光度]:$[\alpha]_D^{20}$ +23.8 → -3.4 (c, 2.5 in H_2O)
[その他のデータ]甘味を呈する

----------文 献----------
Tollens, B. et al., Kurzes Handbuch der Kohlenhydrate, Edwards Bros. Inc., Ann Arbor, 4th Ed., 1935, 425
Begbie, R. et al., Carbohydr. Res., 1966, 2, 272, (分離, 構造決定)

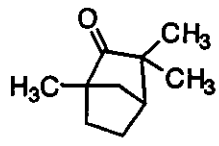
***********プルネラ (Prunella, Self-heal) ***********

§§シソ科ウツボグサ(*Prunella vulgaris* L. var. *lilacina* Nakai (*P. vulgaris* L. subsp. *asiatica* (Nakai) Hara))の花, 葉, 種子。
本調査研究では、成分に関する文献はなかった。

§§シソ科セイヨウウツボグサ(*Prunella vulgaris* L.)の花, 葉, 種子。

§ 2,3-Dihydroxy-12,20(30)-ursadien-28-oic acid; (2 α,3 α)-form
[化合物分類]テルペノイド(Ursane triterpenoids)
[構造式]

[分子式]$C_{30}H_{46}O_4$
[分子量]470.691
[基原]*Prunella vulgaris*
[性状]針状結晶(MeOH) (as Me ester)
[融点]Mp 128-129 ℃ (Me ester)
[比旋光度]:$[\alpha]_D^{23}$ +128 (c, 0.3 in $CHCl_3$) (Me ester)

----------文 献----------
Kojima, H. et al., Phytochemistry, 1987, 26, 1107
Singh, C., Phytochemistry, 1990, 29, 2348, (分離, H-NMR, C13-NMR)
Lee, C.-K. et al., Phytochemistry, 1998, 49, 1119-1122, (3-hydroxycinnamoyl)
Sanoko, R. et al., Phytochemistry, 1999, 51, 1043-1047, (Alternanthera repens saponins)

§ Fenchone; (+)-form
[CAS No.]7787-20-4
[化合物分類]テルペノイド(Fenchane monoterpenoids)
[構造式]

[分子式]$C_{10}H_{16}O$
[分子量]152.236
[基原]植物に広く分布する, 例えば, ウイキョウ(*Foeniculum vulgare*), *Blumea lacera*, *Prunella vulgaris*
[用途]脱水素機構における水素の受容体として用いることができる. 香料原料
[性状]樟脳臭を持つオイル
[融点]Mp 3-5 ℃. 凝固点:Fp 5-6 ℃
[沸点]Bp 193.5 ℃
[比旋光度]:$[\alpha]_D^{29}$ +63. $[\alpha]_D^{21}$ +48 (c, 0.2 in CCl_4)

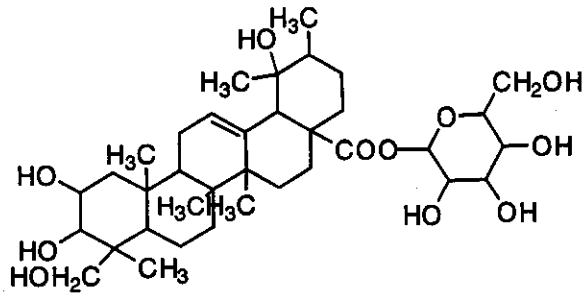
[溶解性]水に難溶, エタノールに易溶; BERDY SOL: メタノール, ヘキサンに可溶; 水に難溶
[販売元]Aldrich:W50770-9; Fluka:46200; Rare Chemicals Library:S57022-2

----------文 献----------

Opdyke, D.L.J., Food Cosmet. Toxicol., 1976, 14, 769, (レビュー, 毒性)
Wijekoon, W.M.D. et al., J. Phys. Chem., 1983, 87, 3034, (H-NMR, C13-NMR, UV, CD)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 278, (レビュー)

§ 2,3,19,24-Tetrahydroxy-12-ursen-28-oic acid; (2 α,3 α)-form, β-D-Glucopyranosyl ester

[化学名・別名]Pruvuloside B
[CAS No.]153753-66-3
[化合物分類]テルペノイド(Ursane triterpenoids)
[構造式]



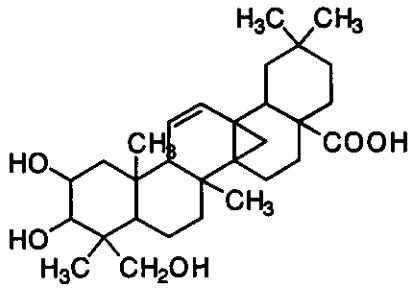
[分子式]$C_{36}H_{58}O_{11}$
[分子量]666.848
[基原]*Prunella vulgaris*, *Rosa transmorrisonensis*, *Rubus xanthocarpus*
[性状]無定型の粉末
[融点]Mp 226-228 ℃
[比旋光度]:$[\alpha]_D^{20}$ -27 (c, 0.32 in MeOH)

----------文 献----------

Sakakibara, J. et al., Phytochemistry, 1983, 22, 2547-2552, (2 α,3 α-form)
Yamagishi, T. et al., Phytochemistry, 1988, 27, 3213-3216, (Hyptatic acid B)
Kojima, H. et al., Phytochemistry, 1989, 28, 1703-1710, (H-NMR, 構造決定)
Kao, S.-F. et al., J. Chin. Chem. Soc. (Taipei), 1993, 40, 597, (glucosyl ester)
Zhang, Y.-J. et al., CA, 1996, 124, 170601t, (Pruvuloside B)

§ 2,3,24-Trihydroxy-13,27-cyclo-11-oleanen-28-oic acid; (2 α,3 α,13 α)-form

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



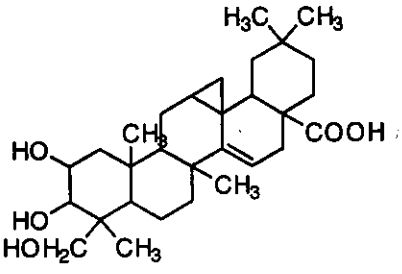
[分子式]$C_{30}H_{46}O_5$
[分子量]486.69
[基原]*Prunella vulgaris*
[性状]結晶(MeOH) (as Me ester)
[融点]Mp 310 ℃ (Me ester)
[比旋光度]:$[\alpha]_D^{24}$ +21.2 (c, 0.17 in $CHCl_3$) (Me ester)

----------文 献----------

Kojima, H. et al., Phytochemistry, 1988, 27, 2921

§ 2,3,24-Trihydroxy-12,27-cyclo-14-taraxeren-28-oic acid; (2 α,3 α)-form

[CAS No.]117581-15-4
[化合物分類]テルペノイド(Nor-, seco- and cyclotaraxerane triterpenoids)
[構造式]



[分子式]$C_{30}H_{46}O_5$
[分子量]486.69
[基原]*Prunella vulgaris*
[性状]結晶(MeOH) (as Me ester)
[融点]Mp 276-278 ℃ (Me ester)
[比旋光度]:$[\alpha]_D^{24}$ +24 (c, 0.5 in $CHCl_3$) (Me ester)

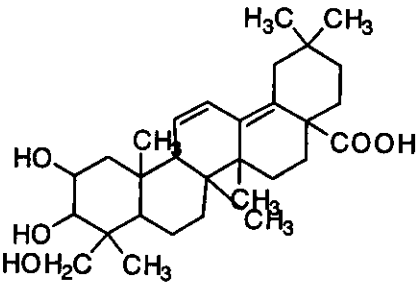
----------文 献----------

Wang, N. et al., Phytochemistry, 1988, 27, 299
Kojima, H. et al., Phytochemistry, 1988, 27, 2921

§ 2,3,24-Trihydroxy-11,13(18)-oleanadien-28-oic acid; (2 α,3 α)-form

[化合物分類]テルペノイド(Oleanane triterpenoids)

[構造式]

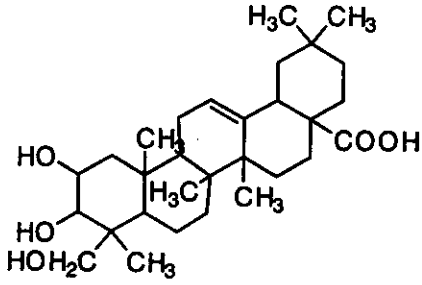


[分子式] $C_{30}H_{46}O_5$
[分子量] 486.69
[基原] *Prunella vulgaris*
[性状] 針状結晶 (MeOH) (as Me ester)
[融点] Mp 267-269 ℃ (Me ester)
[比旋光度]: $[\alpha]_D^{24}$ -156 (c, 0.3 in $CHCl_3$) (Me ester)

----------文 献----------

Kojima, H. et al., Phytochemistry, 1987, 26, 1107

§ 2,3,23-Trihydroxy-12-oleanen-28-oic acid; (2 α,3 β)-form

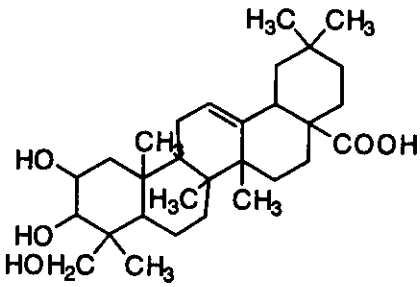


[化学名・別名] Arjunolic acid
[CAS No.] 465-00-9
[化合物分類] テルペノイド (Oleanane triterpenoids)
[構造式]
[分子式] $C_{30}H_{48}O_5$
[分子量] 488.706
[基原] *Terminalia arjuna*, *Tristania conferta*, *Prunella vulgaris*, *Polygala japonica*, *Metrosideros umbellata*, *Psidium guajava*, *Mitragyna ciliata*, その他
[性状] 結晶 (Me_2CO)
[融点] Mp 337-340 ℃
[比旋光度]: $[\alpha]_D^{19}$ +63.5 (c, 0.5 in EtOH)

----------文 献----------

Kojima, H. et al., Phytochemistry, 1986, 25, 729; 1989, 28, 1703, (H-NMR, 構造決定, Arjunolic acid)
Ara acute u jo, F.W.L. et al., J. Nat. Prod., 1990, 53, 1436, (Arjunolic acid)
Tripathi, V.K. et al., Phytochemistry, 1992, 31, 349, (Arjunolitin)
Liang, L. et al., Yaoxue Xuebao, 1993, 28, 836; CA, 120, 101999j, (Arjunolic acid 3-glucoside)

§ 2,3,24-Trihydroxy-12-oleanen-28-oic acid; (2 α,3 α)-form

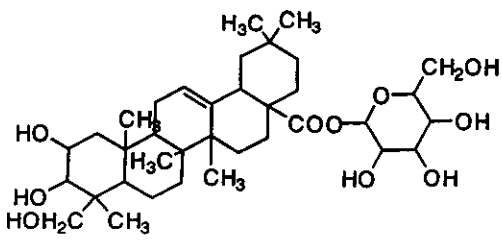


[CAS No.] 88586-19-0
[化合物分類] テルペノイド (Oleanane triterpenoids)
[構造式]
[分子式] $C_{30}H_{48}O_5$
[分子量] 488.706
[基原] 次の植物から分離: *Polygala japonica*, *Prunella vulgaris*
[性状] 結晶 (MeOH) (as Me ester)
[融点] Mp 280-282 ℃ (Me ester)
[比旋光度]: $[\alpha]_D^{27}$ +59.6 (c, 1 in $CHCl_3$) (Me ester)

----------文 献----------

Kojima, H. et al., Phytochemistry, 1986, 25, 729; 1987, 26, 1107, (分離, 構造決定, C13-NMR)
Ngounou, F.N. et al., Phytochemistry, 1987, 26, 3080, (分離, 構造決定)
Yamagishi, T. et al., Phytochemistry, 1988, 27, 3213, (分離, 結晶構造)
Sashida, Y. et al., Phytochemistry, 1994, 35, 377, (分離, H-NMR, C13-NMR)
Maeda, C. et al., Phytochemistry, 1994, 37, 1131, (Scheffoleoside F)
Tian, J. et al., Yaoxue Xuebao, 2000, 35, 29-31, (Vulgarsaponin A)

§ 2,3,24-Trihydroxy-12-oleanen-28-oic acid; (2 α,3 α)-form, 28-*O*-β-D-Glucopyranosyl ester



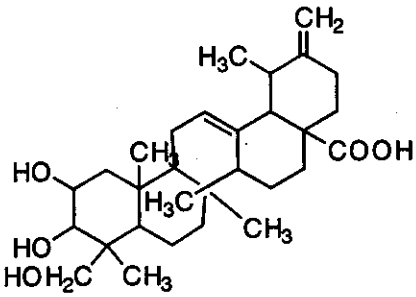
[化学名・別名] Vulgarsaponin A
[CAS No.] 274673-56-2
[化合物分類] テルペノイド (Oleanane triterpenoids)
[構造式]
[分子式] $C_{36}H_{58}O_{10}$
[分子量] 650.848

[基原]*Prunella vulgaris*
[比旋光度]:[α]$_D^{25}$ +28.6 (MeOH)

----------文 献----------

Tian, J. et al., Yaoxue Xuebao, 2000, 35, 29-31, (Vulgarsaponin A)

§ 2,3,24-Trihydroxy-12,20(30)-ursadien-28-oic acid; (2 α,3 α)-form
[化合物分類]テルペノイド(Ursane triterpenoids)
[構造式]

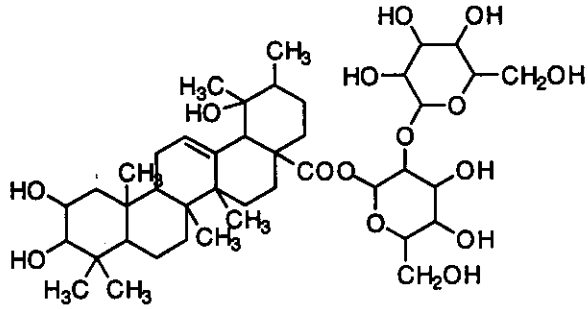


[分子式]$C_{30}H_{46}O_5$
[分子量]486.69
[基原]次の植物から分離: *Prunella vulgaris*
[性状]針状結晶(MeOH) (as Me ester)
[融点]Mp 212-213 ℃ (Me ester)
[比旋光度]:[α]$_D^{19}$ +121.2 (c, 0.5 in $CHCl_3$) (Me ester)

----------文 献----------

Kojima, H. et al., Phytochemistry, 1987, 26, 1107

§ 2,3,19-Trihydroxy-12-ursen-28-oic acid; (2 α,3 α,19 α)-form, 28-*O*-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl] ester
[化学名・別名]Pruvuloside A
[CAS No.]173933-45-4
[化合物分類]テルペノイド(Ursane triterpenoids)
[構造式]

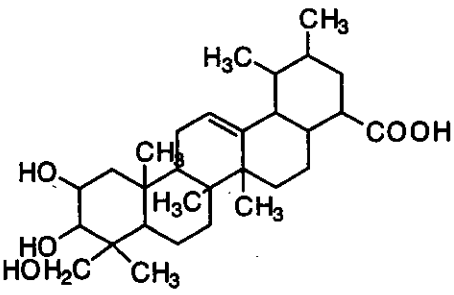


[分子式]$C_{42}H_{68}O_{15}$
[分子量]812.99
[基原]*Prunella vulgaris*

----------文 献----------

Zhang, Y.J. et al., CA, 1996, 124, 170601t, (Pruvuloside A)

§ 2,3,23-Trihydroxy-12-ursen-28-oic acid; (2 α,3 α)-form
[化学名・別名]Esculentic acid ‡. Dammarolic acid
[CAS No.]76964-07-3
[化合物分類]テルペノイド(Ursane triterpenoids)
[構造式]



[分子式]$C_{30}H_{48}O_5$
[分子量]488.706
[基原]*Nepeta hindostana*, *Diplazium esculentum*, *Hedyotis lawsoniae*, *Prunella vulgaris*
[性状]結晶(MeOH)
[融点]Mp 270 ℃
[比旋光度]:[α]$_D$ +51 (EtOH)
[その他のデータ]The sample from *N. hindostana* was originally assigned the (2 β,3 α)-config.

----------文 献----------

Polonsky, J. et al., Bull. Soc. Chim. Fr., 1959, 880; 1961, 1586, (分離, 構造決定)
Singh, B. et al., Phytochemistry, 1969, 8, 917, (分離)
Ahmad, V.U. et al., Phytochemistry, 1986, 25, 1487, (分離)
Furuya, T. et al., Phytochemistry, 1987, 26, 715, (分離, H-NMR, C13-NMR)
Sashida, Y. et al., Phytochemistry, 1992, 31, 2801, (誘導体)