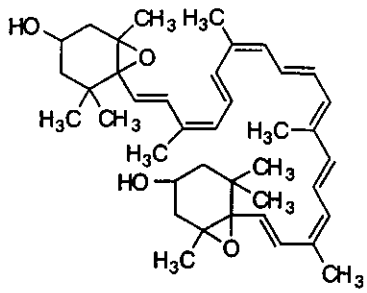
§ Violaxanthin; (13Z)-form
[CAS No.]75715-58-1
[化合物分類]テルペノイド(Tetraterpenoids)
[構造式]

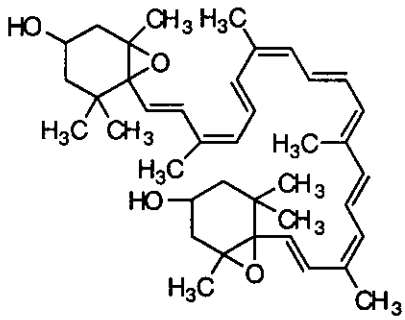


[基原]*Viola tricolor*
[性状]淡黄色の板状結晶(C_6H_6/petrol)
[融点]Mp 108 ℃
[UV]:[neutral] λ_{max} 337 (log ε 4.77); 419 (log ε 4.91); 445 (log ε 5.06); 475 (log ε 5) (C_6H_6)

----------文献----------

Stransky, H. et al., Arch. Microbiol., 1970, 71, 164, (分離, deoxy)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1842, (生育)
Koreeda, N. et al., J.A.C.S., 1973, 95, 239, (絶対構造)
Sapozhnikov, D.I., Pure Appl. Chem., 1973, 35, 47, (レビュー)
Molnár, P. et al., Phytochemistry, 1980, 19, 623, (mono-*cis* isomers)
Molnár, P. et al., Phytochemistry, 1986, 25, 195, (分離)
Straub, O. et al., Key to Carotenoids, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 259, (成書)

§ Violaxanthin; (15Z)-form
[CAS No.]24620-97-1
[化合物分類]テルペノイド(Tetraterpenoids)
[構造式]



[基原]*Viola tricolor*
[性状]黄色の結晶 (C_6H_6/petrol)
[融点]Mp 109 ℃
[UV]:[neutral] λ_{max} 337 (log ε 4.77); 423 (log ε 4.83); 448 (log ε 4.98); 479 (log ε 4.91) (C_6H_6)

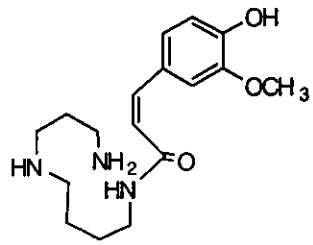
----------文献----------

Stransky, H. et al., Arch. Microbiol., 1970, 71, 164, (分離, deoxy)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1842, (生育)
Koreeda, N. et al., J.A.C.S., 1973, 95, 239, (絶対構造)
Sapozhnikov, D.I., Pure Appl. Chem., 1973, 35, 47, (レビュー)
Lessertois, D. et al., Phytochemistry, 1978, 17, 411, (分離, deoxy)
Molnár, P. et al., Phytochemistry, 1980, 19, 623, (mono-*cis* isomers)
Molnár, P. et al., Phytochemistry, 1986, 25, 195, (分離)
Straub, O. et al., Key to Carotenoids, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 259, (成書)

*********パイナップル (Pineapple) *********

§§パイナップル科パイナップル(*Ananas comosus* Merrill)の果実。

§ 4-Coumaroylspermidine; 3'-Methoxy
[化学名・別名]Feruloylspermidine
[CAS No.]70185-60-3
[化合物分類]アルカロイド化合物(Acyclic spermidine alkaloids)
[構造式]



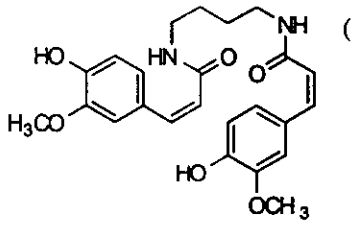
[分子式]$C_{17}H_{27}N_3O_3$
[分子量]321.419
[正確な分子量]321.205242

[基原]次の植物から得られるアルカロイド: *Ananas comosus*, *Lycopersicon esculentum*（パイナップル科, ナス科）

----------文献----------

Deleacutetang, J., Ann. Tab., Sect. 2, 1974, 11, 123; CA, 84, 147656m,（構造決定）
Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927,（生育）

§ Di-4-coumaroylputrescine; 3,3'-Dimethoxy

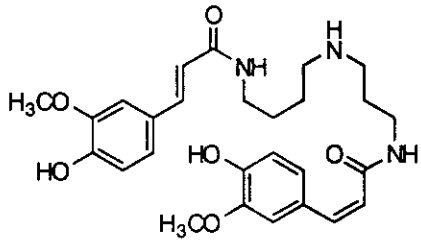


[化学名・別名]Diferuloylputrescine. *N*,*N'*-Bis 4-hydroxy-3-methoxycinnamoyl)-1,4-butanediamine
[CAS No.]42369-86-8
[化合物分類]アルカロイド化合物(Putrescine alkaloids)
[構造式]
[分子式]$C_{24}H_{28}N_2O_6$
[分子量]440.495
[正確な分子量]440.194738
[基原]次の植物から得られるアルカロイド: *Ananas comosus*, *Triticum vulgare*, *Gomphrena globosa*, *Dianthus caryophyllus*, *Vicia faba*, *Lycopersicon esculentum*, *Petunia* sp., *Nicotiana tabacum*（パイナップル科, イネ科, ヒユ科, ナデシコ科, マメ科, ナス科）

----------文献----------

Martin-Tanguy, J. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1973, 276, 1433,（UV, 構造決定, 合成法, Diferuloylputrescine）
Cabanne, F. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1976, 282, 1959,（UV, 構造決定, Dicaffeoylputrescine）
Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927,（生育, 誘導体）

§ N^1,N^{10}-Dicoumaroylspermidine; 3',3''-Dimethoxy

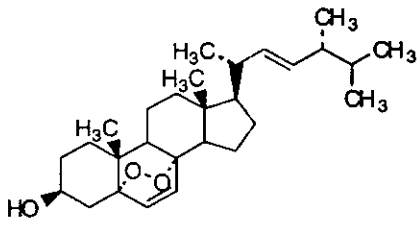


[化学名・別名]N^1,N^{10}-Diferuloylspermidine
[CAS No.]70185-61-4
[化合物分類]アルカロイド化合物(Acyclic spermidine alkaloids)
[構造式]
[分子式]$C_{27}H_{35}N_3O_6$
[分子量]497.59
[正確な分子量]497.252587
[基原]次の植物から得られるアルカロイド: *Corylus avellana* の花粉, また *Ananas comosus*, *Dianthus caryophyllus*, *Vicia faba* and *Lunaria esculentum*（Corylaceae, パイナップル科, ナデシコ科, マメ科, ナス科）

----------文献----------

Deleacutetang, J., Ann. Tab., Sect. 2, 1974, 11, 123; CA, 84, 147656m,（UV, H-NMR, 構造決定, Dicaffeoylspermidine）
Cabanne, F. et al., Physiol. Veg., 1977, 15, 429; CA, 88, 86095m,（UV, 構造決定）
Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927,（生育）
Meurer, B. et al., Phytochemistry, 1986, 25, 433,（Caffeoylferuloylspermidine, Diferuloylspermidine）

§ Ergosterol peroxide



[化学名・別名]5,8-Epidioxy-5 α,8 α-ergosta-6,22*E*-dien-3 β-ol. 5 α,8 α-Peroxygosterol
[CAS No.]2061-64-5
[化合物分類]ステロイド(Vitamin D2 (ergocalciferol). metabolites and analogces)., ステロイド(Ergostane steroids;excluding withanolides and brassinolides). (C28).
[構造式]
[分子式]$C_{28}H_{44}O_3$
[分子量]428.654
[正確な分子量]428.329045
[基原]カビと苔に広く分布する. また *Ananas comosus* の葉, *Ajuga remota*, 海綿 *Axinella cannabina*, *Typha latifolia*, その他の生物学的基原

[用途]Active against mycobacterium tuberculosis. 強い抗腫瘍作用
[性状]結晶(MeOH)
[融点]Mp 181.5-183 ℃ (176-198 ℃)
[比旋光度]:[α]$_D$ -29 (c, 0.8 in $CHCl_3$)
[化学物質毒性データ総覧(RTECS)登録番号]KE7289000

----------文献----------

Windaus, A. et al., Annalen, 1928, 460, 225, (分離)
Windaus, A., Z. Phys. Chem., 1942, 276, 280, (分離, 構造決定)
Wieland, P. et al., Helv. Chim. Acta, 1947, 30, 1028, (分離)
Bauslaugh, G. et al., Nature (London), 1964, 202, 1218, (分離)
Takahashi, R. et al., Phytochemistry, 1972, 11, 1850, (分離)
Della Greca, M. et al., Gazz. Chim. Ital., 1990, 120, 391, (分離, H-NMR, C13-NMR, 成書)
Bok, J.W. et al., Phytochemistry, 1999, 51, 891, (配糖体)
Cantrell, C.L. et al., Planta Med., 1999, 65, 732, (分離, 活性)

*****RTECS (化学物質毒性データ) *****

生体影響物質　　: 生殖影響物質. ホルモン.

*****健康障害に関するデータ*****

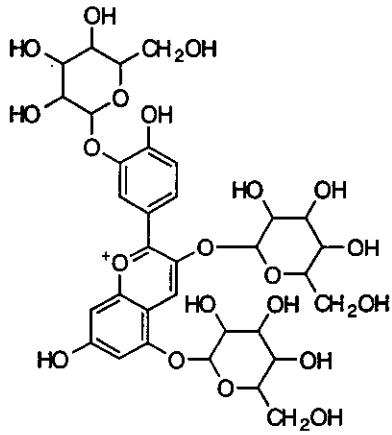
*****生殖に関するデータ*****

〈〈試験方法〉〉 最小毒性量(TDLo)試験.
曝露経路　　: 経口投与.
被験動物　　: げっ歯類-マウス
投与　　: 30 mg/kg
雌雄投与期間 : 雌 1 日間(交配後)
毒性影響　　: 〔生殖〕 [受精能]着床前死亡率. (e.g. reduction in number of implants per female; total number of implants per corpora lutea)
参照文献
JRPFA4 Journal of Reproduction and Fertility. (Biochemical Soc. Book Depot, POB 32, Commerce Way, Colchester, Essex CO2 8HP, UK) V.1- 1960- [Vol.,頁,年(19-)]46,461,1976

〈〈試験方法〉〉 最小毒性量(TDLo)試験.
曝露経路　　: 経口投与.
被験動物　　: げっ歯類-マウス
投与　　: 60 mg/kg
雌雄投与期間 : 雌 6-7 日間(交配後)
毒性影響　　: 〔生殖〕 [受精能]流産.
参照文献
JRPFA4 Journal of Reproduction and Fertility. (Biochemical Soc. Book Depot, POB 32, Commerce Way, Colchester, Essex CO2 8HP, UK) V.1- 1960- [Vol.,頁,年(19-)]46,461,1976

§ 3,3',4',5,7-Pentahydroxyflavylium(1+); 3,3',5-Tri-*O*-β-D-glucopyranoside

[化学名・別名]Cyanidin 3,3',5-triglucoside
[CAS No.]88110-66-1
[化合物分類]フラボノイド(Anthocyanidins and anthocyanins; 5 × O-置換基)
[構造式]



[分子式]$C_{33}H_{41}O_{21}^{(+)}$
[分子量]773.674
[正確な分子量]773.21404
[基原]次の植物から分離: パイナップル科, 例えば, *Ananas comosus*

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1713; 1715; 1716, (生育)

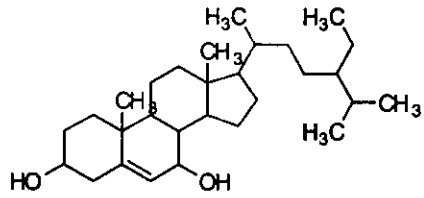
Iacobucci, G.A. et al., Tetrahedron, 1983, 39, 3005, (レビュー)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Tamura, H. et al., Agric. Biol. Chem., 1989, 53, 1971, (誘導体)

§ Spermine; Bis(4-hydroxy-3-methoxycinnamoyl)
[化学名・別名]Diferuloylspermine
[CAS No.]70208-06-9
[化合物分類]アルカロイド化合物(Alkaloids 構造は一部又は全てが未知), アルカロイド化合物(Acyclic spermine alkaloids)
[構造式]有効な構造式はない
[分子式]$C_{30}H_{42}N_4O_6$
[分子量]554.685
[正確な分子量]554.310436
[基原]次の植物から得られるアルカロイド: *Ananas comosus*, *Gomphrena globosa*
[その他のデータ]正確な構造式は未知.

----------文献----------

Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927, (Diferuloylspermine, Disinapoylspermine)
Polyamines in the Gastrointestinal Tract, (eds. Dowling, R.H. et al), Kluwer Academic Publishers, Dordrecht, 1992, (専門書)

§ Stigmast-5-ene-3,7-diol; (3 β,7 α,24*R*)-form
[化学名・別名]Ikshusterol. 7 α-Hydroxysitosterol
[CAS No.]34427-61-7
[化合物分類]薬物: 抗フイブリノゲン薬(Antifibrinogens), ステロイド(Stigmastane steroids). (C29).
[構造式]

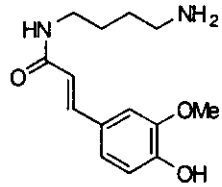


[基原]サトウキビ(*Saccharum officinarum*), 次の植物の葉: *Ananas comosus*, *Spatholobus suberetus*, 海綿 *Corallistes undulatus*
[用途]繊維素溶解薬
[性状]結晶(MeOH)
[融点]Mp 129-133 ℃ (202-204 ℃)
[比旋光度]:[α]$_D$ -27 ($CHCl_3$)

----------文献----------

Das, B. et al., Phytochemistry, 1992, 31, 2427; 4371, (Poriferast-5-ene-3,7-diol)

§ Subaphylline
[化学名・別名]*N*-(4-Hydroxy-3-methoxycinnamoyl)-1,4-butanediamine. Feruloylputrescine
[CAS No.]501-13-3
[化合物分類]アルカロイド化合物(Putrescine alkaloids)
[構造式]



[分子式]$C_{14}H_{20}N_2O_3$
[分子量]264.324
[正確な分子量]264.147393
[基原]次の植物から得られるアルカロイド: *Ananas comosus*, *Pennisetum*, *Triticum*, *Gomphrena*, *Salix*, *Persea*, その他の属(パイナップル科, イネ科, ヒユ科, ヤナギ科, クスノキ科, ナス科, ミカン科, アカザ科). Also isol. from elicitor-treated cell suspension cultures and fungus-infected leaves of *Solanum tuberum* (ナス科)
[性状]結晶(C_6H_6 or MeOH)
[融点]Mp 171.5-172 ℃
[化学物質毒性データ総覧(RTECS)登録番号]GD6981000

----------文献----------

Ryabinin, A.A. et al., Dokl. Akad. Nauk SSSR, 1949, 67, 513; 1951, 76, 689; CA, 44, 1455h; 45, 8479d, (分離, 構造決定)
Wheaton, T.A. et al., Nature (London), 1965, 206, 620, (分離, UV, IR, Mass, 構造決定)
Stoessl, A. et al., Tet. Lett., 1969, 2807, (Feruloyl-2-hydroxyputrescine)

Mizusaki, S. et al., Phytochemistry, 1971, 10, 1347, (分離, 合成法)
Keller, H. et al., Phytochemistry, 1996, 42, 389, (分離, H-NMR)

***RTECS (化学物質毒性データ) ***

生体影響物質　　: 医薬品.

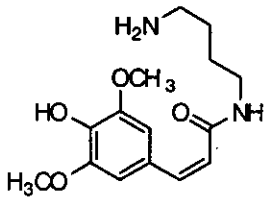
健康障害に関するデータ

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　　: 腹腔内投与
被験動物　　: げっ歯類-マウス
投与量・期間 : 225 mg/kg
毒性影響　　: 〔行動〕筋収縮または痙直.
〔血管〕自律性の切断を伴わない血圧の低下.
参照文献

FATOAO Farmakologiya i Toksikologiya (Moscow). For English translation, see PHTXA6 and RPTOAN. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) V.2- 1939- [Vol.,頁,年(19-)]18 (6),9,1955

§ Subaphylline; 5'-Methoxy
[化学名・別名]Sinapoylputrescine. *N*-(3,4-Dihydroxy-5-methoxycinnamoyl)-1,4-butanediamine
[CAS No.]70185-57-8
[化合物分類]アルカロイド化合物(Putrescine alkaloids)
[構造式]



[分子式]$C_{15}H_{22}N_2O_4$
[分子量]294.35
[正確な分子量]294.157958
[基原]次の植物から得られるアルカロイド: *Ananas comosus*, *Lilium* sp. (パイナップル科, ユリ科)

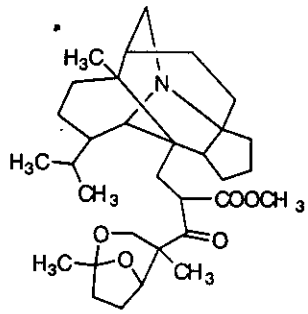
----------文献----------

Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927, (生育, Subaphylline, Sinapoylputresine)
Keller, H. et al., Phytochemistry, 1996, 42, 389, (分離, H-NMR)

*********ハイビスカス (Hibiscus, Roselle) *********

§§ アオイ科ロゼル(*Hibiscus sabdariffa* L.)の萼と総苞弁。

§ Daphnimacropine; 16-Deoxy, 22-acetoxy
[化学名・別名]Daphniphylline. Daphniphyllamine
[CAS No.]15007-67-7
[化合物分類]アルカロイド化合物(Daphniphylline alkaloids)
[構造式]



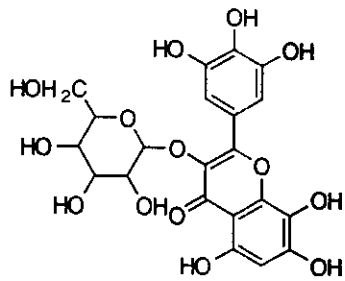
[分子式]$C_{32}H_{49}NO_5$
[分子量]527.743
[正確な分子量]527.361074
[基原]次の植物から得られる主なアルカロイドの一つ: *Daphniphyllum macropodum*, *Daphniphyllum teijsmanni*. また次の植物からも分離される: *Daphniphyllum gracile* の樹皮, *Hibiscus sabdariffa* の乾燥萼と包葉 (ユズリハ科, アオイ科)
[性状]非結晶性

----------文献----------

Sakabe, N. et al., Tet. Lett., 1966, 965, (Daphniphylline)
Sasaki, K. et al., J.C.S.(B), 1971, 1565, (Daphniphylline, 絶対構造)
Toda, M. et al., Tetrahedron, 1974, 30, 2683, (Daphniphylline)

Yamamura, S. et al., Chem. Lett., 1980, 393, (Daphniphylline)
Morita, H. et al., Tetrahedron, 1999, 55, 12549, (Daphnezomine E)

§ 3,3',4',5,5',7,8-Heptahydroxyflavone; 3-*O*-β-D-Glucopyranoside



[化学名・別名]Hibiscitrin
[化合物分類]フラボノイド(Flavonols; 7 × O-置換基)
[構造式]
[分子式]$C_{21}H_{20}O_{14}$
[分子量]496.381
[正確な分子量]496.08531
[基原]次の植物から得られる配糖体: *Hibiscus sabdariffa*
[性状]結晶(EtOH)
[融点]Mp 238-240 ℃

----------文献----------

Rao, P.S. et al., Proc. - Indian Acad. Sci., Sect. A, 1942, 15, 148; 1948, 27, 209, (分離)
Chow, P.W. et al., Aust. J. Chem., 1968, 21, 2529, (分離, UV)
Whalen, M.D. et al., Phytochemistry, 1979, 18, 263, (誘導体)
Bohlmann, F. et al., Phytochemistry, 1979, 18, 1081, (分離, UV, IR, H-NMR)
Whalen, M.D. et al., Phytochemistry, 1983, 22, 2107, (分離, H-NMR, UV, Mass)
Fang, N. et al., Phytochemistry, 1985, 24, 2693; 1986, 25, 927, (分離)
Horie, T. et al., Phytochemistry, 1988, 27, 1491, (合成法, 構造決定)
Ferracin, R.J. et al., Phytochemistry, 1998, 47, 393, (Hydroxyhexamethoxyflavones)

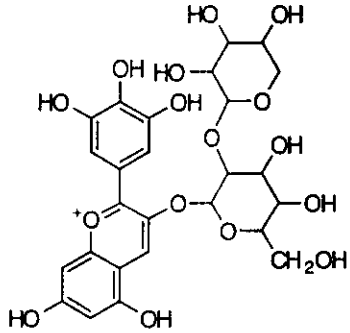
§ 3,3',4',5,5',7-Hexahydroxyflavylium(1+); 3-*O*-[4-Hydroxycinnamoyl-(→?)-[3,4,5-trihydroxybenzoyl-(→?)]-β-D-glucopyranoside]

[CAS No.]83063-59-6
[化合物分類]フラボノイド(Anthocyanidins and anthocyanins; 6 × O-置換基), フラボノイド(Flavonoids 構造は一部又は全てが未知)
[構造式]有効な構造式はない
[分子式]$C_{37}H_{31}O_{18}^{(+)}$
[分子量]763.641
[正確な分子量]763.151045
[基原]次の植物から分離: *Abrus precatorius*, *Hibiscus sabdariffa*

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1727; 1730; 1734; 1735; 1737; 1739, (Delphinidin, Myrtillin B, Hibiscin, Nasunin A, Gentianin, Delphinin)
Iacobucci, G.A. et al., Tetrahedron, 1983, 39, 3005, (レビュー)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Andersen, O.M., Phytochemistry, 1989, 28, 495, (Podocarpin A)

§ 3,3',4',5,5',7-Hexahydroxyflavylium(1+); 3-*O*-[β-D-Xylopyranosyl-(1 → 2)-β-D-glucopyranoside]



[化学名・別名]Delphinidin 3-sambubioside
[CAS No.]53158-73-9
[化合物分類]フラボノイド(Anthocyanidins and anthocyanins; 6 × O-置換基)
[構造式]

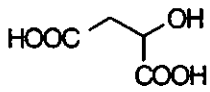
[分子式]$C_{26}H_{29}O_{16}^{(+)}$
[分子量]597.505
[正確な分子量]597.145565
[基原]次の植物から分離: *Abrus precatorius*, *Hibiscus sabdariffa*

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1727; 1730; 1734; 1735; 1737; 1739, (Delphinidin, Myrtillin B, Hibiscin, Nasunin A,

Gentianin, Delphinin)
Yoshitama, K. et al., Phytochemistry, 1977, 16, 591, (Delphin)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Andersen, O.M., Phytochemistry, 1989, 28, 495, (Podocarpin A)
Toki, K. et al., Phytochemistry, 1995, 39, 243; 1996, 42, 1055, (3-xylosylrhamnosylglucoside, Ranunculus anthocyanin)

§ 3,3',4',5,5',7-Hexahydroxyflavylium(1+); Glycoside
[化学名・別名]Hibiscin
[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(Anthocyanidins and anthocyanins; 6 × O-置換基)
[構造式]有効な構造式はない
[分子式]$C_{26}H_{29}O_{16}^{(+)}$
[分子量]597.505
[正確な分子量]597.145565
[基原]次の植物の果実から分離: *Hibiscus sabdariffa*
[性状]赤-茶色の針状結晶, もしくはプリズム結晶 (as chloride)
[融点]Mp 178 ℃ (chloride)
[その他のデータ]Hydrol. gives Delphinidin + 1 Glc and 1 pentose
----------文献----------
Rakhimkhanov, Z.B. et al., Khim. Prir. Soedin., 1970, 6, 129; Chem. Nat. Compd. (Engl. Transl.), 1970, 6, 123, (Cannabinidin)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1727; 1730; 1734; 1735; 1737; 1739, (Delphinidin, Myrtillin B, Hibiscin, Nasunin A, Gentianin, Delphinin)
Iacobucci, G.A. et al., Tetrahedron, 1983, 39, 3005, (レビュー)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Andersen, O.M., Phytochemistry, 1989, 28, 495, (Podocarpin A)

§ Malic acid; (*R*)-form
[化学名・別名]D-form
[CAS No.]636-61-3


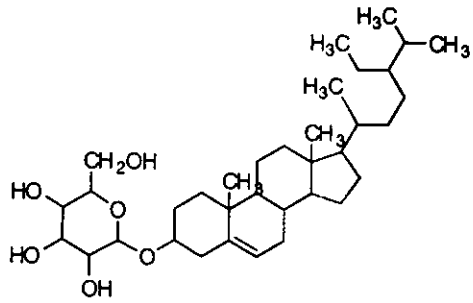
[化合物分類]炭水化物(Aldaric acids)
[構造式]
[基原] *Hibiscus sabdariffa*
[性状]結晶(Et_2O)
[融点]Mp 101 ℃ (97-99 ℃)
[比旋光度]:$[\alpha]_D$ +2.92 (MeOH). $[\alpha]_b^{20}$ +28.4 (c, 5.5 in Py) (>99.8% ee)
[溶解性]水, エタノール, アセトンに可溶
[PKa 値]pK_{a1} 5.26 (25 ℃, H_2O)
[化学物質毒性データ総覧(RTECS)登録番号]ON7260000
----------文献----------
Pratt, D.S., Philipp. J. Sci., 1912, 7, 201; Chem. Zentralbl., 1913, 645, (分離, R-form)
Rodd's Chem. Carbon Compd. (2nd edn.), 1976, 1E, 224, (レビュー)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, 13, 1063, (レビュー)
Eck, R. et al., Tetrahedron, 1994, 50, 13641, (合成法, R-form, S-form)

*****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-ウサギ.
投与量・期間 : 5500 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

IECHAD Industrial and Engineering Chemistry. (Washington, DC) V.15-62, 1923-70. For publisher information, see CHMTBL. [Vol.,頁,年(19-)]15,628,1923

§ Stigmast-5-en-3-ol; (3 β,24*R*)-form, *O*-β-D-Galactopyranoside



[CAS No.]55057-29-9
[その他の CAS No.]
[化合物分類]ステロイド(Stigmastane steroids). (C29).
[構造式]
[分子式]$C_{35}H_{60}O_6$
[分子量]576.855
[正確な分子量]576.43899
[基原]*Hibiscus sabdariffa*
[性状]結晶($CHCl_3$)
[融点]Mp 275-277 ℃
[比旋光度]:[α]$_D$ -63 (c, 0.52 in Py)

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2071, (生育)

***********麦芽 (Malt) ***********

§§イネ科オオムギ(*Hordeum vulgare* L.)の発芽種子。
「コウジ」参照

§§イネ科ジジョウオオムギ(*Hordeum vulgare* Linne var. *vulgare*)の発芽種子。
該当物質なし

***********ハコベ (Hakobe, Common chickweed) ***********

§§ナデシコ科ハコベ(*Stellaria media* Cry.)の全草。

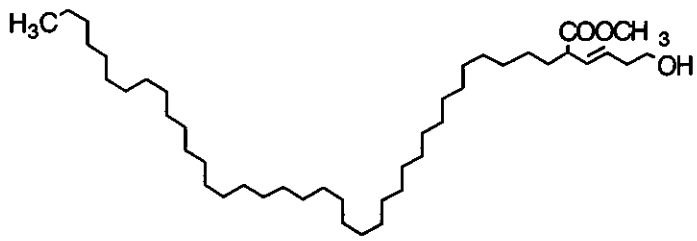
§ 6,7-Dimethylheptacosane
[CAS No.]165675-38-7
[化合物分類]脂肪族化合物(Branched aliphatic hydrocarbons)
[構造式] $H_3C(CH_2)_{19}CH(CH_3)CH(CH_3)(CH_2)_4CH_3$
[分子式]$C_{29}H_{60}$
[分子量]408.793
[正確な分子量]408.4695
[基原]*Stellaria media*
[融点]Mp 60 ℃

----------文献----------

Pande, A. et al., Phytochemistry, 1995, 39, 709, (分離, H-NMR, Mass)

§ 3-Dotetracontene-1,5-diol; 5-Ac
[CAS No.]165675-40-1
[化合物分類]脂肪族化合物(Unbranched alkenic acetates)

[構造式]

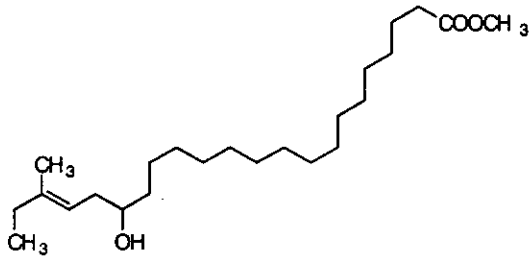


[分子式]$C_{44}H_{86}O_3$
[分子量]663.162
[正確な分子量]662.657695
[基原]*Stellaria media*

----------文献----------

Pande, A. et al., Phytochemistry, 1995, 39, 709,（分離, IR, H-NMR, Mass）

§ 19-Methyl-18-heneicosene-1,16-diol; 1-Ac
[CAS No.]165675-39-8
[化合物分類]脂肪族化合物(Branched alkenic acetates)
[構造式]



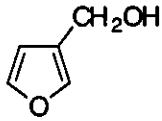
[分子式]$C_{24}H_{46}O_3$
[分子量]382.626
[正確な分子量]382.344695
[基原]*Stellaria media*

----------文献----------

Pande, A. et al., Phytochemistry, 1995, 39, 709,（分離, H-NMR, Mass）

§§ナデシコ科ウシハコベ(*Stellaria aquatica* Scopoli)の全草。

§ 3-Furanmethanol(CAS 名)
[化学名・別名]3-Furancarbinol. 3-Furfuryl alcohol. 3-(Hydroxymethyl)furan
[CAS No.]4412-91-3
[化合物分類]含酸素複素環式化合物(Furans)



[構造式]
[分子式]$C_5H_6O_2$
[分子量]98.101
[正確な分子量]98.03678
[基原]*Aloe arborescens*, *Eucommia ulmoides*, *Stellaria aquatica*
[性状]液体
[沸点]Bp_{17} 79-80 ℃
[濃度]d^{20}_4 1.139
[屈折率]n^{20}_D 1.4842

----------文献----------

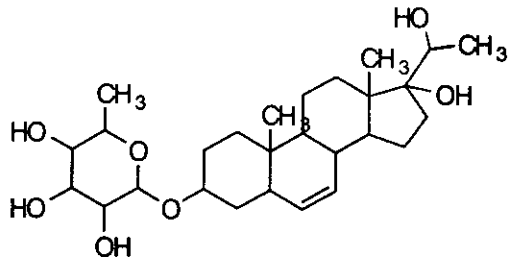
Kitagawa, I. et al., Chem. Pharm. Bull., 1983, 31, 664,（配糖体）
Reinecke, M.G. et al., J. Nat. Prod., 1988, 51, 1236; 1989, 52, 375,（pyrrole-2-carboxylate）
Marstokk, K.M. et al., Acta Chem. Scand., 1993, 47, 849,（microwave, 構造決定）

***********バシクルモン（Basikurumon）***********

§§キョウチクトウ科バシクルモン(*Apocynum venetum*（L.）var. *basikurumon*（Hara）Hara)の茎葉。

§ Pregn-6-ene-3,17,20-triol;（3 β,5 α,17 α *OH*,20*R*)-form, 3-*O*-Fucopyranoside

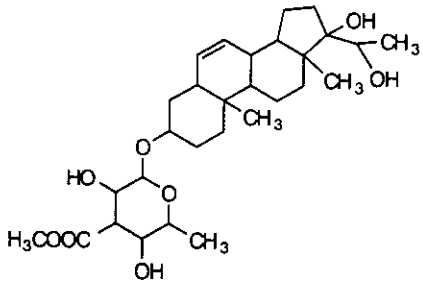
[化学名・別名]Basikoside A
[CAS No.]112667-05-7
[化合物分類]ステロイド(Pregnane steroids). (C21).
[構造式]
[分子式]$C_{27}H_{44}O_7$
[分子量]480.64
[正確な分子量]480.308705
[基原]*Apocynum venetum* var. *basikurumon*
[性状]結晶(MeOH)
[融点]Mp 260-265 ℃
[比旋光度]:[α]$_D^{26}$ -101.8 (c, 0.4 in MeOH)



----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1981, 29, 416; 1987, 35, 4087, (Basikosides)

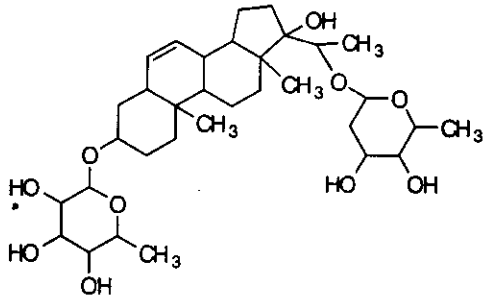
§ Pregn-6-ene-3,17,20-triol; (3 β,5 α,17 α *OH*,20*R*)-form, 3-*O*-(3-*O*-Acetyl-β-D-fucopyranoside)
[化学名・別名]Basikoside B
[CAS No.]112667-06-8
[化合物分類]ステロイド(Pregnane steroids). (C21).
[構造式]
[分子式]$C_{29}H_{46}O_8$
[分子量]522.678
[正確な分子量]522.31927
[基原]*Apocynum venetum* var. *basikurumon*
[性状]プリズム結晶 (MeOH)
[融点]Mp 240-246 ℃
[比旋光度]:[α]$_D^{26}$ -47.7 (c, 0.3 in MeOH)



----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1981, 29, 416; 1987, 35, 4087, (Basikosides)

§ Pregn-6-ene-3,17,20-triol; (3 β,5 α,17 α *OH*,20*R*)-form, 3-*O*-β-D-Fucopyranoside, 20-(2,6-dideoxy-β-D-*arabino*-hexopyranoside)
[化学名・別名]Basikoside C
[CAS No.]112667-07-9
[化合物分類]ステロイド(Pregnane steroids). (C21).
[構造式]
[分子式]$C_{33}H_{54}O_{10}$
[分子量]610.784
[正確な分子量]610.3717
[基原]*Apocynum venetum* var. *basikurumon*
[性状]結晶
[融点]Mp 215-220 ℃
[比旋光度]:[α]$_D^{26}$ -92.2 (c, 0.7 in MeOH)

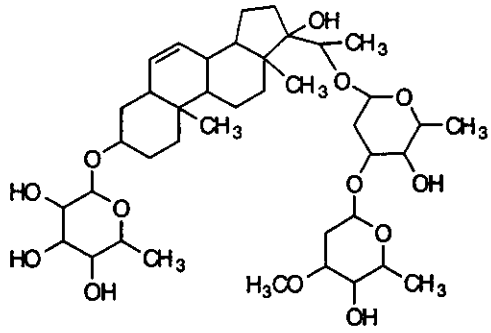


----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1981, 29, 416; 1987, 35, 4087, (Basikosides)

§ Pregn-6-ene-3,17,20-triol; (3 β,5 α,17 α *OH*,20*R*)-form, 3-*O*-β-D-Fucopyranoside, 20-*O*-[2,6-dideoxy-3-*O*-methyl-β-D-*lyxo*-hexopyranosyl-(1 → 3)-2,6-dideoxy-β-D-*arabino*-hexopyranoside]
[化学名・別名]Basikoside D

[CAS No.]112667-08-0
[化合物分類]ステロイド(Pregnane steroids). (C21).
[構造式]
[分子式]$C_{40}H_{66}O_{13}$
[分子量]754.954
[正確な分子量]754.450345
[基原]*Apocynum venetum* var. *basikurumon*
[性状]粉末
[比旋光度]:[α]$_D^{26}$ -97 (c, 0.4 in MeOH)

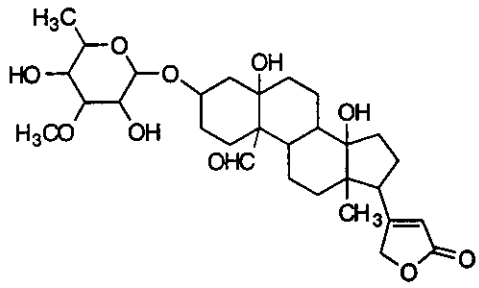


----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1981, 29, 416; 1987, 35, 4087, (Basikosides)

§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3 β,5 β,14 β)-form, 3-*O*-(6-Deoxy-3-*O*-methyl-β-D-galactopyranoside)

[化学名・別名]Strophanthidin digitaloside
[CAS No.]65681-32-5
[その他の CAS No.]119179-09-8
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]
[分子式]$C_{30}H_{44}O_{10}$
[分子量]564.672
[正確な分子量]564.29345
[基原]*Adonis vernalis*, *Apocynum venetum* var. *basikurumon*
[性状]塊
[比旋光度]:[α]$_D^{22}$ +5.2 (c, 0.2 in MeOH)

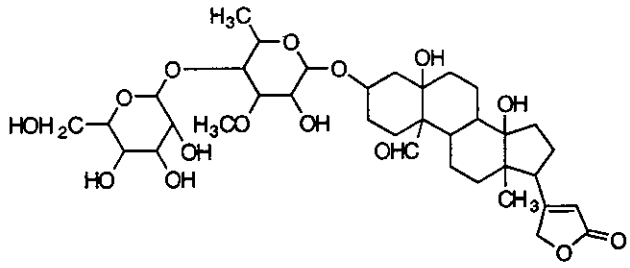


----------文献----------

Mauli, R. et al., Helv. Chim. Acta, 1957, 40, 284, (Glucostrophanthidin)
Marakevich, I.F. et al., Khim. Prir. Soedin., 1966, 2, 416; 1969, 5, 508; 1970, 6, 57; 1972, 8, 180; 1974, 10, 607; Chem. Nat. Compd. (Engl. Transl.), 1966, 2, 341; 1969, 5, 427; 1970, 6, 52; 1972, 8, 184; 1974, 10, 612; 619, (3-Epistrophanthidin, Erychoside, Cheirotoxin, Strophanthoside, Neoglucoerysimoside, Glucostrophalloside)
Timmermans, M. et al., Biochem. Syst. Ecol., 1992, 20, 343, (Strophanthidin allosides)
Wichtl, M. et al., Arch. Pharm. (Weinheim, Ger.), 1977, 310, 905, (digitaloside)

§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3 β,5 β,14 β)-form, 3-*O*-[β-D-Glucopyranosyl-(1→4)-6-deoxy-3-*O*-methyl-β-D-galactopyranoside]

[CAS No.]119182-48-8
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]
[分子式]$C_{36}H_{54}O_{15}$
[分子量]726.814
[正確な分子量]726.346275
[基原]*Apocynum venetum* var. *basikurumon*
[性状]塊
[比旋光度]:[α]$_D^{26}$ +14.3 (c, 0.3 in MeOH)



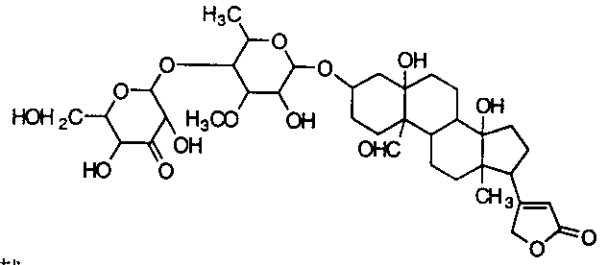
----------文献----------

Mauli, R. et al., Helv. Chim. Acta, 1957, 40, 284, (Glucostrophanthidin)
612; 619, (3-Epistrophanthidin, Erychoside, Cheirotoxin, Strophanthoside, Neoglucoerysimoside, Glucostrophalloside)
Allgeir, H. et al., Helv. Chim. Acta, 1967, 50, 456, (Strophothevoside)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 2249; 2251-2254, (生育)

Timmermans, M. et al., Biochem. Syst. Ecol., 1992, 20, 343, (Strophanthidin allosides)

§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3 β,5 β,14 β)-form, 3-*O*-[β-D-Glucos-3-ulosyl-(1 → 4)-2,6-dideoxy-3-*O*-methyl-β-D-*ribo*-hexopyranoside]

[化学名・別名]Basikuloside
[CAS No.]119144-85-3
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]



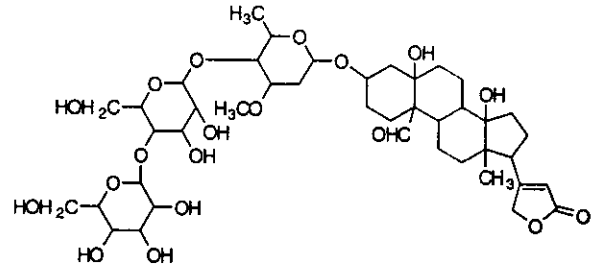
[基原]*Apocynum venetum* var. *basikurumon*
[性状]塊
[比旋光度]:[α]$_D^{26}$ +12.8 (c, 0.5 in MeOH)

----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1988, 36, 3811, (Apobasinoside, Basikuloside, Cellostrophanthoside)

§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3 β,5 β,14 β)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 4)-β-D-glucopyranosyl-(1 → 4)-2,6-dideoxy-3-*O*-methyl-β-D-*ribo*-hexopyranoside]

[化学名・別名]Cellostrophanthoside
[CAS No.]18829-75-9
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]



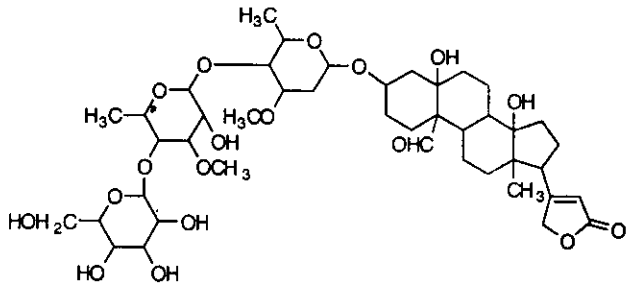
[分子式]$C_{32}H_{64}O_{19}$
[分子量]872.956
[正確な分子量]872.404185
[基原]*Apocynum venetum* var. *basikurumon*, *Adonis wolgensis*
[融点]Mp 179-182 ℃
[比旋光度]:[α]$_D^{26}$ +15.6 (c, 0.5 in MeOH)

----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1988, 36, 3811, (Apobasinoside, Basikuloside, Cellostrophanthoside)

§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3 β,5 β,14 β,17 α)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 4)-β-D-6-deoxy-3-*O*-methyl-β-D-galactopyranosyl-(1 → 4)-2,6-dideoxy-3-*O*-methyl-β-D-*ribo*-hexopyranoside]

[化学名・別名]Apobasinoside
[CAS No.]119179-08-7
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]



[分子式]$C_{43}H_{66}O_{18}$
[分子量]870.984
[正確な分子量]870.42492
[基原]*Apocynum venetum* var. *basikurumon*
[性状]塊
[比旋光度]:[α]$_D^{23}$ +23.1 (c, 0.06 in MeOH)

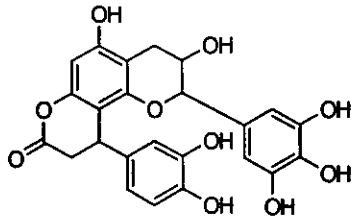
----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1988, 36, 3811, (Apobasinoside, Basikuloside, Cellostrophanthoside)

§§ キョウチクトウ科(*Apocynum venetum* L.)の茎葉。

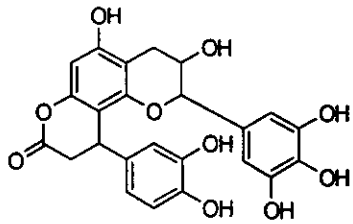
§ Cinchonain Ia; 5'-Hydroxy

[化学名・別名]Apocynin C
[化合物分類]フラボノイド(Neoflavonoids), フラボノイド(Flavan-3-ols)

[構造式]

[分子式]$C_{24}H_{20}O_{10}$
[分子量]468.416
[正確な分子量]468.10565
[基原]*Apocynum venetum*
[性状]茶色の塊
[比旋光度]:[α]$_D^{25}$ -57.6 (c, 0.28 in MeOH)
[UV]:[neutral] λ $_{max}$ 210 (log ε 4.84); 230 (sh) (); 270 (log ε 4) (MeOH)

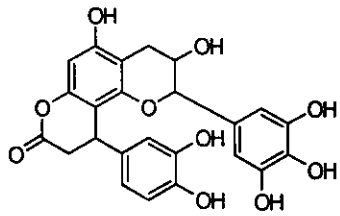
----------文献----------

Fan, W. et al., Chem. Pharm. Bull., 1999, 47, 1049, (Apocynins)

§ Cinchonain Ia; 3-Epimer, 5'-hydroxy
[化学名・別名]Apocynin A
[化合物分類]フラボノイド(Neoflavonoids), フラボノイド(Flavan-3-ols)
[構造式]

[分子式]$C_{24}H_{20}O_{10}$
[分子量]468.416
[正確な分子量]468.10565
[基原]*Apocynum venetum*
[性状]茶色の塊
[比旋光度]:[α]$_D^{25}$ -46.9 (c, 0.19 in MeOH)
[UV]:[neutral] λ $_{max}$ 210 (log ε 4.74); 230 (sh) (); 270 (log ε 4.02) (MeOH)

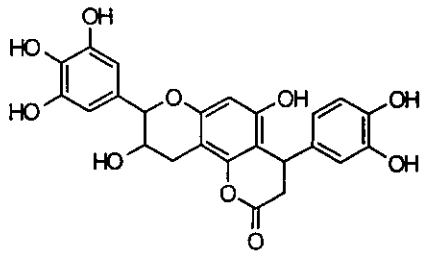
----------文献----------

Fan, W. et al., Chem. Pharm. Bull., 1999, 47, 1049, (Apocynins)

§ Cinchonain Ia; 3,10-Diepimer, 5'-hydroxy
[化学名・別名]Apocynin B
[化合物分類]フラボノイド(Flavan-3-ols), フラボノイド(Neoflavonoids)
[構造式]

[分子式]$C_{24}H_{20}O_{10}$
[分子量]468.416
[正確な分子量]468.10565
[基原]*Apocynum venetum*
[性状]茶色の粉末
[比旋光度]:[α]$_D^{25}$ +49.9 (c, 0.46 in MeOH)
[UV]:[neutral] λ $_{max}$ 218 (log ε 4.59); 230 (sh) (); 270 (log ε 3.86) (MeOH)

----------文献----------

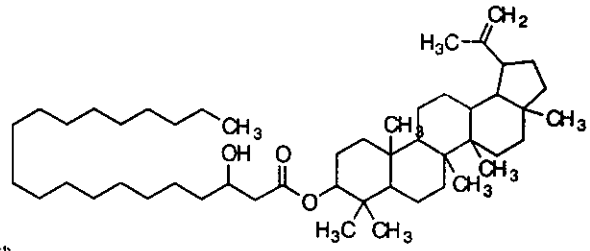
Fan, W. et al., Chem. Pharm. Bull., 1999, 47, 1049, (Apocynins)

§ Cinchonain Ic; 3-Epimer, 5'-hydroxy
[化学名・別名]Apocynin D
[CAS No.]246152-24-9
[化合物分類]フラボノイド(Flavan-3-ols), フラボノイド(Neoflavonoids)
[構造式]

[分子式]$C_{24}H_{20}O_{10}$
[分子量]468.416
[正確な分子量]468.10565
[基原]*Apocynum venetum*
[性状]茶色の塊
[比旋光度]:[α]$_D^{25}$ +45.5 (c, 0.23 in MeOH)
[UV]:[neutral] λ $_{max}$ 210 (log ε 4.52); 230 (sh) (); 270 (log ε 3.75) (MeOH)

----------文献----------

Fan, W. et al., Chem. Pharm. Bull., 1999, 47, 1049, (Apocynin D)

§ 20(29)-Lupen-3-ol; 3 β-form, 3-Hydroxyeicosanoyl
[CAS No.]98891-90-8
[化合物分類]テルペノイド(Lupane triterpenoids)
[構造式]

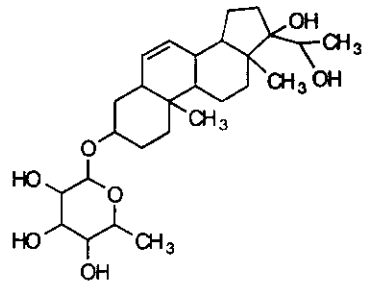


[分子式]$C_{50}H_{88}O_3$
[分子量]737.243
[正確な分子量]736.673345
[基原]*Apocynum venetum, Parahancornia amapa*

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2023,(生育)

§ Pregn-6-ene-3,17,20-triol; (3 β,5 α,17 α *OH*,20*R*)-form, 3-*O*-Fucopyranoside
[化学名・別名]Basikoside A
[CAS No.]112667-05-7
[化合物分類]ステロイド(Pregnane steroids). (C21).
[構造式]

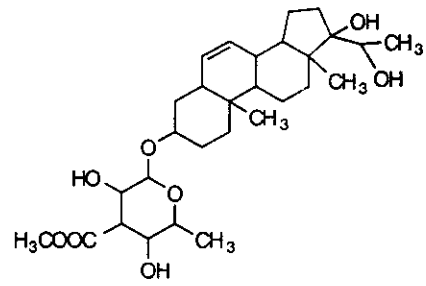


[分子式]$C_{27}H_{44}O_7$
[分子量]480.64
[正確な分子量]480.308705
[基原]*Apocynum venetum* var. *basikurumon*
[性状]結晶(MeOH)
[融点]Mp 260-265 ℃
[比旋光度]:[α]$_D^{26}$ -101.8 (c, 0.4 in MeOH)

----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1981, 29, 416; 1987, 35, 4087,(Basikosides)

§ Pregn-6-ene-3,17,20-triol; (3 β,5 α,17 α *OH*,20*R*)-form, 3-*O*-(3-*O*-Acetyl-β-D-fucopyranoside)
[化学名・別名]Basikoside B
[CAS No.]112667-06-8
[化合物分類]ステロイド(Pregnane steroids). (C21).
[構造式]

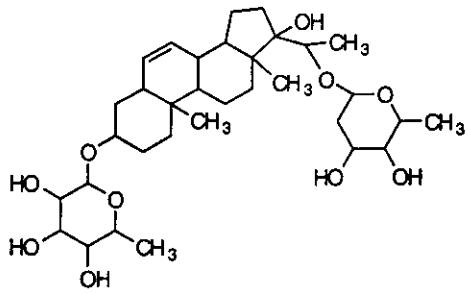


[分子式]$C_{29}H_{46}O_8$
[分子量]522.678
[正確な分子量]522.31927
[基原]*Apocynum venetum* var. *basikurumon*
[性状]プリズム結晶 (MeOH)
[融点]Mp 240-246 ℃
[比旋光度]:[α]$_D^{26}$ -47.7 (c, 0.3 in MeOH)

----------文献----------

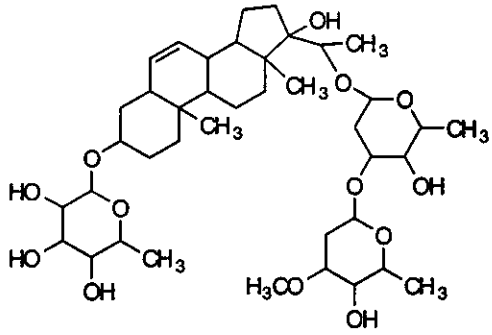
Abe, F. et al., Chem. Pharm. Bull., 1981, 29, 416; 1987, 35, 4087,(Basikosides)

§ Pregn-6-ene-3,17,20-triol; (3 β,5 α,17 α *OH*,20*R*)-form, 3-*O*-β-D-Fucopyranoside, 20-

(2,6-dideoxy-β-D-*arabino*-hexopyranoside)
[化学名・別名]Basikoside C
[CAS No.]112667-07-9
[化合物分類]ステロイド(Pregnane steroids). (C21).
[構造式]

[分子式]$C_{33}H_{54}O_{10}$
[分子量]610.784
[正確な分子量]610.3717
[基原]*Apocynum venetum* var. *basikurumon*
[性状]結晶
[融点]Mp 215-220 ℃
[比旋光度]:[α]$_D^{26}$ -92.2 (c, 0.7 in MeOH)

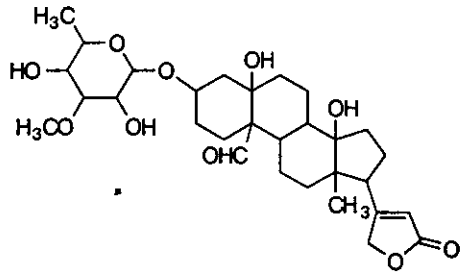
----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1981, 29, 416; 1987, 35, 4087, (Basikosides)

§ Pregn-6-ene-3,17,20-triol; (3 β,5 α,17 α *OH*,20*R*)-form, 3-*O*-β-D-Fucopyranoside, 20-*O*-[2,6-dideoxy-3-*O*-methyl-β-D-*lyxo*-hexopyranosyl-(1 → 3)-2,6-dideoxy-β-D-*arabino*-hexopyranoside]
[化学名・別名]Basikoside D
[CAS No.]112667-08-0
[化合物分類]ステロイド(Pregnane steroids). (C21).
[構造式]

[分子式]$C_{40}H_{66}O_{13}$
[分子量]754.954
[正確な分子量]754.450345
[基原]*Apocynum venetum* var. *basikurumon*
[性状]粉末
[比旋光度]:[α]$_D^{26}$ -97 (c, 0.4 in MeOH)

----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1981, 29, 416; 1987, 35, 4087, (Basikosides)

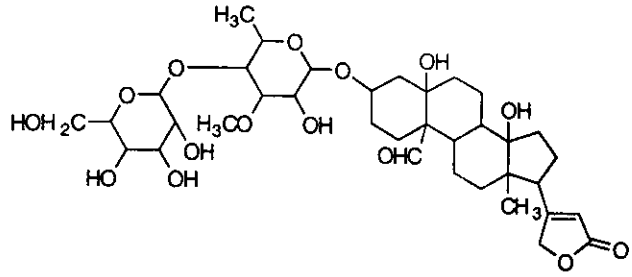
§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3 β,5 β,14 β)-form, 3-*O*-(6-Deoxy-3-*O*-methyl-β-D-galactopyranoside)
[化学名・別名]Strophanthidin digitaloside
[CAS No.]65681-32-5
[その他の CAS No.]119179-09-8
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]

[分子式]$C_{30}H_{44}O_{10}$
[分子量]564.672
[正確な分子量]564.29345
[基原]*Adonis vernalis*, *Apocynum venetum* var. *basikurumon*
[性状]塊
[比旋光度]:[α]$_D^{22}$ +5.2 (c, 0.2 in MeOH)

----------文献----------

Mauli, R. et al., Helv. Chim. Acta, 1957, 40, 284, (Glucostrophanthidin)
612; 619, (3-Epistrophanthidin, Erychoside, Cheirotoxin, Strophanthoside, Neoglucoerysimoside, Glucostrophalloside)
Allgeir, H. et al., Helv. Chim. Acta, 1967, 50, 456, (Strophothevoside)
Timmermans, M. et al., Biochem. Syst. Ecol., 1992, 20, 343, (Strophanthidin allosides)

§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3 β,5 β,14 β)-form, 3-*O*-[β-D-Glucopyranosyl-(1

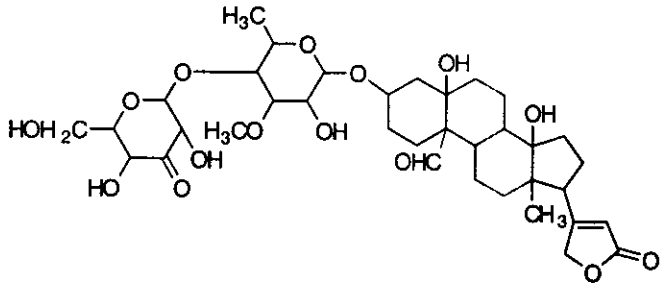
→ 4)-6-deoxy-3-*O*-methyl-β-D-galactopyranoside]
[CAS No.]119182-48-8
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]
[分子式]$C_{36}H_{54}O_{15}$
[分子量]726.814
[正確な分子量]726.346275
[基原]*Apocynum venetum* var. *basikurumon*
[性状]塊
[比旋光度]:[α]$_D^{26}$ +14.3 (c, 0.3 in MeOH)



----------文献----------

Mauli, R. et al., Helv. Chim. Acta, 1957, 40, 284, (Glucostrophanthidin)
612; 619, (3-Epistrophanthidin, Erychoside, Cheirotoxin, Strophanthoside, Neoglucoerysimoside, Glucostrophalloside)
Allgeir, H. et al., Helv. Chim. Acta, 1967, 50, 456, (Strophothevoside)
Timmermans, M. et al., Biochem. Syst. Ecol., 1992, 20, 343, (Strophanthidin allosides)

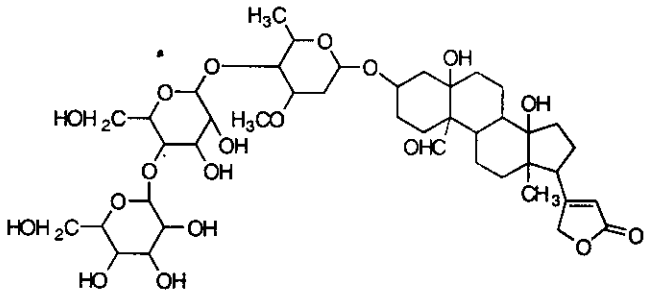
§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3β,5β,14β)-form, 3-*O*-[β-D-Glucos-3-ulosyl-(1 → 4)-2,6-dideoxy-3-*O*-methyl-β-D-*ribo*-hexopyranoside]
[化学名・別名]Basikuloside
[CAS No.]119144-85-3
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]
[分子式]$C_{36}H_{52}O_{14}$
[分子量]708.798
[正確な分子量]708.33571
[基原]*Apocynum venetum* var. *basikurumon*
[性状]塊
[比旋光度]:[α]$_D^{26}$ +12.8 (c, 0.5 in MeOH)



----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1988, 36, 3811, (Apobasinoside, Basikuloside, Cellostrophanthoside)

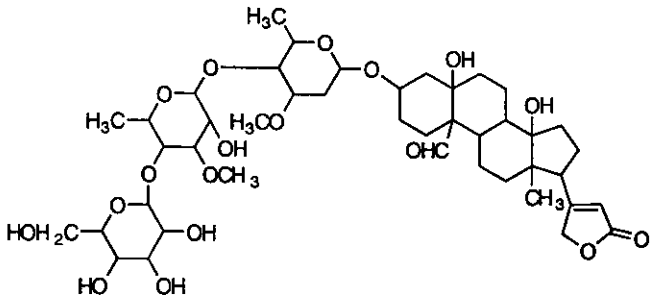
§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3β,5β,14β)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 4)-β-D-glucopyranosyl-(1 → 4)-2,6-dideoxy-3-*O*-methyl-β-D-*ribo*-hexopyranoside]
[化学名・別名]Cellostrophanthoside
[CAS No.]18829-75-9
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]
[分子式]$C_{42}H_{64}O_{19}$
[分子量]872.956
[正確な分子量]872.404185
[基原]*Apocynum venetum* var. *basikurumon*, *Adonis wolgensis*
[融点]Mp 179-182 ℃
[比旋光度]:[α]$_D^{26}$ +15.6 (c, 0.5 in MeOH)



----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1988, 36, 3811, (Apobasinoside, Basikuloside, Cellostrophanthoside)

§ 3,5,14-Trihydroxy-19-oxocard-20(22)-enolide; (3β,5β,14β,17α)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 4)-β-D-6-deoxy-3-*O*-methyl-β-D-galactopyranosyl-(1 → 4)

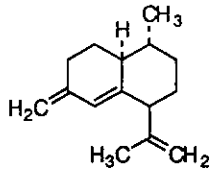
-2,6-dideoxy-3-*O*-methyl- β -D-*ribo*-hexopyranoside]
[化学名・別名]Apobasinoside
[CAS No.]119179-08-7
[化合物分類]ステロイド(Cardanolide steroids). (C23).
[構造式]

[分子式]$C_{43}H_{66}O_{18}$
[分子量]870.984
[正確な分子量]870.42492
[基原]*Apocynum venetum* var. *basikurumon*
[性状]塊
[比旋光度]:$[\alpha]_D^{23}$ +23.1 (c, 0.06 in MeOH)

----------文献----------

Abe, F. et al., Chem. Pharm. Bull., 1988, 36, 3811, (Apobasinoside, Basikuloside, Cellostrophanthoside)

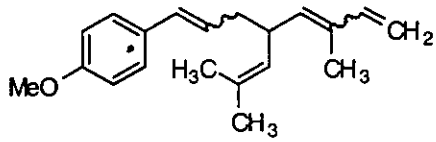
**********バジル (Basil) **********

§ § シソ科メボウキ(*Ocimum basilicum* L.)の茎葉または花。

§ 4(15),5,11-Cadinatriene
[化学名・別名]1-Epibicyclosesquiphellandrene. 1-*epi*-Bicyclosesquiphellandrene
[CAS No.]54274-73-6
[化合物分類]テルペノイド(Cadinane sesquiterpenoids)
[構造式]

[分子式]$C_{15}H_{22}$
[分子量]202.339
[正確な分子量]202.17215
[基原]*Ocimum basilicum*
[性状]オイル

----------文献----------

Terhune, S.J. et al., Phytochemistry, 1974, 13, 1183, (分離, 構造決定)
Vig, O.P. et al., J. Indian Chem. Soc., 1976, 53, 593, (合成法)

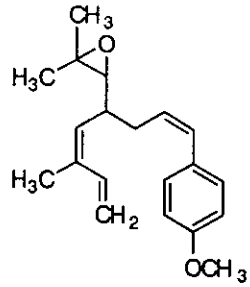
§ Juvocimene 1
[化学名・別名]1-Methoxy-4-[6-methyl-4-(2-methyl-1-propenyl)-1,5,7-octatrienyl]benzene(CAS 名)
[CAS No.]75539-64-9
[関連 CAS No.]94668-94-7, 94668-95-8, 94668-96-9
[化合物分類]脂肪族化合物(Long-chain aromatic systems)
[構造式]

[分子式]$C_{20}H_{26}O$
[分子量]282.425
[正確な分子量]282.198365
[基原]*Ocimum basilicum* のオイル
[用途]昆虫の幼若ホルモン類似物質

----------文献----------

Nishida, R. et al., J. Chem. Ecol., 1984, 10, 1435, (分離, 合成法)

§ Juvocimene 1; 1'',2''-Epoxide

[化学名・別名]Juvocimene 2
[CAS No.]75539-63-8
[化合物分類]脂肪族化合物(Long-chain aromatic systems)
[構造式]
[分子式]$C_{20}H_{26}O_2$
[分子量]298.424
[正確な分子量]298.19328
[基原]*Ocimum basilicum* のオイル
[用途]昆虫の幼若ホルモン類似物質



----------文献----------

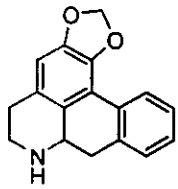
Nishida, R. et al., J. Chem. Ecol., 1984, 10, 1435, (分離, 合成法)

§§シソ科ブッシュバジル(*Ocimum minimum* L.)の茎葉または花。
該当物質なし

***********ハス (Lotus) ***********

§§スイレン科ハス(*Nelumbo nucifera* Gaertner)の果実, 葉または地下茎。

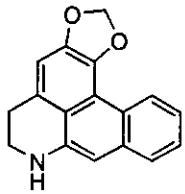
§ Anonaine; (*R*)-form
[CAS No.]1862-41-5
[化合物分類]アルカロイド化合物(Aporphine alkaloids)
[構造式]
[基原]次の植物から得られるアルカロイド: *Annona reticulata*, *Annona muricata* (バンレイシ科), *Nelumbo nucifera* (ハス科), また, クスノキ科, モクレン科, モニミア科, ケシ科, クロウメモドキ科, ツヅラフジ科からも得られる.
[用途]殺虫作用を示す. Serotonin receptor antagonist
[融点]Mp 122-123 ℃
[比旋光度]:$[\alpha]_D^{31}$ -68 (c, 0.77 in EtOH)



----------文献----------

Gopinath, K.W. et al., Chem. Ber., 1959, 92, 776, (分離)
Johns, S.R. et al., Aust. J. Chem., 1968, 21, 1383, (分離, H-NMR)
Bhakuni, D.S. et al., Phytochemistry, 1972, 11, 1819, (Mass, H-NMR, UV, 分離)
Hufford, C.D. et al., Phytochemistry, 1976, 15, 1169, (*N*-Acetylanonaine)
Sashida, Y. et al., Yakugaku Zasshi, 1976, 96, 659; CA, 88, 3043u, (*N*-Acetylanonaine)
Gray, A.I. et al., Planta Med., 1980, 39, 209, (*N*-Acetylanonaine)
Ren, L. et al., Yaoxue Xuebao, 1981, 16, 672; CA, 96, 48974e, (*N*-Acetylanonaine)
Achenbach, H. et al., Annalen, 1982, 1623, (*N*-Formylanonaine, *N*-Carbamoylanonaine)
Hasrat, J.A. et al., Phytomedicine, 1997, 4, 133, (活性)

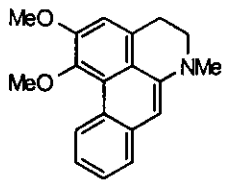
§ Anonaine; (*R*)-form, 6*a*,7-Didehydro
[化学名・別名]Dehydroanonaine
[CAS No.]41679-82-7
[化合物分類]アルカロイド化合物(Aporphine alkaloids)
[構造式]
[分子式]$C_{17}H_{13}NO_2$
[分子量]263.295
[正確な分子量]263.094629
[基原]次の植物の葉から得られるアルカロイド: *Nelumbo nucifera* (ハス科)



----------文献----------

Kunitomo, J. et al., Phytochemistry, 1973, 12, 699, (Dehydroanonaine)
Atanes, N. et al., J.O.C., 1991, 56, 2984, (合成法, Dehydroanonaine)

§ Dehydronuciferine

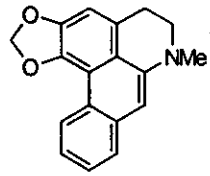


[CAS No.] 7630-74-2
[化合物分類] アルカロイド化合物 (Aporphine alkaloids)
[構造式]
[分子式] $C_{19}H_{19}NO_2$
[分子量] 293.365
[正確な分子量] 293.141579
[基原] 次の植物から得られるアルカロイド: *Nelumbo nucifera* の葉, *Colubrina faralaotra* subsp. *faralaotra*, *Colubrina faralaotra* subsp. *trichocarpa* (ハス科, クロウメモドキ科)
[性状] 結晶 (EtOH)
[融点] Mp 130-131 ℃

----------文献----------

Lenz, G.R. et al., J.C.S. Perkin 1, 1984, 1273, (Dehydronornuciferine, 合成法, UV, IR, H-NMR, C13-NMR)
Cortes, D. et al., J. Nat. Prod., 1986, 49, 878, (Dehydronornuciferine, 分離)
Atanes, N. et al., J.O.C., 1991, 56, 2984, (合成法, Dehydronornuciferine)

§ Dehydroroemerine

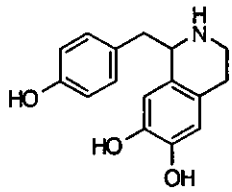


[化学名・別名] Dehydroaporheine
[CAS No.] 36285-03-7
[化合物分類] アルカロイド化合物 (Aporphine alkaloids)
[構造式]
[分子式] $C_{18}H_{15}NO_2$
[分子量] 277.322
[正確な分子量] 277.110279
[基原] 次の植物から得られるアルカロイド: *Nelumbo nucifera*, *Stephania sasakii*, *Stephania micrantha*, *Stephania kwangsiensis*, *Papaver glaucum*, *Papaver rhoeas*, *Papaver spicatum* var. *spicatum*, *Papaver spicatum* var. *luschanii*, *Liriodendron tulipifera*, *Colubrina faralaotra* ssp. *faralaotra*, *Colubrina faralaotra* ssp. *sinuata* (ハス科, ツヅラフジ科, ケシ科, モクレン科, クロウメモドキ科)
[融点] Mp 88-89 ℃

----------文献----------

Preininger, V. et al., Planta Med., 1973, 23, 233, (Didehydroroemerine)
Guinaudeau, H. et al., Planta Med., 1975, 27, 304; 1976, 30, 201, (分離)
Min, Z. et al., Yaoxue Xuebao, 1980, 15, 532; CA, 94, 117773m, (分離)
Phillipson, J.D. et al., J. Nat. Prod., 1981, 44, 296, (生育)
Sariyar, G. et al., Plant. Med. Phytother., 1981, 15, 160; CA, 96, 119030g, (分離)
Kunitomo, J. et al., Yakugaku Zasshi, 1981, 101, 431; CA, 95, 204236c, (分離)
Min, Z. et al., Yaoxue Xuebao, 1981, 16, 557; CA, 97, 3595m, (分離)

§ Higenamine; (*R*)-form

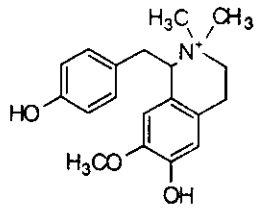


[CAS No.] 106032-53-5
[化合物分類] アルカロイド化合物 (Benzylisoquinoline alkaloids)
[構造式]
[基原] 次の植物の種子胚から得られるアルカロイド: *Nelumbo nucifera* (ハス科)
[性状] プリズム結晶 (EtOH)
[融点] Mp 242-244 ℃で分解
[比旋光度]: $[\alpha]_D^{26.5}$ +16 (c, 1 in MeOH)
[その他のデータ] 絶対構造は証明されていない

----------文献----------

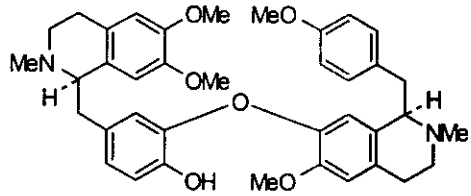
Albonico, S.M. et al., J.C.S. (C), 1966, 1340, (UV, ord, 絶対構造, Colletine, Magnocurarine)
Johns, S.R. et al., Aust. J. Chem., 1967, 20, 1729, (分離, H-NMR, Mass, Coclaurine)
Ida, Y. et al., Phytochemistry, 1994, 35, 209, (*N*-Methylhigenamine 7-glucoside)
Xu, Q. et al., J. Nat. Prod., 1999, 62, 1025, (*N*-Methylhigenamine oxide)

§ Higenamine; (*R*)-form, *O*^{7},*N*,*N*-Tri-Me

[化学名・別名]Lotusine
[CAS No.]6871-67-6
[化合物分類]アルカロイド化合物(Benzylisoquinoline alkaloids)
[構造式]

[分子式]$C_{19}H_{24}NO_3^{(+)}$
[分子量]314.404
[正確な分子量]314.175619
[基原]次の植物から得られる４基のアルカロイド: *Nelumbo nucifera* の胚, *Tiliacora racemosa* (ハス科)
[融点]Mp 213-215 ℃ (as chloride)
[比旋光度]:[α]$_D$ -15 (MeOH) (chloride)

----------文献----------

Furukawa, H., Yakugaku Zasshi, 1965, 85, 335; 472; CA, 63, 4351d; 5692d, (4'-Methyl-*N*-methylcoclaurine, Lotusine)

§ **Neferine**
[化学名・別名]12'-*O*-Methylliensinine
[CAS No.]2292-16-2
[化合物分類]アルカロイド化合物(Bisbenzylisoquinoline alkaloids; one ether link)
[構造式]

[分子式]$C_{38}H_{44}N_2O_6$
[分子量]624.775
[正確な分子量]624.319938
[基原]次の植物の種子胚から得られるアルカロイド:
Nelumbo nucifera (ハス科)
[性状]オイル
[比旋光度]:[α]$_D^{28}$ -37.8 (c, 1.43 in $CHCl_3$). [α]$_D^{27}$ -100 (c, 0.24 in MeOH)
[化学物質毒性データ総覧(RTECS)登録番号]SM9495000

----------文献----------

Chao, Y.C. et al., Sci. Sin. (Engl. edn.), 1962, 11, 215; CA, 57, 7383i, (分離, Liensinine)
Hsieh, Y.Y. et al., Sci. Sin. (Engl. edn.), 1964, 12, 2018; CA, 62, 9183h, (絶対構造, Liensinine)
Tomita, M. et al., Tet. Lett., 1964, 2637, (Isoliensinine)
Furukawa, H., Yakugaku Zasshi, 1965, 85, 335; 353; CA, 63, 4351ad, (分離, IR, H-NMR, 構造決定)
Yang, T.-H. et al., J. Chin. Chem. Soc. (Taipei), 1970, 17, 235; CA, 74, 100254g, (分離, UV, IR, H-NMR)
Kametani, T. et al., J. Het. Chem., 1970, 7, 181, (分離, H-NMR)

*****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　　: 静脈注射
被験動物　　: げっ歯類-マウス
投与量・期間 : 26 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

CTYAD8 Zhongcaoyao. Chinese Traditional and Herbal Medicine. (China International Book Trading Corp., POB 2820, Beijing, Peop. Rep. China) V.11- 1980- [Vol.,頁,年(19-)]19,217,1988

§ **Neferine; *O*^{7}-De-Me**
[化学名・別名]Isoliensinine
[CAS No.]6817-41-0
[化合物分類]アルカロイド化合物(Bisbenzylisoquinoline alkaloids; one ether link)