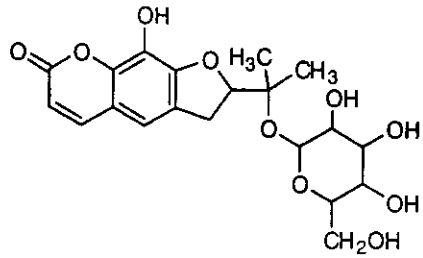
[その他の CAS No.]68692-60-4
[化合物分類]ベンゾピラノイド(Dihydrofuranocoumarins), ベンゾピラノイド(7,8-Dioxygenated coumarins)
[構造式]

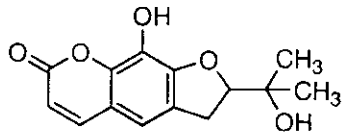


[分子式]$C_{20}H_{24}O_{10}$
[分子量]424.404
[基原]*Ruta graveolens*
[性状]結晶
[融点]Mp 275-276 ℃ (245-248 ℃)
[比旋光度]:[α]$_D$ -40 (c, 0.4 in MeOH)

文献

Schneider, G. et al., Arch. Pharm. (Weinheim, Ger.), 1967, 300, 73; 913, (分離, IR, UV, H-NMR, Mass)
Shagova, L.I. et al., Khim. Prir. Soedin., 1973, 9, 665; Chem. Nat. Compd. (Engl. Transl.), 1973, 9, 631, (分離)
Varga, E. et al., Acta Pharm. Hung., Suppl. No. 36, 1974, 44 ; CA, 82, 13996, (分離)
Kong, L. et al., Chin. Chem. Lett., 1993, 4, 37, (Qianhucoumarin G)
Srivastava, S.K. et al., Fitoterapia, 1994, 65, 301-303, (rutinoside)

§ Rutaretin; (*S*)-form
[化合物分類]ベンゾピラノイド(Dihydrofuranocoumarins), ベンゾピラノイド(7,8-Dioxygenated coumarins)
[構造式]

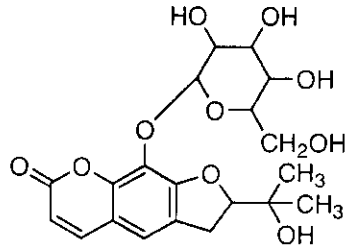


[分子式]$C_{14}H_{14}O_5$
[分子量]262.262
[天然基原]次の植物から分離: *Herba rutae*, *Apium graveolens* と *Ruta graveolens* の種子
[性状]青白い黄色の針状結晶
[融点]Mp 198 ℃
[比旋光度]:[α]$_D^{19}$ -30.4 (c, 0.79 in $CHCl_3$)

文献

Schneider, G. et al., Arch. Pharm. (Weinheim. Ger.), 1967, 300, 73; 913, (分離, IR, UV, H-NMR, Mass)
Shagova, L.I. et al., Khim. Prir. Soedin., 1973, 9, 665; Chem. Nat. Compd. (Engl. Transl.), 1973, 9, 631, (分離)
Varga, E. et al., Acta Pharm. Hung., Suppl. No. 36, 1974, 44 ; CA, 82, 13996, (分離)
Srivastava, S.K. et al., Fitoterapia, 1994, 65, 301-303, (rutinoside)

§ Rutaretin; (*S*)-form, 9-*O*-β-D-Glucopyranoside
[化学名・別名]Rutarin, Campesenin
[CAS No.]20320-81-4
[化合物分類]ベンゾピラノイド(7,8-Dioxygenated coumarins), ベンゾピラノイド(Dihydrofuranocoumarins)
[構造式]

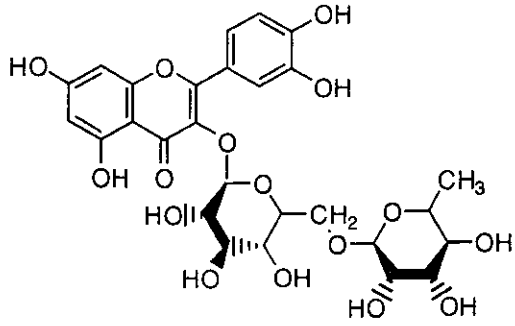


[分子式]$C_{20}H_{24}O_{10}$
[分子量]424.404
[天然基原]*Ruta graveolens*, *Seseli campestre*
[性状]結晶
[融点]Mp 145-148 ℃
[比旋光度]:[α]$_D^{22}$ -47.1 (c, 0.106 in EtOH)
[溶解性]BERDY SOL: ヘキサンに難溶

文献

Schneider, G. et al., Arch. Pharm. (Weinheim, Ger.), 1967, 300, 73; 913, (分離, IR, UV, H-NMR, Mass)
Shagova, L.I. et al., Khim. Prir. Soedin., 1973, 9, 665; Chem. Nat. Compd. (Engl. Transl.), 1973, 9, 631, (分離)
Varga, E. et al., Acta Pharm. Hung., Suppl. No. 36, 1974, 44 ; CA, 82, 13996, (分離)
Srivastava, S.K. et al., Fitoterapia, 1994, 65, 301-303, (rutinoside)

[CAS No.] 153-18-4
[関連 CAS No.] 22519-99-9
[化合物分類] 薬物: 止血剤(Haemostatic agents), 薬物: 抗血栓薬(Antithrombotic agents), 薬物: 抗 HIV 薬(Anti-HIV agents), フラボノイド(Flavonols; 5 × O-置換基), 薬物: 抗ウイルス物質(Antiviral agents), 薬物: 鎮痙薬(Antispasmodics), 薬物: 抗炎症薬(Antiinflammatory agents), PA4800, PM6148, 薬物: 抗低血圧症薬(Antihypotensive agents), 炭水化物(Disaccharides)



[構造式]
[分子式] $C_{27}H_{30}O_{16}$
[分子量] 610.524
[一般的性質] The synonym Rutinion refers to the Na salt. The name Vitamin P appears to be loosely applied to various biflavonoids or mixtures of which Rutin is one component
[天然基原] 多くの植物から得られる. 30 以上の科に存在し, 大部分は双子葉植物, demonstrated by 1955. 最初に *Ruta graveolens* から分離された(Weiss, 1842)
[用途] Used as 1m *M* soln. in 50% MeOH for photometric detn. of Mo (λ_{max} 400 nm, ε 22100), W (λ_{max} 405 nm, ε 40300). 抗酸化剤. Antioedemic, 抗炎症, 抗血栓症薬. 強い抗低血圧症, 鎮痙作用がある. 抗出血作用; 抗-HIV 活性を示す
[性状] 黄色の結晶・三水和物 (H_2O)
[融点] Mp 214-215 ℃で分解 (無水物)
[比旋光度]: $[\alpha]_D^{23}$ +13.82 (EtOH)
[Log P 計算値] Log P -3.97 (未確認値)(計算値)
[傷害・毒性] 50 %致死量(LD_{50})(ラット, 腹膜内) 2000 mg/kg
[化学物質毒性データ総覧(RTECS)登録番号] VM2975000
[販売元] Fluka:84082; Sigma:R5143

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1536, (成書)
Voelter, W. et al., D-(β-Hydroxyethyl)rutosides: New Results, Eds,. Springer-Verlag, Berlin, 1983, (専門書)
Khalifa, T.I. et al., Anal. Profiles Drug Subst., 1983, 12, 623, (レビュー)

***RTECS (化学物質毒性データ) ***
生体影響物質 : 催腫瘍物質. 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 : 腹腔内投与.
被験動物 : げっ歯類-モルモット.
投与量・期間 : 2 gm/kg
毒性影響 : 致死量以外に毒性影響に関する報告はない.
参照文献
Eksperimentalna Meditsina i Morfologiya.19,207,1980

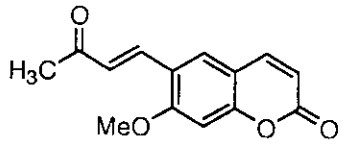
催腫瘍性に関するデータ

<<試験方法>> 最小毒性量(TDLo).
曝露経路 : 経口投与.
被験動物 : げっ歯類-ラット.
投与量・期間 : 973 gm/kg/3 年間継続投与
毒性影響 : 〔催腫瘍性〕 RTECS 基準による催腫瘍性.
〔肝臓〕 腫瘍.
参照文献
Proceedings of the American Association for Cancer Research. 25,95,1984

変異原性に関するデータ

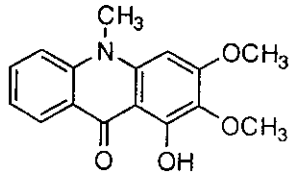
<<試験方法>> 微生物を用いた突然変異試験.
試験系 : 大腸菌 Salmonella typhimurium
投与量・期間 : 80 ug/plate
参照文献
Food and Chemical Toxicology.23,669,1985

試験系　　：大腸菌 Salmonella typhimurium
投与量・期間：80 ug/plate
参照文献
Food and Chemical Toxicology.23,669,1985
〈〈試験方法〉〉DNA 修復.
試験系　　：大腸菌 Escherichia coli
投与量・期間：100 mg/L
参照文献
Food and Cosmetics Toxicology.18,223,1980

§ Suberenone
[化学名・別名]7-Methoxy-6-(3-oxo-1-butenyl)-2*H*-1-benzopyran-2-one(CAS 名), 7-Methoxy-6-(3-oxo-1-butenyl)coumarin
[CAS No.]35897-95-1
[化合物分類]ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted)
[構造式]

[分子式]$C_{14}H_{12}O_4$
[分子量]244.246
[天然基原]*Ruta graveolens*, *Boenninghausenia albiflora*
[性状]黄色の針状結晶 (MeOH/petrol)
[融点]Mp 225 ℃

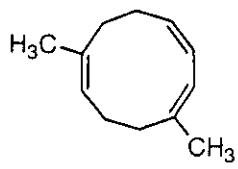
文 献

Minker, E. et al., Magy. Kem. Foly., 1972, 78, 6, (分離, 構造決定)
Talapatra, S.K. et al., Phytochemistry, 1975, 14, 836, (分離, 構造決定)
Ju-ichi, M. et al., Heterocycles, 1988, 27, 1451, (Funadonin)

§ 1,2,3-Trihydroxyacridone; 2,3,10-*O*,*O*,*N*-Tri-Me
[化学名・別名]Arborinine
[CAS No.]5489-57-6
[化合物分類]アルカロイド化合物(Acridone alkaloids), 薬物: 鎮痙薬(Antispasmodics), 薬物: 抗炎症薬(Antiinflammatory agents)
[構造式]

[分子式]$C_{16}H_{15}NO_4$
[分子量]285.299
[天然基原]次の植物から得られるアルカロイド: *Glycosmis arborea*, *Fagara leprieurii*, *Evodia xanthoxyloides*, *Ruta graveolens*, その他のミカン科の属
[用途]抗ヒスタミン, 抗炎症, 鎮痙薬
[性状]結晶 (EtOH)
[融点]Mp 175-176 ℃
[Log P 計算値]Log P 1.11 (計算値)

文 献

Hughes, G.K. et al., Aust. J. Sci. Res., Ser. A, 1952, 5, 401; 406, (分離, 合成法)
Chakravati, D. et al., J.C.S., 1953, 3337, (分離, Arborinine)

§ 11,12,13-Trinor-1(10),4,6-germacratriene; (1(10)*E*,4*E*,6*Z*)-form
[化学名・別名]Pregeijerene
[化合物分類]テルペノイド(Nor- and homogermacrane sesquiterpenoids)
[構造式]

[天然基原]*Geijera parviflora*, *Ruta graveolens*, *Rubus rosifolius*
[性状]オイル
[沸点]Bp_5 82 ℃

文 献

Jones, R.V.H. et al., Aust. J. Chem., 1968, 21, 2255
Coggon, P. et al., J.C.S.(B), 1970, 1024, (結晶構造)
Kubeczka, K.H., Phytochemistry, 1974, 13, 2017

§ 2-Undecanone

[分子式] $C_{11}H_{22}O$
[分子量] 170.294
[天然基原] ヤシの仁のオイル，大豆油，ヘンルーダオイル(*Ruta graveolens*)の重要成分であり，多くのその他の精油に見られる．Constit. of alarm pheromone of weaver ant *Oecophylla longinoda*
[用途] 香水と香料に用いられる．抗カビ剤
[融点] Fp 15 ℃
[沸点] Bp 228 ℃．Bp_{12} 105-106 ℃
[傷害・毒性] 50 %致死量(LD_{50})(ラット，経口) 5000 mg/kg．引火点:89 ℃
[化学物質毒性データ総覧(RTECS)登録番号] YQ2820000
[販売元] Aldrich:U130-3; Fluka:68160

----------文献----------

Haller, A. et al., C. R. Hebd. Seances Acad. Sci., 1910, 151, 698,（分離）
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 425,（生育）
Opdyke, D.L.J., Food Cosmet. Toxicol., 1975, 13, 869,（レビュー，毒性）

RTECS（化学物質毒性データ）

生体影響物質　　：農業化学品．生殖影響物質．

健康障害に関するデータ

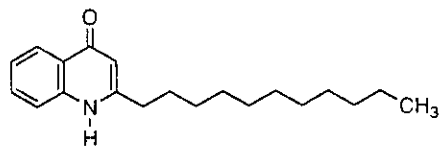
急性毒性に関するデータ

<<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：5 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
Farm Chemicals Handbook.C201,1991

生殖に関するデータ

<<試験方法>> 最小毒性量(TDLo)．
曝露経路　　：腹腔内投与．
被験動物　　：げっ歯類-マウス．
投与　　：1 gm/kg
雌雄投与期間：雌 1-20 日間(交配後)
毒性影響　　：〔生殖〕[受精能への影響]雌受精能の指標(たとえば精子陽性の雌のうち妊娠した雌の数，交配させた雌のうち妊娠した雌の数)．
参照文献
Journal of Medicinal Chemistry.18,1024,1975

§ 2-Undecyl-4(1*H*)-quinolinone(CAS 名)



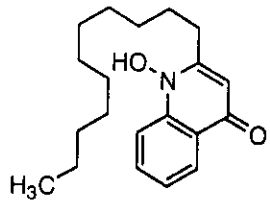
[化学名・別名] 4-Hydroxy-2-undecylquinoline
[CAS No.] 56183-46-1
[化合物分類] アルカロイド化合物(Simple quinoline alkaloids)
[構造式]
[分子式] $C_{20}H_{29}NO$
[分子量] 299.455
[天然基原] 次の植物から得られるアルカロイド: *Ptelea trifoliata*, *Ruta graveolens* の根(as the main component of an inseparable mixt. of 2-alkylquinolones contg. the 2-dodecyl, 2-tridecyl and 2-tetradecyl homologues)(ミカン科)
[用途] Antagonist of Dihydrostreptomycin
[性状] 結晶 (Me_2CO)
[融点] Mp 130-132 ℃

----------文献----------

Cornforth, J.W. et al., Biochem. J., 1956, 63, 124,（分離）
Reisch, T. et al., Phytochemistry, 1975, 14, 840,（分離, IR, H-NMR）
Sugimoto, T. et al., Chem. Pharm. Bull., 1988, 36, 4453,（分離, UV, IR, H-NMR, C13-NMR, Mass, 誘導体）

Sugimoto, T. et al., Chem. Pharm. Bull., 1988, 36, 4453, (分離, UV, IR, H-NMR, C13-NMR, Mass, 誘導体)

§ 2-Undecyl-4(1*H*)-quinolinone; *N*-Oxide

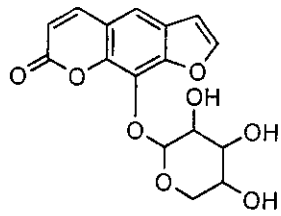


[化学名・別名]2-Undecyl-4(1*H*)-quinolinone *N*-oxide
[CAS No.]2503-86-8
[化合物分類]アルカロイド化合物(Simple quinoline alkaloids)
[構造式]
[分子式]$C_{20}H_{29}NO_2$
[分子量]315.455
[天然基原]Metab. of *Pseudomonas pyocyanea* の代謝物. 次の植物から分離: *Ptelea trifoliata* の花, *Ruta graveolens* の根(ミカン科)
[性状]葉状結晶
[融点]Mp 148.5-149.5 ℃

----------文 献----------

Cornforth, J.W. et al., Biochem. J., 1956, 63, 124, (分離)
Reisch, T. et al., Phytochemistry, 1975, 14, 840, (分離, IR, H-NMR)
Sugimoto, T. et al., Chem. Pharm. Bull., 1988, 36, 4453, (分離, UV, IR, H-NMR, C13-NMR, Mass, 誘導体)

§ Xanthotoxol; *O*-β-L-Arabinopyranoside



[化学名・別名]Xanthotoxol arabinoside
[CAS No.]160845-06-7
[化合物分類]ベンゾピラノイド(7,8-Dioxygenated coumarins)、ベンゾピラノイド(Furanocoumarins)
[構造式]
[分子式]$C_{16}H_{14}O_8$
[分子量]334.282
[天然基原]*Ruta graveolens*
[性状]針状結晶
[融点]Mp 180-182 ℃
[比旋光度]:$[\alpha]_D^{25}$ +12 (MeOH)
UV: [neutral] λ_{max} 220 ; 250 ; 260 ; 300 (溶媒の報告はない)

----------文 献----------

Späth, E. et al., Monatsh. Chem., 1938, 72, 179, (分離, 合成法)
Gellert, M. et al., Phytochemistry, 1972, 11, 2894, (分離)
Sharma, B.R. et al., Indian J. Chem., Sect. B, 1980, 19, 162, (分離)
Jain, A.K. et al., J. Indian Chem. Soc., 1991, 68, 452, (配糖体)
Srivastava, S.K. et al., Fitoterapia, 1994, 65, 301-303, (arabinoside)

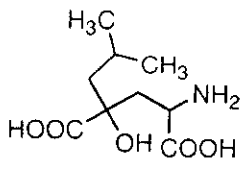
*********ルリジサ (Borage) *********

§§ムラサキ科ルリジサ(*Borago officinalis* L.)の花, 茎葉または根。
本調査研究では、成分に関する文献はなかった。

*********レセダ (Reseda) *********

§§モクセイソウ科モクセイソウ(*Reseda odorata* L.)の花。

§ 2-Amino-4-hydroxy-4-(2-methylpropyl)pentanedioic acid; (2*S*,4*S*)-form

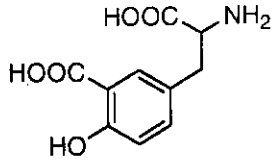


[化学名・別名]L-*erythro*-form
[CAS No.]50632-61-6
[化合物分類]アミノ酸とペプチド(Non-protein α-aminoacids)
[構造式]
[分子式]$C_9H_{17}NO_5$
[分子量]219.237
[天然基原]*Reseda odorata* の花の D-galactopyranoside として見つかる
[比旋光度]:$[\alpha]_D^{25}$ -13 (c, 0.4 in H_2O), $[\alpha]_D^{25}$ +2 (c, 0.2 in 6 *M* HCl)
[PKa 値]pK_{a1} 1.7; pK_{a2} 3.5; pK_{a3} 9.7

----------文 献----------

Kaas, K. et al., Acta Chem. Scand., Ser. A, 1977, 31, 364, (結晶構造, 絶対構造)

§ 3-Carboxytyrosin; (*S*)-form

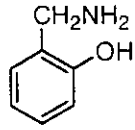


[化学名・別名]L-form
[CAS No.]4303-95-1
[化合物分類]アミノ酸とペプチド(Non-protein α-aminoacids)
[構造式]
[分子式]$C_{10}H_{11}NO_5$
[分子量]225.201
[天然基原]*Reseda odorata*, *Lunaria annua* の種子
[性状]結晶 (H_2O)
[融点]Mp 273 ℃で分解
[比旋光度]:$[\alpha]_D^{24}$ -30.5 (c, 0.6 in 0.2M phosphate buffer at pH 7)

---文献---

Larsen, P.O. et al., Acta Chem. Scand., Ser. B, 1977, 31, 109; 826

§ 2-Hydroxybenzylamine

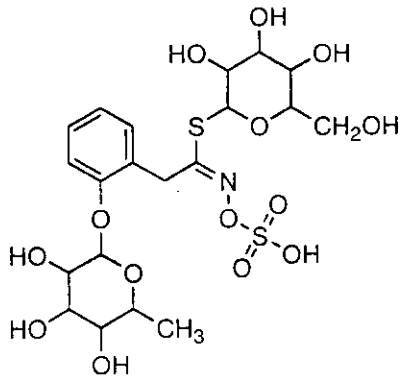


[化学名・別名]2-(Aminomethyl)phenol(CAS 名). α-Amino-*o*-cresol(旧 CAS 名). Salicylamine
[CAS No.]932-30-9
[化合物分類]アルカロイド化合物(Simple acyclic amine alkaloids; 1 × N), 単環芳香族(Simple phenols)
[構造式]
[分子式]C_7H_9NO
[分子量]123.154
[天然基原]*Reseda odorata* の花
[性状]結晶 (EtOH/petrol)もしくは塊
[融点]Mp 97-99 ℃. Mp 129 ℃ (prob. refers to a hydrate)
[その他のデータ]Sublimes

---文献---

Sorensen, H., Phytochemistry, 1970, 9, 865-870, (分離)
Olsen, O. et al., Phytochemistry, 1980, 19. 1783-1787, (分離, H-NMR, C13-NMR)
Reany, O. et al., J.C.S. Perkin 2, 2000, 1819-1831, (合成法, H-NMR, C13-NMR, Mass)

§ Isoglucosinalbin; *O*-α-L-Rhamnopyranoside

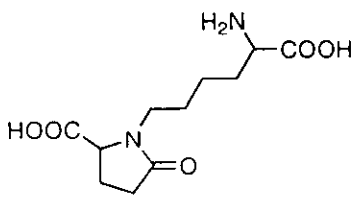


[化学名・別名]2-(α-L-Rhamnopyranosyloxy)benzyl glucosinolate
[CAS No.]73518-99-7
[化合物分類]炭水化物(Glycosinolates)
[構造式]
[分子式]$C_{20}H_{29}NO_{14}S_2$
[分子量]571.579
[天然基原]次の植物から分離: *Reseda odorata*
UV: [neutral] λ_{max} 270 ; 276 (溶媒の報告はない)

---文献---

Olsen, O. et al., Phytochemistry, 1979, 18, 1547-1552, (分離, C13-NMR, H-NMR)

§ Pyrosaccharopine; (2*S*,2'*S*)-form



[CAS No.]38495-84-0
[化合物分類]アミノ酸とペプチド(Non-protein α-aminoacids)
[構造式]
[分子式]$C_{11}H_{18}N_2O_5$
[分子量]258.274
[天然基原]色々なキノコから分離; *Fagopyrum esculentum*, *Reseda odorata*
[性状]結晶 (Me_2CO 溶液); 針状結晶(EtOH 溶液)
[融点]Mp 245-248 ℃で分解 (225-227 ℃)
[比旋光度]:$[\alpha]_D$ +9.3 (c, 0.5 in H_2O). $[\alpha]_D$ +18.2 (c, 0.9 in 1 *M* HCl)

[融点]Mp 245-248 ℃で分解 (225-227 ℃)
[比旋光度]:[α]$_D$ +9.3 (c, 0.5 in H_2O). [α]$_D$ +18.2 (c, 0.9 in 1 *M* HCl)
[その他のデータ]Possibly an artifact in some cases

----------文 献----------

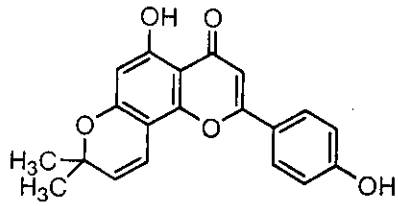
Larsen, P.O. et al., Acta Chem. Scand., 1972, 26, 2562, (合成法)
Soerensen, H., Phytochemistry, 1976, 15, 1527, (分離)
Aoyagi, Y. et al., Agric. Biol. Chem., 1982, 46, 987, (分離)
Burkard, U. et al., Annalen, 1986, 1030, (合成法, C13-NMR, H-NMR)

*********レモン (Lemon) *********

§§ミカン科レモン(*Citrus limon* (L.) Burman f.)の果実。

§ Atalantoflavone

[化学名・別名]5-Hydroxy-2-(4-hydroxyphenyl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*']dipyran-4-one (CAS名). Limonianin
[CAS No.]119309-02-3
[化合物分類]フラボノイド(Cyclised C-isopentenylated flavonoids), フラボノイド(Flavones; 3 × O-置換基)
[構造式]



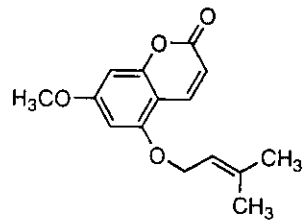
[分子式]$C_{20}H_{16}O_5$
[分子量]336.343
[天然基原]*Atalantia racemosa* の葉, *Citrus limon* の根皮
[性状]黄色の針状結晶 (Me_2CO/hexane)
[融点]Mp 289-290 ℃ (275-277 ℃)
[その他のデータ]Physical data varies between Atalantoflavone and Limonianin

----------文 献----------

Banerji, A. et al., Phytochemistry, 1988, 27, 3637, (分離, 構造決定, 合成法)
Chang, S.-H., Phytochemistry, 1990, 29, 351, (Limonianin)

§ 5,7-Dihydroxy-2*H*-1-benzopyran-2-one; 5-*O*-(3-Methyl-2-butenyl), 7-Me ether

[化学名・別名]7-Methoxy-5-prenyloxycoumarin
[CAS No.]35590-41-1
[化合物分類]ベンゾピラノイド(5,7-Dioxygenated coumarins)
[構造式]



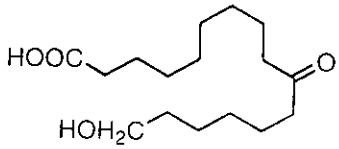
[分子式]$C_{15}H_{16}O_4$
[分子量]260.289
[天然基原]次の植物から分離: *Citrus limon*, *Heracleum* spp.
[融点]Mp 90-92 ℃

----------文 献----------

Talapatra, B. et al., Indian J. Chem., 1975, 13, 835, (分離, 誘導体)
Günther, D.H. et al., Org. Magn. Reson., 1975, 7, 339, (C13-NMR, 誘導体)
Bhardwaj, D.K. et al., Phytochemistry, 1976, 15, 1789, (Lacoumarin)
Gray, A.I. et al., J.C.S. Perkin 2, 1978, 391, (H-NMR)
Gashimov, N.F. et al., Khim. Prir. Soedin., 1978, 14, 653; Chem. Nat. Compd. (Engl. Transl.), 1978, 14, 563, (誘導体)
Joseph-Nathan, P. et al., J. Het. Chem., 1984, 21, 1141, (H-NMR, 誘導体)
Ngadjui, B.J. et al., Phytochemistry, 1989, 28, 585, (Anisocoumarin B)
Ito, C. et al., Chem. Pharm. Bull., 1996, 44, 2231, (5-Geranyloxy-7-hydroxycoumarin)

§ 10,16-Dihydroxyhexadecanoic acid; 10-Ketone

[化学名・別名]16-Hydroxy-10-oxohexadecanoic acid
[CAS No.]53833-25-3
[化合物分類]脂肪族化合物(Saturated unbranched carboxylic acids and lactones)
[構造式]

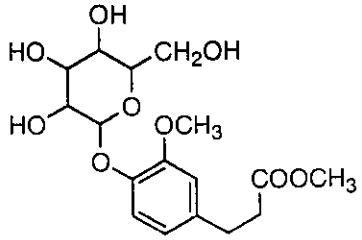


[分子式]$C_{16}H_{30}O_4$
[分子量]286.411

Espelie, K.E. et al., Lipids, 1978, 13, 832, (分離, CD)
Hu, Z. et al., Phytochemistry, 1988, 23, 679, (分離)
Ray, A.K. et al., Phytochemistry, 1995, 38, 1361, (分離, Mass)

§ 3-(3,4-Dihydroxyphenyl)propanoic acid; 3-Me ether, 4-*O*-β-D-glucopyranoside, Me ester

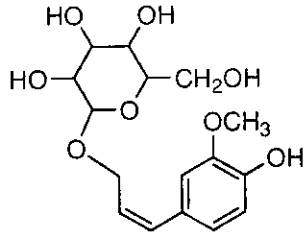
[化学名・別名]Citrusin E
[CAS No.]134860-03-0
[化合物分類]単環芳香族(Simple phenylpropanoids)
[構造式]
[天然基原]次の植物から分離: レモン *Citrus limon* のオイル
[用途]ラットの低血圧症薬
[融点]Mp 108 ℃
[比旋光度]:[α]$_D^{17}$ -35.68 (c, 0.1 in MeOH)



文献
Zetsche, F. et al., Helv. Chim. Acta, 1927, 10, 472, (分離)
Matsubara, Y. et al., Agric. Biol. Chem., 1991, 55, 647, (Citrusins)

§ 3-(3,4-Dihydroxyphenyl)-2-propen-1-ol; (*E*)-form, 3'-Me ether, 1-*O*-β-D-glucopyranoside

[化学名・別名]Citrusin D. Isoconiferin
[CAS No.]65995-51-9
[化合物分類]単環芳香族(Simple phenylpropanoids)
[構造式]
[分子式]$C_{16}H_{22}O_8$
[分子量]342.345
[天然基原]次の植物から分離: *Citrus limon*, *Citrus unshiu*, *Fortunella japonica*, *Pinus sylvestris*
[用途]抗高血圧作用を示す
[比旋光度]:[α]$_D^{20}$ -16.9 (c, 4.1 in MeOH)
UV: [neutral] λ_{max} 275 (ε 5000) (MeOH)



文献
Sawabe, A. et al., Nippon Kagaku Kaishi, 1988, 62, 1067, (Citrusin D)
Greca, M.D. et al., Phytochemistry, 1998, 49, 1299-1304, (Coniferyl alcohol, Citrusin D)

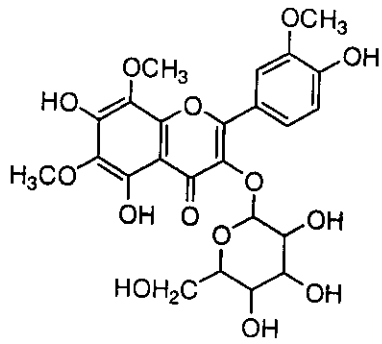
§ Heptadecanal

[CAS No.]629-90-3
[化合物分類]脂肪族化合物(Saturated unbranched aldehydes and ketones)
[構造式]$H_3C(CH_2)_{15}CHO$
[分子式]$C_{17}H_{34}O$
[分子量]254.455
[天然基原]次の植物から分離: レモンオイル(*Citrus limon*)
[性状]結晶 (petrol)
[融点]Mp 36 ℃
[沸点]Bp$_{26}$ 204 ℃

文献
Ikeda, R.M. et al., J. Agric. Food Chem., 1962, 10, 98, (分離)
Rao, P.V. et al., J. Lipid Res., 1967, 8, 380, (合成法, ガスクロマト)
Org. Synth., 1971, 51, 39, (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]

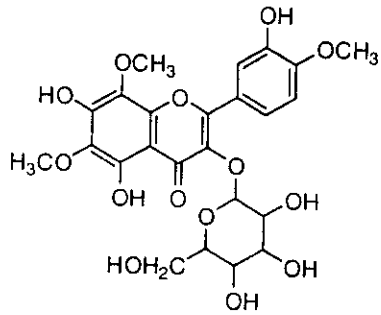


[分子式] $C_{24}H_{26}O_{14}$
[分子量] 538.461
[天然基原] 次の植物から分離: *Citrus limon, Primula officinalis*
[性状] 黄色のプリズム結晶 (H_2O)
[融点] Mp 163 ℃. Mp 203-204 ℃ (dimorph.)

---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)

§ Isolimocitrol 3-glucoside
[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
[天然基原] 次の植物から分離: *Citrus limon*
[性状] 結晶 (MeOH 溶液)
[融点] Mp 220-225 ℃

---文 献---

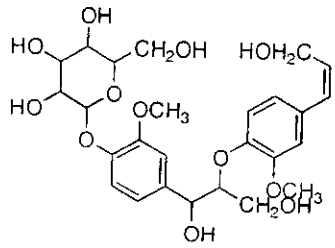
Gentili, B. et al., Tetrahedron, 1964, 20, 2313, (Limocitrol, Isolimocitrol, 3-glucoside)

§ Hexadecanal(CAS 名)
[化学名・別名] Palmitic aldehyde. Palmitaldehyde
[CAS No.] 629-80-1
[化合物分類] 脂肪族化合物(Saturated unbranched aldehydes and ketones)
[構造式] $H_3C(CH_2)_{14}CHO$
[分子式] $C_{16}H_{32}O$
[分子量] 240.428
[天然基原] Occurs as an enol ether of diacylglycerol (plasmalogens). 次の植物から分離: レモンオイル (*Citrus limon*), 細菌脂質. Common constit. of lepidopteran sex pheromones
[融点] Mp 34 ℃
[沸点] Bp_{29} 200-202 ℃
[その他のデータ] Polymerises on standing to the trimer (Mp 73 ℃)
[販売元] Sigma:J6361

---文 献---

Le Sueur, H.R., J.C.S., 1905, 87, 1888, (合成法)
Ikeda, R.M. et al., J. Agric. Food Chem., 1962, 10, 98, (分離)
Goldfine, H., J. Biol. Chem., 1964, 239, 2130, (分離)
Christiansen, K. et al., Lipids, 1969, 4, 421, (Mass, acetal)
Degani, I. et al., J.C.S. Perkin 1, 1976, 323, (合成法)

§ 1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxy-1-propenyl)-2-methoxyphenoxy]-1,3-propanediol; 4-*O*-β-D-Glucopyranoside
[化学名・別名] Citrusin A
[CAS No.] 105279-09-2
[化合物分類] リグナン化合物(Neolignans)
[構造式]



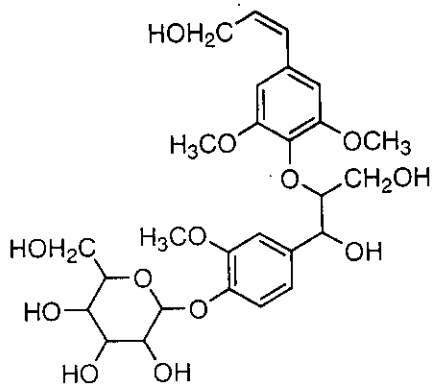
[分子式] $C_{26}H_{34}O_{12}$
[分子量] 538.547
[天然基原] 次の植物から分離: レモン(*Citrus limon*), マルバキンカン

Fortunella japonica)の皮
[融点]Mp 108-109 ℃
[比旋光度]:[α]$_D^{20}$ -17.2 (c, 0.3 in MeOH)

文献

Sawabe, A. et al., Nippon Kagaku Kaishi, 1986, 60, 593, (Citrusins)
Matsubara, Y. et al., Agric. Biol. Chem., 1991, 55, 647, (Citrusin A)

§ 1-(4-Hydroxy-3-methoxyphenyl) -2-[4-(3-hydroxy-1-propenyl) -2-methoxyphenoxy] -1,3-propanediol; 5'-Methoxy, 4-*O*-β-D-glucopyranoside



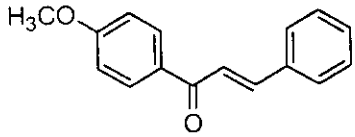
[化学名・別名]Citrusin B
[CAS No.]105279-10-5
[化合物分類]リグナン化合物(Neolignans)
[構造式]

[分子式]$C_{27}H_{36}O_{13}$
[分子量]568.574
[天然基原]次の植物から分離: レモン(*Citrus limon*), マルバキン(*Fortunella japonica*), *Eucommia ulmoides* の樹皮
[融点]Mp 105-106 ℃
[比旋光度]:[α]$_D^{20}$ -11.3 (c, 0.3 in MeOH)

文献

Sawabe, A. et al., Nippon Kagaku Kaishi, 1986, 60, 593, (Citrusins)
Deyama, T. et al., Chem. Pharm. Bull., 1987, 35, 1803, (Citrusin B)

§ 1-(4-Hydroxyphenyl)-3-phenyl-2-propen-1-one; Me ether

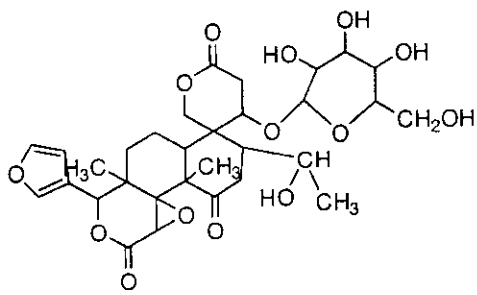


[化学名・別名]4'-Methoxychalcone
[CAS No.]22966-19-4
[その他の CAS No.]959-23-9
[化合物分類]フラボノイド(Chalcone flavonoids; 1 × O-置換基)
[構造式]
[分子式]$C_{16}H_{14}O_2$
[分子量]238.285
[天然基原]*Citrus limon* に存在すると報告された(実証されていない)
[性状]針状結晶(MeOH)
[融点]Mp 107 ℃

文献

Peyron, L., C. R. Hebd. Seances Acad. Sci., 1963, 257, 235, (分離, 誘導体)
Jain, A. et al., Phytochemistry, 1982, 21, 957, (配糖体)
Zhengdong, L. et al., Acta Cryst. C, 1992, 48, 751, (結晶構造, Me ether)

§ Ichangin; 4-*O*-β-D-Glucopyranoside



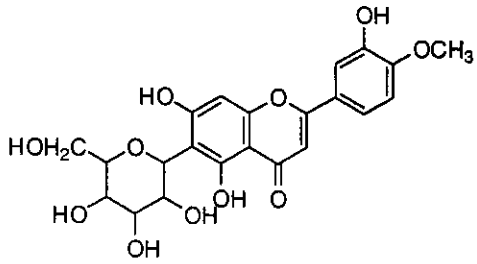
[化合物分類]テルペノイド(Ring cleaved tetranortriterpenoids)
[構造式]

[分子式]$C_{32}H_{42}O_{14}$
[分子量]650.675
[天然基原]次の植物から分離: *Citrus limon*
[性状]結晶
[融点]Mp 268-270 ℃で分解
[比旋光度]:[α]$_D^{20}$ -0.7 (c, 0.72 in MeOH)

文献

Dreyer, D.L., J.O.C., 1966, 31, 2279
Matsubara, Y. et al., Agric. Biol. Chem., 1990, 54, 1143, (誘導体)

§ **Isoorientin; 4'-Me ether**
[化学名・別名]6-β-D-Glucopyranosyldiosmetin
[CAS No.]15822-82-9
[化合物分類]フラボノイド(Flavones; 4 × O-置換基)
[構造式]

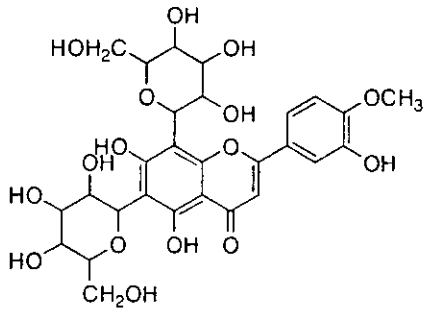


[分子式]$C_{22}H_{22}O_{11}$
[分子量]462.409
[天然基原]次の植物から分離: *Citrus limon*
[性状]結晶 (MeOH)
[融点]Mp 243-245 ℃

文 献

Chulia, A.J. et al., J. Nat. Prod., 1985, 48, 480, (6"-glucosyl derivs)
Congora, C. et al., Helv. Chim. Acta, 1986, 69, 251, (分離)
Kato, T. et al., Chem. Pharm. Bull., 1990, 38, 2277, (Acetylisoorientin)
Kuo, S.-H. et al., Phytochemistry, 1996, 41, 309, (6"-Caffeoylisoorientin)
Zheng, S. et al., Indian J. Chem., Sect. B, 1997, 36, 955-957, (6-Galloylisoorientin)

§ **Lucenin 2; 4'-Me ether**
[化学名・別名]6,8-Diglucopyranosyl-3',5,7-trihydroxy-4'-methoxyflavone. 6,8-Diglucopyranosyldiosmetin. 6,8-Diglucosyldiosmetin
[CAS No.]98813-28-6
[化合物分類]フラボノイド(Flavones; 4 × O-置換基)
[構造式]

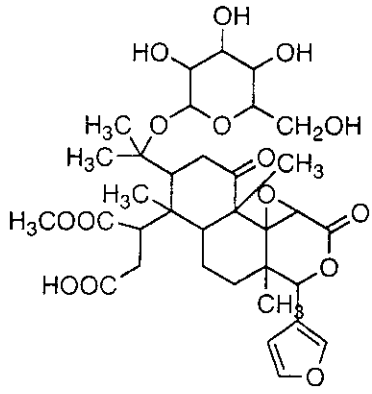


[分子式]$C_{28}H_{32}O_{16}$
[分子量]624.551
[天然基原]次の植物から分離: 皮をむいた *Citrus limon*
[性状]Gelatinous ppt.

文 献

Seikel, M.K. et al., Phytochemistry, 1966, 5, 439, (分離)
Osterdahl, B.G., Acta Chem. Scand., Ser. B, 1978, 32, 93, (分離, 構造決定)
Kumamoto, H. et al., CA, 1985, 103, 183426, (誘導体)

§ **Nomilinic acid; *O*-β-D-Glucopyranoside**
[CAS No.]113301-65-8
[化合物分類]テルペノイド(Ring cleaved tetranortriterpenoids)
[構造式]



[分子式]$C_{34}H_{46}O_{15}$
[分子量]694.728
[天然基原]次の植物から分離: レモン *Citrus limon*
[性状]結晶
[融点]Mp 250-252 ℃で分解
[比旋光度]:$[\alpha]_D^{20}$ +35.44 (c, 0.75 in MeOH)

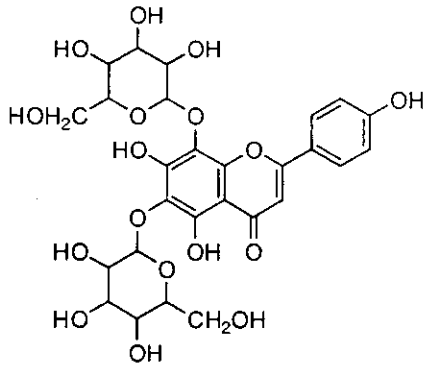
文 献

Dreyer, D.L., J.O.C., 1965, 30, 749, (Deacetylnomilin)
Dreyer, D.L. et al., Phytochemistry, 1966, 5, 367, (レビュー)
Ahmed, F.R. et al., Can. J. Chem., 1978, 56, 1020, (7-Acetoxydihydronomilin)
Herman, Z. et al., Phytochemistry, 1987, 26, 2247, (生合成)

Matsubara, Y. et al., Agric. Biol. Chem., 1990, 54, 1143, (配糖体)
Zhen, S. et al., Indian J. Chem., Sect. B, 1997, 36, 374-376, (Microulins)
Liu, J. et al., Indian J. Heterocycl. Chem., 1999, 9, 69-70, (Deacetylnomilin gallate)

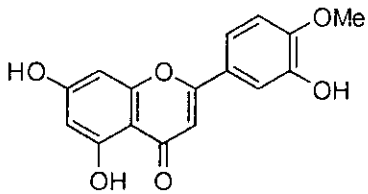
§ Pentadecanal
[CAS No.]2765-11-9
[化合物分類]脂肪族化合物(Saturated unbranched aldehydes and ketones)
[構造式]$H_3C(CH_2)_{13}CHO$
[分子式]$C_{15}H_{30}O$
[分子量]226.401
[天然基原]次の植物から分離: *Cinnamomum micranthum* の精油, レモンオイル(*Citrus limon*)
[融点]Mp 24-25 ℃
[沸点]Bp_{25} 185 ℃, $Bp_{0.2}$ 103-106 ℃
[その他のデータ]Readily forms a polymer Mp 69-70 ℃
----------文献----------
Lauer, W.M. et al., J.A.C.S., 1941, 63, 1153, (合成法)
Fujita, Y. et al., CA, 1944, 41, 3509; 1963, 58, 10506, (分離)
Ikeda, R.M. et al., J. Agric. Food Chem., 1962, 10, 98, (分離)
Org. Synth., 1971, 51, 39, (合成法)
Enders, D. et al., Chem. Eur. J., 1995, 1, 382, (合成法, H-NMR, C13-NMR)

§ 4',5,6,7,8-Pentahydroxyflavone; 6,8-Di-*O*-β-D-glucopyranoside
[CAS No.]90456-53-4
[化合物分類]フラボノイド(Flavones; 5 × O-置換基)
[構造式]



[分子式]$C_{27}H_{30}O_{17}$
[分子量]626.524
[天然基原]*Desmodium styracifolium*, *Citrus limon*
----------文献----------
Kagan, H.B. et al., J.O.C., 1966, 31, 1629, (分離)
Chhabra, S.C. et al., Indian J. Chem., Sect. B, 1971, 14, 651, (Desmethoxysudachin)
Bohlmann, F. et al., Phytochemistry, 1979, 18, 1375, (7-Hydroxy-4',5,6,8-tetramethoxyflavone)
Ward, R.S., Synthesis, 1992, 719, (レビュー, 合成法, 成書)
Wang, J. et al., Nat. Prod. Sci., 1998, 4, 38-41, (6-Me ether, Isothymusin 8-glucoside)
Grayer, R.J. et al., Phytochemistry, 1998, 47, 779-782, (Isothymusin 8-glucoside)

§ 3',5,7-Trihydroxy-4'-methoxyflavone
[化学名・別名]Diosmetin. Salinigricoflavonol. Vitamin P
[CAS No.]520-34-3
[化合物分類]フラボノイド(Flavones; 4 × O-置換基)
[構造式]



[分子式]$C_{16}H_{12}O_6$
[分子量]300.267
[天然基原]次の植物から分離: *Valeriana* spp.の地上部, *Digitalis* spp.の葉, レモンの皮(*Citrus limon*), その他
[用途]Used as 0.01 *M* soln. in MeOH for photometric detn. of Fe(III) (λ_{max} 480 nm, ε 14000, pH 6.5)
[性状]青白い黄色の結晶 (EtOH)
[融点]Mp 258-259 ℃ (250-253 ℃), Mp 228-230 ℃
[溶解性]メタノール, エタノールに可溶
UV: [neutral] λ_{max} 253 (ε 19000); 268 (ε 17800); 345 (ε 21000) (MeOH) (Berdy)
----------文献----------
Horowitz, R.M. et al., J.O.C., 1956, 21, 1184, (分離)

Horowitz, R.M. et al., J.O.C., 1956, 21, 1184, (分離)
Plouvier, V., C. R. Hebd. Seances Acad. Sci. Ser. D, 1966, 263, 439, (分離, 構造決定)
Borisov, M.I. et al., Khim. Prir. Soedin., 1969, 5, 371; Chem. Nat. Compd. (Engl. Transl.), 1969, 5, 309,
Brieskorn, C.H. et al., Arch. Pharm. (Weinheim, Ger.), 1971, 304, 557, (分離)
Le Quesne, P.W. et al., J.C.S. Perkin 1, 1978, 1572, (分離, UV, H-NMR)

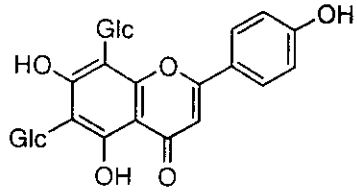
§ Vicenin 2

[化学名・別名] 6,8-Di-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one (CAS 名). 6,8-Di-*C*-glucosyl-4',5,7-trihydroxyflavone. 6,8-Di-*C*-glucopyranosylapigenin. 6,8-Di-*C*-glucosylapigenin

[CAS No.] 23666-13-9

[化合物分類] フラボノイド (Flavones; 3 × O-置換基)

[構造式]



[分子式] $C_{27}H_{30}O_{15}$

[分子量] 594.525

[天然基原] *Vitex lucens* の木部, レモン *Citrus limon*, その他多くの植物属

[性状] 結晶 (H_2O)

[融点] Mp 233-236 ℃ (214-216 ℃)

[比旋光度]: $[\alpha]_D$ +25 (c, 0.21 in Py), $[\alpha]_D$ +71 (c, 0.36 in H_2O)

----------文 献----------

Seikel, M.K. et al., Phytochemistry, 1966, 5, 439, (分離)
Gentili, B. et al., J.O.C., 1968, 33, 1571, (分離, 構造決定, H-NMR)
Bouillant, M.L. et al., Phytochemistry, 1984, 23, 2653, (6"-glucoside)
Baktiar, A. et al., Phytochemistry, 1990, 29, 1339, (6,8-Diglucosylgenkwanin)
Hussein, S.A.M. et al., Phytochemistry, 1997, 45, 1529, (diglucosyl)

*********レモングラス (Lemongrass) *********

§§イネ科レモングラス (*Cymbopogon citratus* (de Candolle) Stapf)

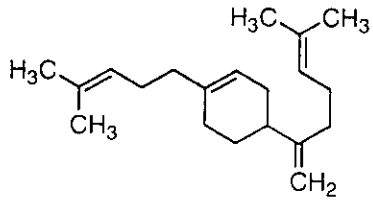
§ α-Camphorene

[化学名・別名] 4-(5-Methyl-1-methylene-4-hexenyl)-1-(4-methyl-3-pentenyl) cyclohexene (CAS 名). Paracamphorene. *p*-Camphorene. Dimyrcene

[CAS No.] 532-87-6

[化合物分類] テルペノイド (Miscellaneous monocyclic diterpenoids)

[構造式]



[分子式] $C_{20}H_{32}$

[分子量] 272.473

[天然基原] 樟脳オイル, *Humulus lupulus* のオイル, また *Nothopanax simplex*, *Dacrydium biforme*, *Cymbopogon citratus*, その他

[性状] オイル

[沸点] $Bp_{0.03}$ 110 ℃

----------文 献----------

Lammens, H. et al., Bull. Soc. Chim. Belg., 1968, 77, 497, (分離)
Vig, O.P. et al., J. Indian Chem. Soc., 1986, 63, 507, (合成法)

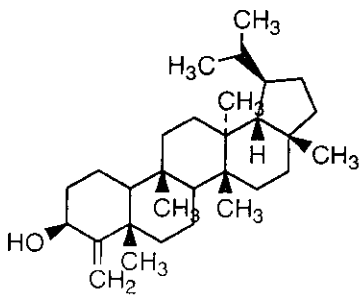
§ Cymbopogonol

[化学名・別名] D:A-Friedo-4(23)-lupen-3 β-ol

[CAS No.] 60816-94-6

[化合物分類] テルペノイド (Nor-, friedo- and secolupane triterpenoids)

[構造式]



[分子式] $C_{30}H_{50}O$

[分子量] 426.724

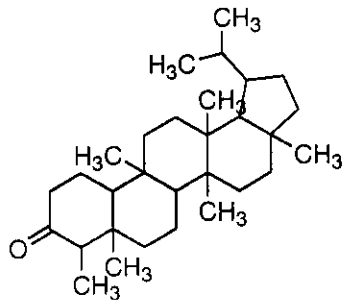
[天然基原] *Cymbopogon citratus*

[性状] 結晶 (EtOH)

[融点] Mp 191-193 ℃

Yokoyama, Y. et al., Tet. Lett., 1980, 3701, (構造決定)

§ Cymbopogonol; 4 α,23-Dihydro, 3-ketone

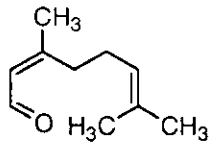


[化学名・別名]Cymbopogone
[CAS No.]57789-30-7
[化合物分類]テルペノイド(Nor-, friedo- and secolupane triterpenoids)
[構造式]
[分子式]$C_{30}H_{50}O$
[分子量]426.724
[天然基原]次の植物から分離: *Cymbopogon citratus*
[性状]結晶 (EtOH)
[融点]Mp 262-265 ℃

----------文献----------

Yokoyama, Y. et al., Chem. Lett., 1979, 1463, (合成法, 結晶構造)
Yokoyama, Y. et al., Tet. Lett., 1980, 3701, (構造決定)

§ 3,7-Dimethyl-2,6-octadienal; (*E*)-form



[CAS No.]141-27-5
[化合物分類]テルペノイド(Acyclic monoterpenoids)
[構造式]
[分子式]$C_{10}H_{16}O$
[分子量]152.236
[天然基原]Occurs in レモングラスオイル(*Cymbopogon citratus*), レモン, オレンジ, その他多くの精油. Sex pheromone of the parasitic wasp *Itoplectis conquisitor*; recruiting pheromone for honey bees, alarm pheromone for various formicine ants, the myrmicine ant *Atta sexdens* and the bee *Lestrimelitta limao*
[用途]食品, 香水工業で重要
[沸点]Bp 229 ℃. Bp_{20} 119 ℃
[屈折率]n^{20}_{D} 1.4898
[化学物質毒性データ総覧(RTECS)登録番号]RG5075100

----------文献----------

Simonsen, J.L. et al., The Terpenes, 2nd Ed., Cambridge Univ. Press, 1947, 1, 83, (レビュー)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 371, (生育)
Vortkevich, S.A., Parfums, Cosmet. Savons Fr., 1972, 2, 407, (レビュー)
Opdyke, D.L.J., Food Cosmet. Toxicol., 1979, 17, 259, (レビュー, 毒性)

***RTECS (化学物質毒性データ) ***

生体影響物質　　: 農業化学品.

健康障害に関するデータ

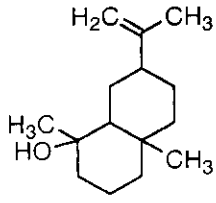
急性毒性に関するデータ

〈〈試験方法〉〉 LD50 試験(50%致死量試験).
曝露経路　　: 経口投与.
被験動物　　: げっ歯類-ラット.
投与量・期間 : 500 mg/kg
毒性影響　　: 致死量以外に毒性影響に関する報告はない.

参照文献
French Demande Patent Document.2448856

§§ イネ科東インドレモングラス(*Cymbopogon flexuosus* (de Candolle) Stapf)の全草。

§ 11-Eudesmen-4-ol; (4 α,5 α,7 α,10 β)-form



[化学名・別名]Isointermedeol
[CAS No.]71963-78-5
[化合物分類]テルペノイド(Simple eudesmane sesquiterpenoids)
[構造式]
[分子式]$C_{15}H_{26}O$
[分子量]222.37
[天然基原]*Cymbopogon flexuosus*

[分子式] $C_{15}H_{26}O$
[分子量] 222.37
[天然基原] *Cymbopogon flexuosus*
[性状] 塊
[融点] Mp 40-41 ℃
[比旋光度]: $[\alpha]_D$ +2 (c, 3.3 in MeOH)

----------文 献----------

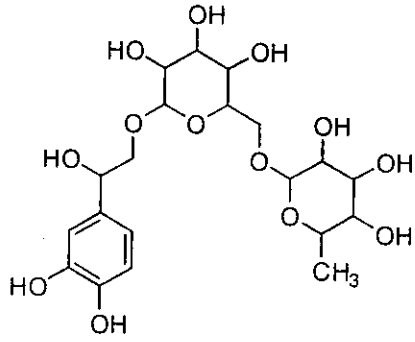
Thappa, R.K. et al., Phytochemistry, 1979, 18, 671, (Isointermedeol)
Sakar, M.K. et al., Fitoterapia, 1999, 70, 103-105, (Intermedeol, H-NMR, C13-NMR)

*********レンギョウ (Rengyo) *********

§§モクセイ科レンギョウ(*Forsythia suspensa* Vahl)の果実。

§ 1-(3,4-Dihydroxyphenyl)-1,2-ethanediol; (*S*)-form, 2-*O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside]

[化学名・別名] Forsythoside D
[CAS No.] 84233-74-9
[化合物分類] 単環芳香族(Simple phenols)
[構造式]



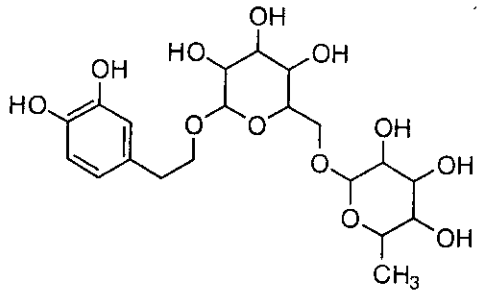
[分子式] $C_{29}H_{36}O_{15}$
[分子量] 478.449
[天然基原] *Forsythia suspensa* の果実
[比旋光度]: $[\alpha]_D$ -30.5 (MeOH)
[溶解性] BERDY SOL: メタノールに可溶; ヘキサンに難溶
UV: [neutral] λ_{max} 220 ; 233 ; 250 ; 290 ; 331 (MeOH) (Berdy)

----------文 献----------

Endo, K. et al., Heterocycles, 1982, 19, 2033, (Forsythoside D)

§ 2-(3,4-Dihydroxyphenyl)ethanol; 1-*O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside]

[化学名・別名] Forsythoside E
[CAS No.] 93675-88-8
[化合物分類] 単環芳香族(Simple phenols)
[構造式]



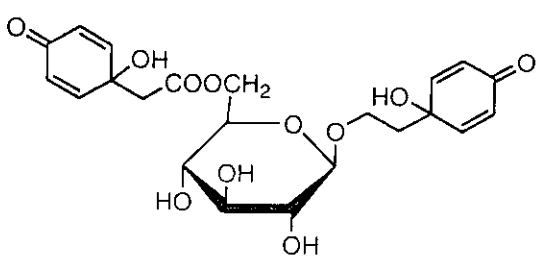
[分子式] $C_{29}H_{36}O_{14}$
[分子量] 462.45
[天然基原] 次の植物から分離: *Forsythia suspensa* の果実
[性状] 青白い黄色の無定型の塊
[比旋光度]: $[\alpha]_D$ -35.3 (c, 0.41 in MeOH)

----------文 献----------

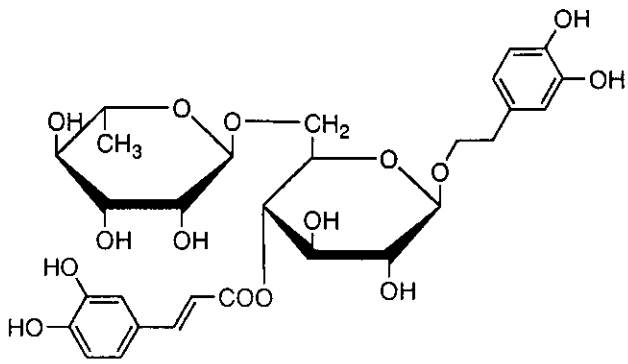
Endo, K. et al., Can. J. Chem., 1984, 62, 2011, (Forsythoside E)
Jimenez, C. et al., Nat. Prod. Rep., 1994, 591, (レビュー, 配糖体)

§ Forsythenside B

[CAS No.] 202721-10-6
[化合物分類] 脂肪族化合物(Monocarbocyclic aldehydes and ketones)
[構造式]

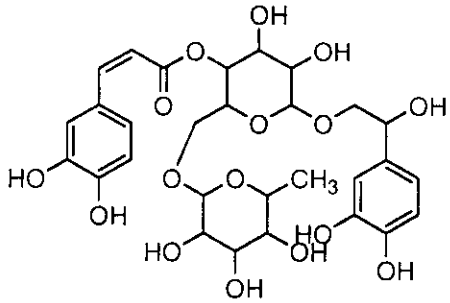


[分子式] $C_{23}H_{26}O_{11}$
[分子量] 466.441
[天然基原] *Forsythia suspensa* の果実
[性状] 無定型の塊 (as penta-Ac)
[比旋光度]: $[\alpha]_D^{20}$ -14.2 (c, 0.1 in MeOH) (penta-Ac)

§ Forsythiaside
[化学名・別名]Forsythoside A
[CAS No.]79916-77-1
[化合物分類]炭水化物(Disaccharides)
[構造式]

[分子式]$C_{29}H_{36}O_{15}$
[分子量]624.594
[天然基原]次の植物から分離: *Forsythia suspensa* の果実
[用途]抗菌作用を示す
[性状]青白く黄色がかった粉末・二水和物
[融点]Mp 144-150 ℃
[比旋光度]:$[\alpha]_D^{20}$ -18.6 (EtOH)

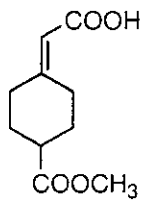
文献

Nishibe, S. et al., Chem. Pharm. Bull., 1982, 30, 1048; 4549

§ Forsythiaside; 2'-Hydroxy
[化学名・別名]Suspensaside. Forsythoside C
[CAS No.]84213-44-5
[化合物分類]AF9200, 炭水化物(Disaccharides)
[構造式]

[分子式]$C_{29}H_{36}O_{16}$
[分子量]640.594
[天然基原]次の植物から分離: *Forsythia suspensa* の果実
[用途]抗菌作用を示す
[性状]粉末
[融点]Mp 177-181 ℃
[比旋光度]:$[\alpha]_D^{18}$ -18.7 (c, 1.7 in MeOH)

文献

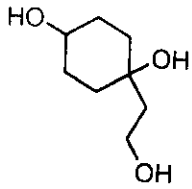
Nishibe, S. et al., Chem. Pharm. Bull., 1982, 30, 1048; 4549

§ (4-Hydroxycyclohexylidene)acetic acid; (ξ)-form, Ac
[化学名・別名](4-Acetoxycyclohexylidene)acetic acid. Suspenolic acid
[CAS No.]202721-07-1
[化合物分類]脂肪族化合物(Monocarbocyclic carboxylic acids and lactones)
[構造式]

[分子式]$C_{10}H_{14}O_4$
[分子量]198.218
[天然基原]*Forsythia suspensa* の果実
[性状]無定型の塊
[融点]Mp 74-76 ℃
[比旋光度]:$[\alpha]_D^{20}$ +4.7 (c, 0.1 in $CHCl_3$)

文献

Walborsky, H.M. et al., J.A.C.S., 1987, 109, 6719-6726, (合成法, H-NMR)
Gawronski, J.K. et al., J.A.C.S., 1987, 109, 6726-6730, (誘導体)
Endo, K. et al., Tetrahedron, 1987, 43, 2681-2688, (合成法, ester)
Ming, D.-S. et al., J. Nat. Prod., 1998, 61, 377-379, (分離, IR, H-NMR, C13-NMR, Mass)

§ **1-(2-Hydroxyethyl)-1,4-cyclohexanediol; (1*RS*,4*RS*)-form**

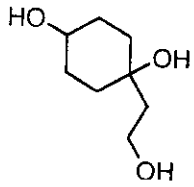


[化学名・別名]Isorengyol
[CAS No.]101489-38-7
[化合物分類]脂肪族化合物(Monocarbocyclic alcohols)
[構造式]
[分子式]$C_8H_{16}O_3$
[分子量]160.213
[天然基原]*Isoplexis chalcantha, Millingtonia hortensis, Forsythia suspensa*
[性状]結晶 ($CHCl_3$)
[融点]Mp 105-106 ℃

----------文 献----------

Endo, K. et al., Can. J. Chem., 1984, 62, 2011, (分離)
Abdallahi, H. et al., Phytochemistry, 1986, 25, 2821, (分離)
Naowsaren, K. et al., Aust. J. Chem., 1989, 42, 1397, (分離, 結晶構造)
Hase, T. et al., Phytochemistry, 1995, 39, 235, (Isorengyoside A)

§ **1-(2-Hydroxyethyl)-1,4-cyclohexanediol; (1*RS*,4*SR*)-form**

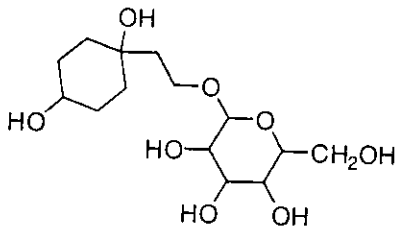


[化学名・別名]Rengyol
[CAS No.]93675-85-5
[化合物分類]脂肪族化合物(Monocarbocyclic alcohols)
[構造式]
[分子式]$C_8H_{16}O_3$
[分子量]160.213
[天然基原]*Isoplexis chalcantham Forsythia suspensa*
[性状]結晶 ($CHCl_3$)
[融点]Mp 118-121 ℃, Mp 123-124 ℃

----------文 献----------

Endo, K. et al., Can. J. Chem., 1984, 62, 2011, (分離)
Abdallahi, H. et al., Phytochemistry, 1986, 25, 2821, (分離)
Naowsaren, K. et al., Aust. J. Chem., 1989, 42, 1397, (分離, 結晶構造)
Seya, K. et al., Phytochemistry, 1989, 28, 1495, (Rengyosides)

§ **1-(2-Hydroxyethyl)-1,4-cyclohexanediol; (1*RS*,4*SR*)-form, 2'-β-D-Glucopyranoside**

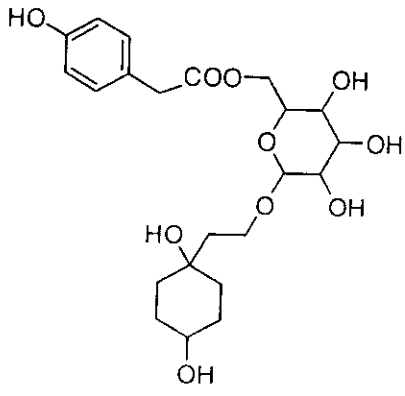


[化学名・別名]Rengyoside A
[CAS No.]101489-32-1
[化合物分類]脂肪族化合物(Monocarbocyclic alcohols)
[構造式]
[分子式]$C_{14}H_{26}O_8$
[分子量]322.355
[天然基原]*Forsythia suspensa*
[性状]無定型の塊
[比旋光度]:$[\alpha]_D^{17}$ -21 (c, 0.2 in MeOH) (-11)

----------文 献----------

Seya, K. et al., Phytochemistry, 1989, 28, 1495, (Rengyosides)

§ **1-(2-Hydroxyethyl)-1,4-cyclohexanediol; (1*RS*,4*SR*)-form, 2'-[4-Hydroxyphenylacetyl-(→6)-β-D-glucopyranoside]**



[化学名・別名]Rengyoside C
[CAS No.]123563-45-1
[化合物分類]脂肪族化合物(Monocarbocyclic alcohols)
[構造式]

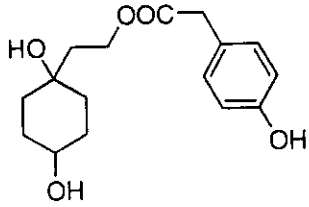
[分子式]$C_{22}H_{32}O_{10}$
[分子量]456.489
[天然基原]*Forsythia suspensa*
[性状]粉末
[比旋光度]:$[\alpha]_D^{23}$ -21.9 (c, 0.06 in 2-propanol)

文献

Naowsaren, K. et al., Aust. J. Chem., 1989, 42, 1397, (分離, 結晶構造)
Seya, K. et al., Phytochemistry, 1989, 28, 1495, (Rengyosides)

§ 1-(2-Hydroxyethyl)-1,4-cyclohexanediol; (1*RS*,4*SR*)-form, 2'-(4-Hydroxyphenylacetyl)

[CAS No.]239135-59-2
[化合物分類]脂肪族化合物(Monocarbocyclic alcohols)
[構造式]



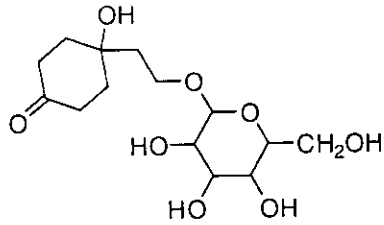
[分子式]$C_{16}H_{22}O_5$
[分子量]294.347
[天然基原]*Forsythia suspensa*

文献

Endo, K. et al., Can. J. Chem., 1984, 62, 2011, (分離)
Abdallahi, H. et al., Phytochemistry, 1986, 25, 2821, (分離)
Naowsaren, K. et al., Aust. J. Chem., 1989, 42, 1397, (分離, 結晶構造)
Seya, K. et al., Phytochemistry, 1989, 28, 1495, (Rengyosides)

§ 1-(2-Hydroxyethyl)-1,4-cyclohexanediol; (1*RS*,4*SR*)-form, 4-Ketone, 2'-β-D-glucopyranoside

[化学名・別名]Rengyoside B
[CAS No.]123563-44-0
[化合物分類]脂肪族化合物(Monocarbocyclic alcohols)
[構造式]



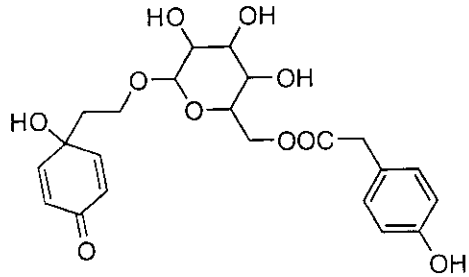
[分子式]$C_{14}H_{24}O_8$
[分子量]320.339
[天然基原]*Forsythia suspensa*
[性状]無定型の塊
[比旋光度]:$[\alpha]_D^{18}$ -17.6 (c, 0.8 in EtOH) (-10.4)

文献

Seya, K. et al., Phytochemistry, 1989, 28, 1495, (Rengyosides)

§ 4-Hydroxy-4-(2-hydroxyethyl)-2,5-cyclohexadien-1-one; 2'-*O*-[6-*O*-(4-Hydroxyphenylacetyl)-β-D-glucopyranoside]

[化学名・別名]Forsythenside A
[化合物分類]脂肪族化合物(Monocarbocyclic aldehydes and ketones)
[構造式]



[分子式]$C_{22}H_{26}O_{10}$
[分子量]450.441
[天然基原]*Forsythia suspensa* の果実
[性状]無定型の塊 (as tetra-Ac)
[比旋光度]:$[\alpha]_D^{20}$ -18.1 (c, 0.1 in MeOH) (tetra-Ac)
[その他のデータ]空気中で非常に不安定

文献

Jensen, S.R. et al., Acta Chem. Scand., 1973, 27, 367, (分離)
Jensen, S.R. et al., Biochem. Syst. Ecol., 1975, 3, 75, (分離)
Eigtved, P. et al., Acta Chem. Scand., Ser. B, 1976, 30, 182, (分離)
Endo, T. et al., Chem. Pharm. Bull., 1978, 26, 2111, (分離)
Ming, D.-S. et al., J. Nat. Prod., 1998, 61, 377-379, (Forsythenside A)

§ 3,3',4',5,7-Pentahydroxyflavone; 3-*O*-[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]

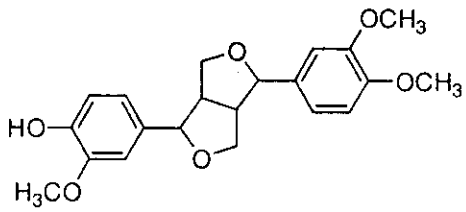
[化学名・別名]Meratin, Meratrin
[CAS No.]27215-04-9
[化合物分類]フラボノイド(Flavonols: 5 × O-置換基), フラボノイド(Flavonoids 構造は一部又は全てが未知)
[構造式]有効な構造式はない

[構造式]有効な構造式はない
[分子式]$C_{27}H_{30}O_{17}$
[分子量]626.524
[天然基原]次の植物から分離: *Meratia praecox*, *Solanum*, *Hibiscus* spp., *Forsythia suspensa*
[性状]淡黄色の針状結晶 (EtOH 溶液)
[融点]Mp 180-183 ℃
[比旋光度]:[α]$_D$ -51.8 (c, 0.49 in MeOH)
[その他のデータ]May be identical with the sophoroside

文 献

Schindler, O., Helv. Chim. Acta, 1945, 28, 1157, (Meratin)
Pakudina, Z.P. et al., Khim. Prir. Soedin., 1965, 1, 67, (分離, 誘導体)
Fraser, A.W. et al., Phytochemistry, 1973, 12, 1787, (分離)
IARC Monog., 1983, 31, 213; Suppl. 7, 71, (レビュー, 毒性)
Vogt, T. et al., Phytochemistry, 1988, 27, (分離)

§ Phillygenin; (+)-form
[CAS No.]487-39-8
[化合物分類]リグナン化合物(Simple furofuranoid lignans)
[構造式]

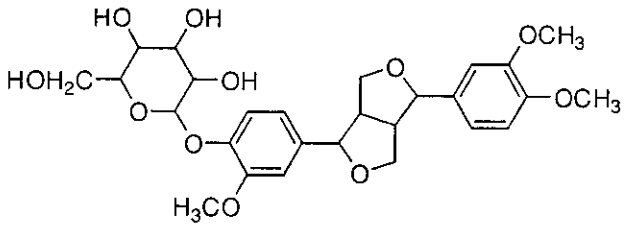


[分子式]$C_{21}H_{24}O_6$
[分子量]372.417
[天然基原]次の植物から分離: *Forsythia suspensa* の果実, また *Phillyrea* spp., *Piper sylvaticum* からも得られる
[融点]Mp 133-134 ℃
[比旋光度]:[α]$_D^{22}$ +120 (c, 0.04 in MeOH)

文 献

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, nos. 1151; 1152, (生育)
Chiba, M. et al., Chem. Pharm. Bull., 1977, 25, 3435, (分離, 構造決定, Phillyrin)
Chiba, M. et al., Phytochemistry, 1980, 19, 335, (分離)
Banerji, A. et al., J. Nat. Prod., 1982, 45, 672, (分離)
Kitagawa, S. et al., Phytochemistry, 1984, 23, 1635, (分離)
Sun, N.-J. et al., Phytochemistry, 1987, 26, 3051, (分離)
Rahman, M.M.A. et al., Phytochemistry, 1990, 29, 1841; 1971, (分離, H-NMR, C13-NMR, 生合成)
Luo, S.Q. et al., Phytochemistry, 1993, 33, 193, (Phillyrin)

§ Phillygenin; (+)-form, *O*-β-D-Glucopyranoside
[化学名・別名]Phillyrin, Forsythin, Phillyroside, Chionanthin
[CAS No.]487-41-2
[化合物分類]リグナン化合物(Simple furofuranoid lignans)
[構造式]

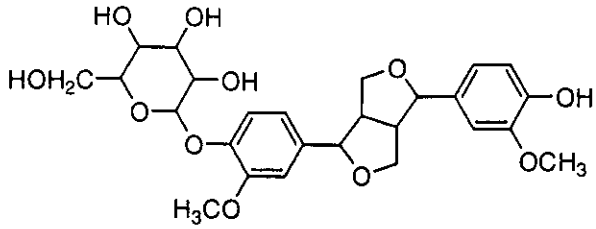


[分子式]$C_{27}H_{34}O_{11}$
[分子量]534.559
[天然基原]*Forsythia suspensa*, *Chionantha virginica*, *Phillyrea latifolia*, *Phillyrea angustifolia*, その他
[融点]Mp 154-155 ℃ (146-148 ℃), Mp 184-185 ℃ (dimorph.)
[比旋光度]:[α]$_D^{21}$ +46.9 (c, 0.25 in MeOH)

文 献

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, nos. 1151; 1152, (生育)
Chiba, M. et al., Chem. Pharm. Bull., 1977, 25, 3435, (分離, 構造決定, Phillyrin)
Luo, S.Q. et al., Phytochemistry, 1993, 33, 193, (Phillyrin)

[CAS No.]69251-96-3
[化合物分類]リグナン化合物(Simple furofuranoid lignans)
[構造式]

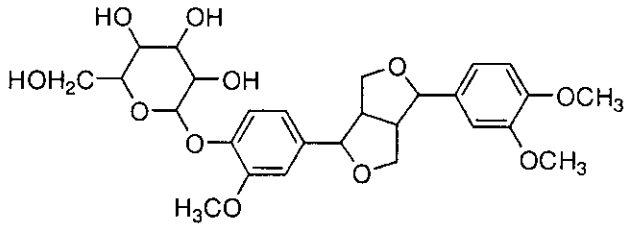


[分子式]$C_{26}H_{32}O_{11}$
[分子量]520.532
[天然基原]*Forsythia suspensa* と *Forsythia koreana* の果実

----------文献----------

Gripenberg, J., Acta Chem. Scand., 1949, 3, 898, (分離)
Weinges, K., Tet. Lett., 1960, No. 20, 1, (分離)
Sih, C.J. et al., J.A.C.S., 1976, 98, 5412, (分離, 誘導体)
Tsukamoto, M. et al., CA, 1984, 100, 117805, (分離, 配糖体)
Batirov, E.Kh. et al., Khim. Prir. Soedin., 1986, 21, 624; Chem. Nat. Compd. (Engl. Transl.), 1986, 21, 584, (Versicoside)
Casabuono, A.C. et al., Phytochemistry, 1994, 35, 479, ((-)-Pinoresinol)

§ Pinoresinol; (+)-form, 4-Me ether, 4'-*O*-β-D-glucopyranoside
[CAS No.]74957-57-6
[化合物分類]リグナン化合物(Simple furofuranoid lignans)
[構造式]

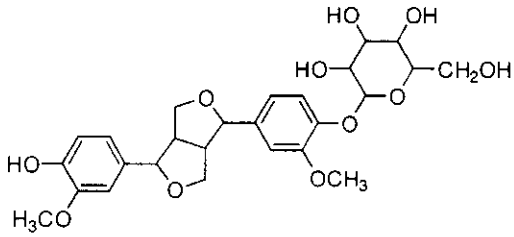


[分子式]$C_{27}H_{34}O_{11}$
[分子量]534.559
[天然基原]*Forsythia suspensa*

----------文献----------

Weinges, K., Tet. Lett., 1960, No. 20, 1, (分離)
Sih, C.J. et al., J.A.C.S., 1976, 98, 5412, (分離, 誘導体)
Tsukamoto, M. et al., CA, 1984, 100, 117805, (分離, 配糖体)

§ Pinoresinol; (+)-form, 7'-Epimer, 4-*O*-β-D-glucopyranoside
[化学名・別名](+)-Epipinoresinol glucoside
[CAS No.]74983-66-7
[化合物分類]リグナン化合物(Simple furofuranoid lignans)
[構造式]

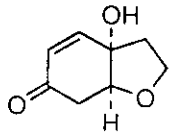


[分子式]$C_{26}H_{32}O_{11}$
[分子量]520.532
[天然基原]*Forsythia suspensa*

----------文献----------

Casabuono, A.C. et al., Phytochemistry, 1994, 35, 479, ((-)-Pinoresinol)
Yang, S.-J. et al., J. Chin. Chem. Soc. (Taipei), 1999, 46, 811-820, (3'-*O*-Demethylepipinoresinol)
Chen, I.S. et al., J. Nat. Prod., 1999, 62, 833-837, (*O*-Prenylpinoresinols)

§ Rengyolone
[化学名・別名]3,3*a*,7,7*a*-Tetrahydro-3*a*-hydroxy-6(2*H*)-benzofuranone(CAS 名), Halleridone, Cleroindicin F
[CAS No.]93675-87-7
[その他の CAS No.]94535-01-0
[化合物分類]ベンゾフラノイド(Benzofurans)
[構造式]



[分子式]$C_8H_{10}O_3$
[分子量]154.165