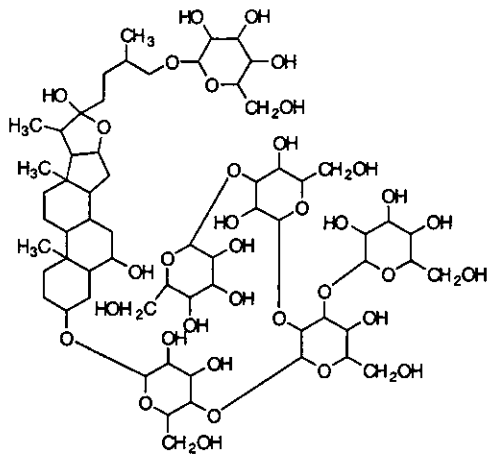
構造式]



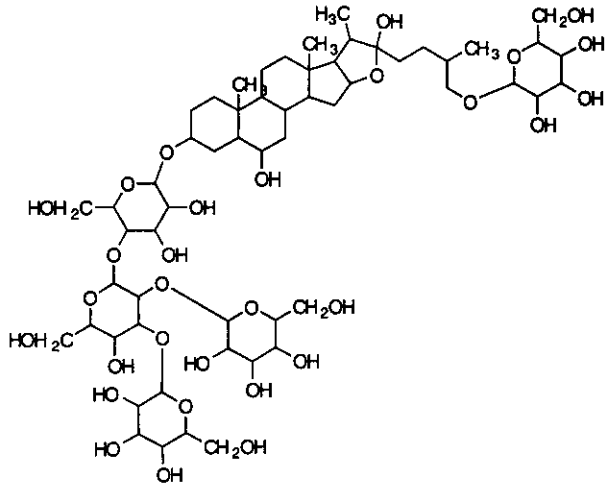
[分子式]$C_{63}H_{106}O_{35}$
[分子量]1423.509
[基原]*Allium sativum*
[性状]粉末 + 4H2O (Me2CO 溶液)
[比旋光度]:[α]$_D^{26}$ -40 (c, 0.39 in H_2O)

----------文献----------

Matsuura, H. et al., Chem. Pharm. Bull., 1989, 37, 1390; 2741; 3435, (Sativoside, Chinenoside I)

§ Furostane-3,6,22,26-tetrol; (3 β,5 α,6 β,22 ξ,25*R*)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-[β-D-glucopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside

[化学名・別名]Protoisoerubioside B
[化合物分類]ステロイド(Furostane steroid).
(C27).
[構造式]



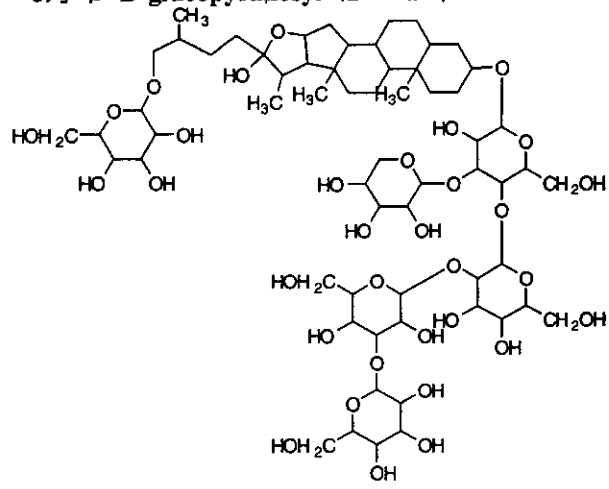
[分子式]$C_{57}H_{96}O_{30}$
[分子量]1261.367
[正確な分子量]1260.59865
[基原]*Allium sativum*
[性状]結晶
[融点]Mp 218-220 ℃
[比旋光度]:[α]$_D^{20}$ -26 (c, 0.1 in Py)

----------文献----------

Peng, J.P. et al., Yaoxue Xuebao, 1996, 31, 607, (Protoisoerubioside B)
Mimaki, Y. et al., Nat. Med. (Tokyo), 1999, 53, 134; CA, 132, 134748c, (Allium ampeloprasum saponin)

§ Furostane-3,22,26-triol; (3 β,5 β,22 ξ,25)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 3)-β-D-glucopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside

[化学名・別名]Sativoside R1
[CAS No.]126594-43-2
[化合物分類]ステロイド(Furostane steroid). (C27).
[構造式]



[分子式]$C_{62}H_{104}O_{33}$
[分子量]1377.484
[正確な分子量]1376.645995
[基原]*Allium sativum* (ニンニク)
[性状]粉末・二水和物 (Me2CO 溶液)
[比旋光度]:[α]$_D^{26}$ -45 (c, 0.59 in Py)

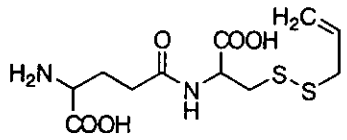
----------文献----------

Matsuura, H. et al., Chem. Pharm. Bull., 1989, 37, 2741, (Sativoside R1)

§ γ-Glutamyl-*S*-allylthiocysteine; L-L-form

[化合物分類]アミノ酸とペプチド(Dipeptide)

[構造式]



[基原]ニンニク (*Allium sativum*)

[性状]微細な針状結晶 (Me_2CO 溶液)

[融点]Mp 148-149 ℃

[比旋光度]:$[\alpha]_D^{23.5}$ -55.1 (c, 0.39 in 6 *M* HCl)

----------文献----------

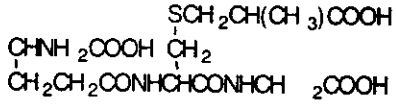
Sugii, M. et al., Chem. Pharm. Bull., 1964, 12, 1114, (分離)

§ γ-L-Glutamyl-*S*-(2-carboxy-1-propyl) cysteinylglycine

[CAS No.]6710-22-1

[化合物分類]アミノ酸とペプチド(Tripeptide)

[構造式]



[分子式]$C_{14}H_{23}N_3O_8S$

[分子量]393.417

[正確な分子量]393.120587

[基原]タマネギ(*Allium cepa*), ニンニク (*Allium sativum*)

[性状]針状結晶

[比旋光度]:$[\alpha]_D^{22}$ -38.1 (H_2O)

----------文献----------

Virtanen, A.J. et al., Z. Physiol. Chem., 1960, 322, 8, (分離)

Suzuki, T. et al., Chem. Pharm. Bull., 1961, 9, 77, (分離)

Tsuboi, S. et al., J. Agric. Food Chem., 1989, 37, 611, (HPLC)

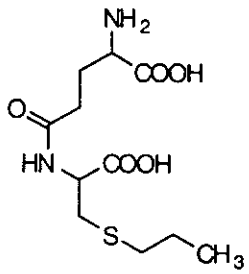
§ *N*-γ-Glutamylcysteine; L-L-form, *S*-Propyl

[化学名・別名]*N*-γ-Glutamyl-*S*-propylcysteine

[CAS No.]91212-00-9

[化合物分類]アミノ酸とペプチド(Dipeptide)

[構造式]



[分子式]$C_{11}H_{20}N_2O_5S$

[分子量]292.355

[正確な分子量]292.109293

[基原]次の植物から分離: *Allium sativum*, *Allium schoenoprasum*

----------文献----------

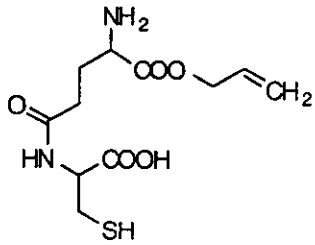
Matikkala, E.J. et al., Acta Chem. Scand., 1962, 16, 2461; 1963, 17, 1799, (S-propenyl, S-propyl, 分離)

§ *N*-γ-Glutamylcysteine; L-L-form, *S*-(*E*)-1-Propenyl

[CAS No.]134677-41-1

[化合物分類]アミノ酸とペプチド(Dipeptide)

[構造式]



[分子式]$C_{11}H_{18}N_2O_5S$

[分子量]290.34

[正確な分子量]290.093643

[基原]*Allium sativum*

[比旋光度]:$[\alpha]_D^{20}$ -12.3 (c, 0.39 in H_2O)

----------文献----------

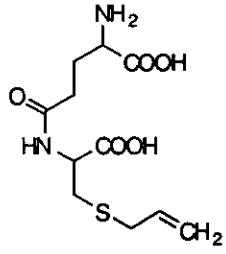
Matikkala, E.J. et al., Acta Chem. Scand., 1962, 16, 2461; 1963, 17, 1799, (S-propenyl, S-propyl, 分離)

§ *N*-γ-Glutamylcysteine; L-L-form, *S*-(2-Propenyl)

[化学名・別名]*N*-γ-Glutamyl-*S*-allylcysteine

[化合物分類]アミノ酸とペプチド(Dipeptide)

[構造式]

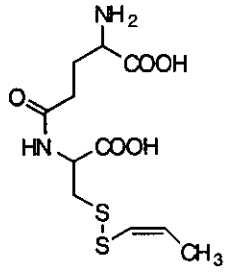


[分子式]$C_{11}H_{18}N_2O_5S$
[分子量]290.34
[正確な分子量]290.093643
[基原]次の植物から分離: ニンニクとエゾネギ(*Allium sativum*, *Allium schoenoprasum*)
[融点]Mp 156-158.5 ℃で分解
[比旋光度]:[α]$_D^{23}$ -17.1 (H_2O)

----------文献----------

Matikkala, E.J. et al., Acta Chem. Scand., 1962, 16, 2461; 1963, 17, 1799, (S-propenyl, S-propyl, 分離)

§ *N*-γ-Glutamylcysteine; L-L-form, *S*-(2-Propenylthio)

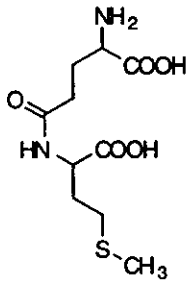


[化学名・別名]*N*-γ-Glutamyl-*S*-(allylthio)cysteine
[CAS No.]94504-37-7
[化合物分類]アミノ酸とペプチド(Dipeptide)
[構造式]
[分子式]$C_{11}H_{18}N_2O_5S_2$
[分子量]322.406
[正確な分子量]322.065713
[基原]*Allium sativum*
[比旋光度]:[α]$_D^{20}$ -64.8 (c, 0.26 in H_2O)

----------文献----------

Matikkala, E.J. et al., Acta Chem. Scand., 1962, 16, 2461; 1963, 17, 1799, (S-propenyl, S-propyl, 分離)
Enneking, D. et al., Phytochemistry, 1998, 48, 643, (S-vinyl, 分離)

§ *N*-γ-Glutamylmethionine; L-L-form

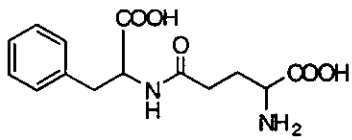


[CAS No.]17663-87-5
[化合物分類]アミノ酸とペプチド(Dipeptide)
[構造式]
[基原]次の植物から分離: タマネギ(*Allium cepa*)の種子, インゲン豆(*Phaseolus vulgari*), mung bean (*Vigna radiata*), ニンニク (*Allium sativum*) and black gram (*Vigna mungo*)
[用途]金属又は腎毒性医薬品に対する抗腎臓毒性に使用する
[融点]Mp 203-205 ℃. Mp 228-231 ℃
[比旋光度]:[α]$_D^{20}$ -9 (c, 1.4 in H_2O)

----------文献----------

Virtanen, A.I. et al., Suom. Kemistil. B, 1961, 34, 53; CA, 56, 716, (分離)
Morris, C.J. et al., J. Biol. Chem., 1963, 238, 650, (分離, 合成法)
Kasai, T. et al., Agric. Biol. Chem., 1971, 35, 1603; 1972, 36, 967, (分離)
Kristensen, I. et al., Phytochemistry, 1974, 13, 2803, (分離)
Otoul, E. et al., Phytochemistry, 1975, 14, 173, (分離)
Wu, S.H., J. Chromatogr., 1982, 245, 268, (分離, HPLC)
Anderson, M.E. et al., Proc. Natl. Acad. Sci. U.S.A., 1986, 83, 5029, (生化学)

§ *N*-γ-Glutamylphenylalanine; L-L-form

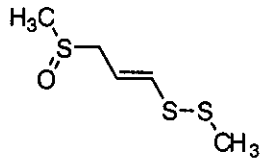


[CAS No.]6810-81-7
[化合物分類]アミノ酸とペプチド(Dipeptide)
[構造式]
[基原]タマネギ(*Allium cepa*), ダイズに存在. また, *Allium sativum*, *Lupinus* spp.からも得られる
[融点]Mp 164-174 ℃で分解
[比旋光度]:[α]$_D$ +17.3 (H_2O)

----------文献----------

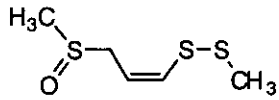
Virtanen, A.I. et al., Hoppe Seyler's Z. Physiol. Chem., 1960, 322, 8, (分離)

Virtanen, A.I. et al., Suom. Kemistil. B, 1960, 33, 83; 34, 44; 53, (分離)
Morris, C.J. et al., Biochemistry, 1962, 1, 706, (分離)

§ Methyl 3-(methylthio)-1-propenyl disulfide; (*E*)-form, 7-Oxide
[化学名・別名]Methyl 3-(methylsulfinyl)-1-propenyl disulfide
[CAS No.]104228-50-4
[その他の CAS No.]104228-67-3
[化合物分類]脂肪族化合物(Disulfides, trisulfide)
[構造式]

[分子式]$C_5H_{10}OS_3$
[分子量]182.331
[正確な分子量]181.989375
[基原]*Allium sativum*, *Allium ursinum*
[性状]オイル

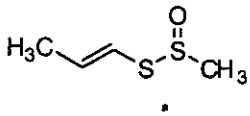
----------文献----------

Block, E. et al., J.A.C.S., 1986, 108, 7045, (合成法, IR, H-NMR)
Sendl, A. et al., Planta Med., 1991, 57, 361; 1992, 58, 1, (分離)

§ Methyl 3-(methylthio)-1-propenyl disulfide; (*Z*)-form, 7-Oxide
[CAS No.]104229-00-7
[化合物分類]脂肪族化合物(Disulfides, trisulfide)
[構造式]

[分子量]182.331
[正確な分子量]181.989375
[基原]*Allium sativum*, *Allium ursinum*
[性状]オイル

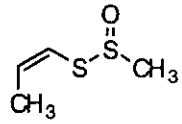
----------文献----------

Block, E. et al., J.A.C.S., 1986, 108, 7045, (合成法, IR, H-NMR)
Sendl, A. et al., Planta Med., 1991, 57, 361; 1992, 58, 1, (分離)

§ Methyl 1-propenyl disulfide; (*E*)-form, 5-Oxide
[化学名・別名]S -1-Propenyl methanesulfinothioate
[CAS No.]119052-99-2
[化合物分類]脂肪族化合物(Disulfides, trisulfide)
[構造式]

[分子式]$C_4H_8OS_2$
[分子量]136.239
[正確な分子量]136.001655
[基原]*Allium cepa*, *Allium sativum*, その他の *Allium* spp.

----------文献----------

Bayer, T. et al., Phytochemistry, 1989, 28, 2373, (誘導体, 分離, H-NMR)
Block, E. et al., Pure Appl. Chem., 1993, 65, 625, (誘導体, 生育)

§ Methyl 1-propenyl disulfide; (*Z*)-form, 5-Oxide
[CAS No.]119053-00-8
[化合物分類]脂肪族化合物(Disulfides, trisulfide)
[構造式]

[分子量]136.239
[正確な分子量]136.001655
[基原]*Allium cepa*, *Allium sativum*, その他の *Allium* spp.

----------文献----------

Bayer, T. et al., Phytochemistry, 1989, 28, 2373, (誘導体, 分離, H-NMR)
Block, E. et al., Pure Appl. Chem., 1993, 65, 625, (誘導体, 生育)

§ Methyl 2-propenyl pentasulfide

[CAS No.] 118023-99-7
[化合物分類] 脂肪族化合物 (Disulfides, trisulfide) 脂肪族化合物 (Unbranched alkenic hydrocarbon)
[構造式] $H_2C=CHCH_2$-S-S-S-S-S-Me
[分子式] $C_4H_8S_5$
[分子量] 216.437
[正確な分子量] 215.92295
[基原] *Allium sativum*. Component of Da Suan

----------文献----------

Ding, Z. et al., CA, 1989, 110, 22443p, (isol)

§ Methyl 2-propenyl tetrasulfide (CAS 名)
[化学名・別名] Allyl methyl tetrasulfide
[CAS No.] 90195-83-8
[化合物分類] 脂肪族化合物 (Unbranched alkenic hydrocarbon), 脂肪族化合物 (Disulfides, trisulfide)
[構造式] $H_2C=CHCH_2$-S-S-S-S-Me
[分子式] $C_4H_8S_4$
[分子量] 184.371
[正確な分子量] 183.95088
[基原] *Adenocalymma alliaceum*, *Allium sativum*. Component of Da Suan

----------文献----------

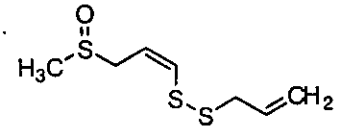
Zoghbi, M.G.B. et al., J. Agric. Food Chem., 1984, 32, 1009-1010, (分離)
Ding, Z. et al., CA, 1989, 110, 22443p, (分離)

§ Methyl 2-propenyl trisulfide (CAS 名)
[化学名・別名] Allyl methyl trisulfide. 4,5,6-Trithia-1-heptene
[CAS No.] 34135-85-8
[化合物分類] 脂肪族化合物 (Unbranched alkenic hydrocarbon), 脂肪族化合物 (Disulfides, trisulfide)
[構造式] $H_2C=CHCH_2$-S-S-S-Me
[分子式] $C_4H_8S_3$
[分子量] 152.305
[正確な分子量] 151.97881
[基原] *Allium sativum* (ニンニクオイル), その他の *Allium* spp.
[用途] 強い細胞毒作用.
[性状] 黄色のオイル
[沸点] $Bp_{0.05}$ 28-30 ℃

----------文献----------

Kameoka, H. et al., Phytochemistry, 1984, 23, 155, (分離)
Vernin, G. et al., Planta Med., 1986, 96, (分離)

§ [3-(Methylsulfinyl)-1-propenyl] 2-propenyl disulfide; (Z)-form
[化合物分類] 脂肪族化合物 (Disulfides, trisulfide)
[構造式]



[基原] 次の植物から分離: ニンニクオイル (*Allium sativum*)
[性状] オイル

----------文献----------

Yoshida, H. et al., Biosci., Biotechnol., Biochem., 1998, 62, 1015, (分離, H-NMR, C13-NMR, Mas)

§ 2-Propen-1-ol (CAS 名)
[化学名・別名] Allyl alcohol
[CAS No.] 107-18-6
[関連 CAS No.] 20907-32-8
[化合物分類] 脂肪族化合物 (Unbranched alkenic alcohol)
[構造式] $H_2C=CHCH_2OH$
[分子式] C_3H_6O

[分子量]58.08
[正確な分子量]58.041865
[基原]ニンニク *Allium sativum* に存在. Manuf. by isomerisation of propylene oxide or by oxidation of propylene with O_2
[性状]刺激性のマスタード様の臭気を持つ液体
[融点]Mp-129 ℃
[沸点]Bp 96-97 ℃
[溶解性]水, アルコール, エーテルに混和する; クロロホルムに可溶
[濃度]d^{20} 0.854
[PKa 値]p*K*a 15.5 (25 ℃)
[屈折率]n^{20}_D 1.4135
[その他のデータ]n 20 D 1.4135. Vp 24 mmHg (25 ℃). 水と混和した溶液は一定の沸点を示す contg.
[傷害・毒性]極めて強い可燃性, 発火温度:21 ℃, 自然発火温度:375 ℃. 硫酸と激しく反応する. 四塩化炭素と反応し, ハロゲン化した不安定な C4-epoxides を生成する. 皮膚,眼(ヒト)と,内分泌系を強く刺激する. 50 %致死量(LD_{50})(ラット, 経口) 64 mg/kg. 50 %致死量(LD_{50})(ウサギ, 皮膚塗布) 45 mg/kg. 肝細胞毒. OES: long-term 2 ppm; short-term 4 ppm (Sk)
[化学物質毒性データ総覧(RTEC)登録番号]BA5075000

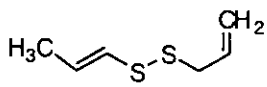
----------文献----------

Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, A1, 431, (レビュー)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, 2, 144, (レビュー, 成書)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 189, (毒性, レビュー)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, AFU750; AFV500; AGK750

*****RTECS (化学物質毒性データ) *****

生体影響物質　　: 農芸化学. 催腫瘍物質. 変異原物質. 一時刺激物質

§ 1-Propenyl 2-propenyl disulfide; (*E*)-form
[CAS No.]122156-02-9
[化合物分類]脂肪族化合物(Disulfides, trisulfide)
[構造式]

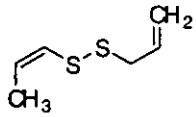


[基原]ニンニク (*Allium sativum*)
[性状]オイル

----------文献----------

Block, E. et al., Pure Appl. Chem., 1993, 65, 625, (誘導体, 生育)
Block, E. et al., J.A.C.S., 1996, 118, 2799, (合成法, H-NMR, C13-NMR)

§ 1-Propenyl 2-propenyl disulfide; (*Z*)-form
[CAS No.]122156-03-0
[化合物分類]脂肪族化合物(Disulfides, trisulfide)
[構造式]

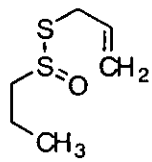


[基原]ニンニク (*Allium sativum*)
[性状]オイル

----------文献----------

Block, E. et al., Pure Appl. Chem., 1993, 65, 625, (誘導体, 生育)
Block, E. et al., J.A.C.S., 1996, 118, 2799, (合成法, H-NMR, C13-NMR)

§ 2-Propenyl propyl disulfide; 4-Oxide
[化学名・別名]S -2-Propenyl 1-propanesulfinothioate
[CAS No.]136516-42-2
[化合物分類]脂肪族化合物(Disulfides, trisulfide)
[構造式]



[分子式]$C_6H_{12}OS_2$
[分子量]164.292
[正確な分子量]164.032955

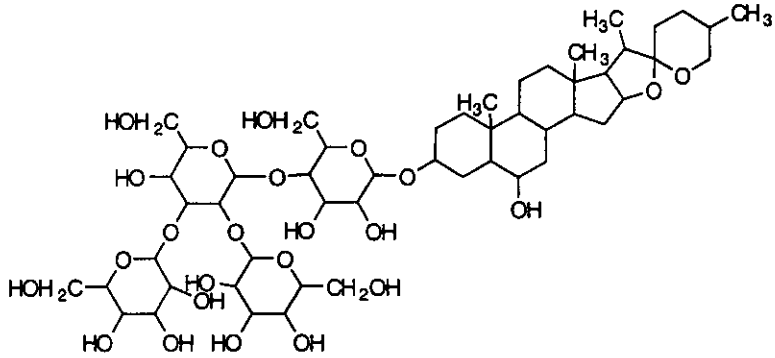
[基原]ニンニク(*Allium sativum*), 野生のセイヨウネギ(*Allium tricoccum*)

----------文献----------

Carson, J.F. et al., J.O.C., 1959, 24, 175, (合成法, ガスクロマト)
Jacobsen, J.V. et al., Arch. Biochem. Biophys., 1964, 104, 473, (IR, ガスクロマト)
Brodnitz, M.H. et al., J. Agric. Food Chem., 1969, 17, 760, (分離, H-NMR, IR, Mass, ガスクロマト)
Calvey, E.M. et al., Phytochemistry, 1998, 49, 359, (誘導体, 分離)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, AGR500

§ Spirostane-3,6-diol; (3 β,5 α,6 α,25)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-[β-D-glucopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]

[化学名・別名]Isoerubioside B
[CAS No.]186545-52-8
[化合物分類]ステロイド (Spirostane steroid). (C27)
[構造式]



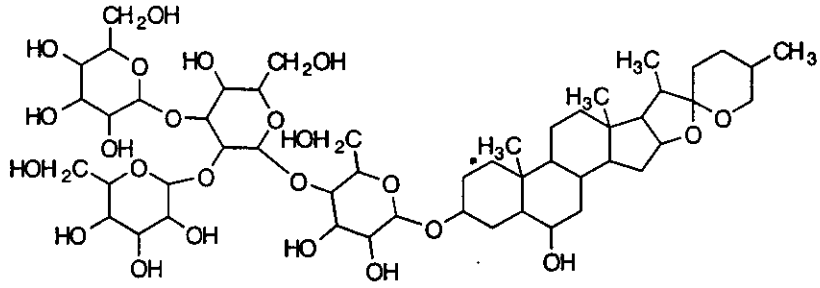
[分子式]$C_{51}H_{84}O_{24}$
[分子量]1081.21
[正確な分子量]1080.53526
[基原]*Allium sativum*
[性状]結晶
[融点]Mp 310-312 ℃
[比旋光度]:$[\alpha]_D^{20}$ -32.8 (c, 1 in Py)

----------文献----------

Blunden, G. et al., Steroids, 1980, 35, 503, (分離, IR, Mass, H-NMR, 3 β 5 β 6 α 25*R*-form)
Carotenuto, A. et al., Phytochemistry, 1999, 51, 1077, (Allium porrum saponin)
Ikeda, T. et al., Chem. Pharm. Bull., 2000, 48, 362, (Allium tuberosum saponin)

§ Spirostane-3,6-diol; (3 β,5 α,6 β,25*R*)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-[β-D-glucopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]

[化学名・別名]Eruboside B
[CAS No.]72994-87-7
[化合物分類]AJ5000, ステロイド(Spirostane steroid). (C27)
[構造式]



[分子式]$C_{51}H_{84}O_{24}$
[分子量]1081.21
[正確な分子量]1080.53526
[基原]*Allium erubescens*, *Allium sativum*
[性状]無定型
[比旋光度]:$[\alpha]_D^{21}$ -61.3 (c, 0.5 in Py)
[溶解性] メタノール, ピリジンに可溶; 水に易溶; アセトン, ヘキサンに難溶

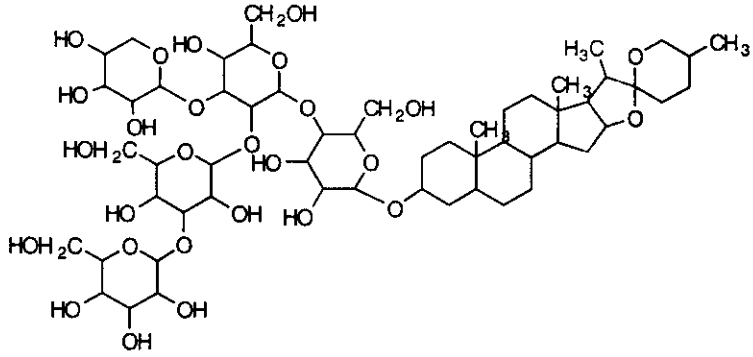
----------文献----------

Chakravarty, A.K. et al., Tet. Lett., 1978, 3875, (分離, 3 β 5 α 6 α 25*S*-form)
Mahmood, U. et al., Phytochemistry, 1985, 24, 2456, (分離)
Carotenuto, A. et al., Phytochemistry, 1999, 51, 1077, (Allium porrum saponin)
Ikeda, T. et al., Chem. Pharm. Bull., 2000, 48, 362, (Allium tuberosum saponin)

§ Spirostan-3-ol; (3 β,5 α,25*R*)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 3)-β-D-glucopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]

[化学名・別名]Sativoside R2
[CAS No.]126643-24-1
[化合物分類]ステロイド(Spirostane steroid). (C27)
[構造式]

[分子式] $C_{56}H_{92}O_{27}$
[分子量] 1197.327
[正確な分子量] 1196.582605
[基原] *Allium sativum*
[性状] 結晶・四水和物
(MeOH/$CHCl_3$)
[融点] Mp 265-270 ℃で分解
[比旋光度]: $[\alpha]_D^{26}$ -51.5 (c, 0.51 in Py)



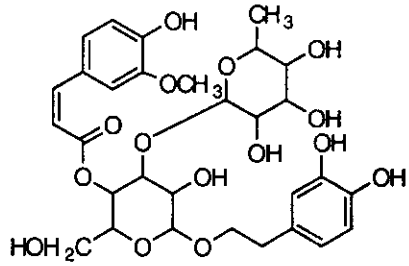
文献

Matsuura, H. et al., Chem. Pharm. Bull., 1989, 37, 2741, (Sativoside R2)

***********ネズミモチ (Nezumimochi) ***********

§§ モクセイ科ネズミモチ(*Ligustrum japonicum* Thunberg)の果実。

§ 2-(3,4-Dihydroxyphenyl) ethanol; 1-*O*-[α-L-Rhamnopyranosyl-(1 → 3)-[4-hydroxy-3-methoxy-*E*-cinnamoyl-(→ 4)]-β-D-glucopyranoside]
[化学名・別名] Leucosceptoside A
[CAS No.] 83529-62-8
[化合物分類] 単環芳香族(Simple phenylpropanoid)
[構造式]

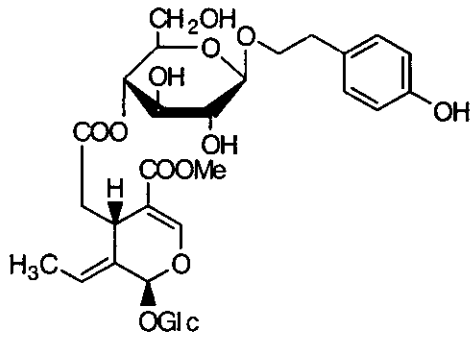


[分子式] $C_{30}H_{38}O_{15}$
[分子量] 638.621
[正確な分子量] 638.221075
[基原] 次の植物から分離: *Ligustrum japonicum*
[性状] 無定型の粉末

文献

Jia, Z.J. et al., Indian J. Chem., Sect. B, 1994, 33, 460, (*cis*-Leucosceptoside, *cis*-Martynoside)
Jimenez, C. et al., Nat. Prod. Rep., 1994, 591, (レビュー, 配糖体)
Duynstee, H.I. et al., Eur. J. Org. Chem., 1999, 2623, (合成法, H-NMR, C13-NMR)
Skrzypek, Z. et al., J. Nat. Prod., 1999, 62, 127, (*cis*-Martynoside, *cis*-Leucosceptoside)

§ Isonuezhenide
[CAS No.] 112693-22-8
[化合物分類] テルペノイド(Secoiridoid monoterpenoid)
[構造式]

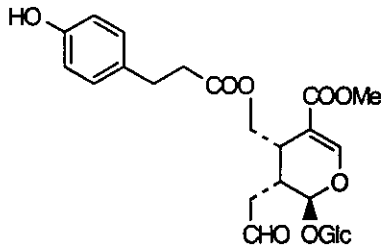


[分子式] $C_{31}H_{42}O_{17}$
[分子量] 686.663
[正確な分子量] 686.242205
[基原] *Ligustrum japonicum*
[性状] 粉末
[比旋光度]: $[\alpha]_D$ -85 (c, 1.15 in EtOH)

文献

Fukuyama, Y. et al., Planta Med., 1987, 53, 427

§ Ligustaloside B
[CAS No.] 85527-08-8
[化合物分類] テルペノイド(Secoiridoid monoterpenoid)
[構造式]

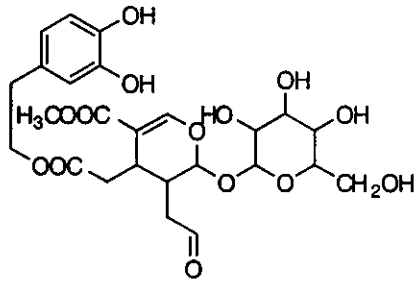


[分子式] $C_{25}H_{32}O_{13}$
[分子量] 540.52
[正確な分子量] 540.184295
[基原] *Ligustrum japonicum*
[性状] 粉末
[比旋光度]: $[\alpha]_D^{20}$ -120 (c, 0.95 in MeOH)

----------文献----------

Inoue, K. et al., Phytochemistry, 1982, 21, 2305
Kuwajima, H. et al., Chem. Pharm. Bull., 1999, 47, 1634, (生合成)

§ Ligustaloside B; 3'-Hydroxy

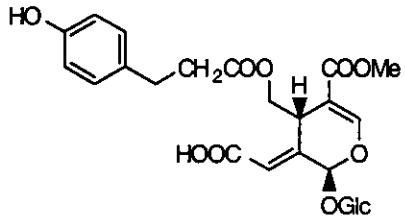


[化学名・別名] Ligustaloside A
[CAS No.] 85527-07-7
[化合物分類] テルペノイド (Secoiridoid monoterpenoid)
[構造式]
[分子式] $C_{25}H_{32}O_{14}$
[分子量] 556.519
[正確な分子量] 556.17921
[基原] *Ligustrum japonicum*
[性状] 粉末
[比旋光度]: $[\alpha]_D^{18}$ -120.1 (c, 1 in MeOH)

----------文献----------

Inoue, K. et al., Phytochemistry, 1982, 21, 2305
Kuwajima, H. et al., Chem. Pharm. Bull., 1999, 47, 1634, (生合成)

§ Ligustrosidic acid

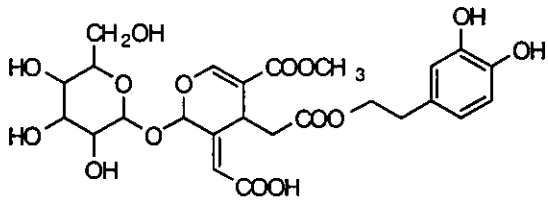


[CAS No.] 96382-89-7
[化合物分類] テルペノイド (Secoiridoid monoterpenoid)
[構造式]
[分子式] $C_{25}H_{30}O_{14}$
[分子量] 554.504
[正確な分子量] 554.16356
[基原] *Ligustrum japonicum*
[性状] 無定型
[比旋光度]: $[\alpha]_D$ -130.2 ($CHCl_3$) (as penta-Ac)

----------文献----------

Kikuchi, M. et al., CA, 1985, 102, 218342, (分離, H-NMR, C13-NMR)

§ Ligustrosidic acid; 3''-Hydroxy



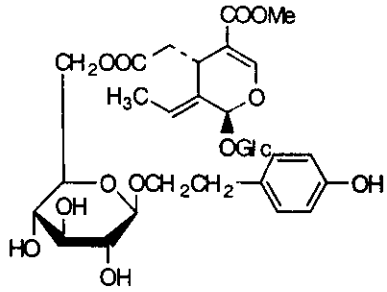
[化学名・別名] Oleuropeinic acid
[CAS No.] 96382-90-0
[化合物分類] テルペノイド (Secoiridoid monoterpenoid)
[構造式]
[分子式] $C_{25}H_{30}O_{15}$
[分子量] 570.503
[正確な分子量] 570.158475
[基原] *Ligustrum japonicum*
[性状] 無定型
[比旋光度]: $[\alpha]_D$ -120.3 ($CHCl_3$)

----------文献----------

Kikuchi, M. et al., CA, 1985, 102, 218342, (分離, H-NMR, C13-NMR)

§ Nuezhenide

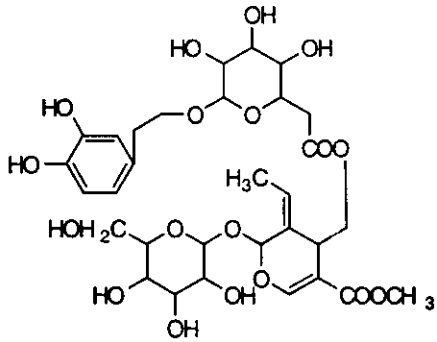
[CAS No.]39011-92-2
[化合物分類]テルペノイド(Secoiridoid monoterpenoid)
[構造式]
[分子式]$C_{31}H_{42}O_{17}$
[分子量]686.663
[正確な分子量]686.242205
[基原]次の植物の熟した果実から分離: *Ligustrum lucidum*, *Ligustrum japonicum*
[性状]結晶(EtOH)
[融点]Mp 125-127 ℃
[比旋光度]:[α]$_D^{17}$ -150 (c, 1 in MeOH)



----------文献----------

Inouye, H. et al., Tetrahedron, 1972, 28, 4231, (分離)
Lalonde, R.T. et al., J.A.C.S., 1976, 98, 3007, (分離)
Kikuchi, M. et al., CA, 1985, 102, 218342j, (Neonuezhenide)

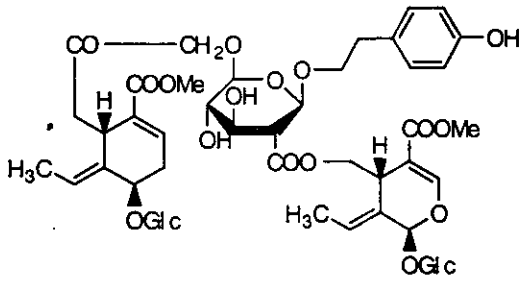
§ Nuezhenide; 3''-Hydroxy
[化学名・別名]Neonuezhenide
[CAS No.]96382-91-1
[化合物分類]テルペノイド(Iridoid monoterpenoid)
[構造式]
[分子式]$C_{31}H_{42}O_{18}$
[分子量]702.662
[正確な分子量]702.23712
[基原]*Ligustrum japonicum*
[性状]結晶(as nona-Ac)
[融点]Mp 85-86 ℃ (nona-Ac)
[比旋光度]:[α]$_D$ -93.5 ($CHCl_3$) (nona-Ac)



----------文献----------

Inouye, H. et al., Tetrahedron, 1972, 28, 4231, (分離)
Lalonde, R.T. et al., J.A.C.S., 1976, 98, 3007, (分離)
Kikuchi, M. et al., CA, 1985, 102, 218342j, (Neonuezhenide)

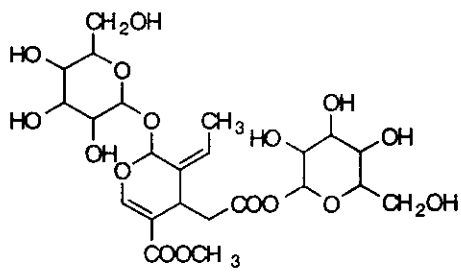
§ Oleonuezhenide
[CAS No.]112693-21-7
[化合物分類]テルペノイド(Secoiridoid monoterpenoid)
[構造式]
[分子式]$C_{48}H_{64}O_{27}$
[分子量]1073.017
[正確な分子量]1072.363505
[基原]*Ligustrum japonicum*
[性状]無定型の粉末
[比旋光度]:[α]$_D$ +62.3 (c, 0.83 in EtOH)



----------文献----------

Fukuyama, Y. et al., Planta Med., 1987, 53, 427

§ Oleoside; 7-β-D-Glucopyranosyl ester, 11-Me ester
[化学名・別名]Methyl glucooleoside
[CAS No.]115623-36-4
[化合物分類]テルペノイド(Secoiridoid monoterpenoid)
[構造式]
[分子式]$C_{23}H_{34}O_{16}$
[分子量]566.512
[正確な分子量]566.18469
[基原]*Ligustrum japonicum*, *Jasminum polyanthum*, *Syringa*

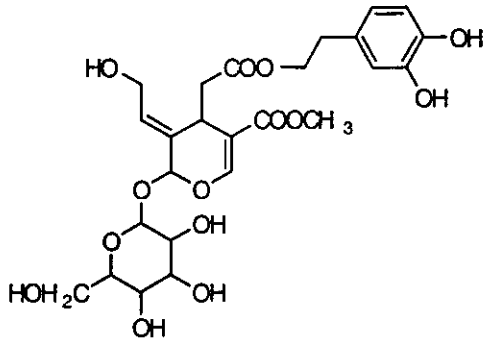


vulgaris, *Fraxinus excelsior*
[性状]粉末
[比旋光度]:[α]$_D^{16}$ -164.7 (c, 0.51 in MeOH)

----------文献----------

Tanahashi, T. et al., Chem. Pharm. Bull., 1987, 35, 5032, (11-Me ester)
Shen, Y.-C. et al., J. Chin. Chem. Soc. (Peking), 1996, 43, 171, (分離, H-NMR, C13-NMR)

§ Oleuropein; 10-Hydroxy

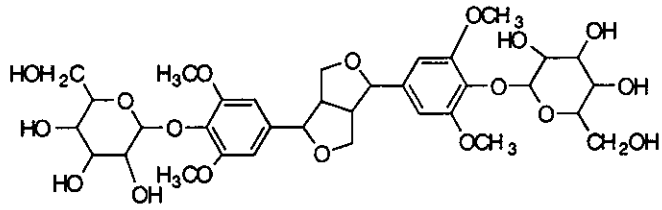


[化学名・別名]10-Hydroxyoleuropein
[CAS No.]84638-44-8
[化合物分類]テルペノイド(Secoiridoid monoterpenoid)
[構造式]
[分子式]$C_{25}H_{32}O_{14}$
[分子量]556.519
[正確な分子量]556.17921
[基原]*Ligustrum japonicum*
[性状]粉末
[比旋光度]:[α]$_D^{20}$ -153.7 (c, 0.38 in MeOH)

----------文献----------

Shasha, B. et al., J.O.C., 1961, 26, 1948, (分離)
Panizzi, L. et al., Gazz. Chim. Ital., 1965, 95, 1279, (分離)
Asaka, Y. et al., Chem. Lett., 1972, 141, (分離, 構造決定)
Inouye, H. et al., Tetrahedron, 1974, 30, 201, (絶対構造)
Kurkin, V.A. et al., Khim. Prir. Soedin., 1990, 695; Chem. Nat. Compd. (Engl. Transl.), 1990, 26, 592,
Damtoft, S. et al., Phytochemistry, 1992, 31, 4197; 1993, 34, 1291; 1995, 40, 785, (生合成, Oleuropein, Ligustroside)
Esti, M. et al., J. Agric. Food Chem., 1998, 46, 32, (生育)

§ Syringaresinol; (-)-form, Di-*O*-β-D-glucopyranoside

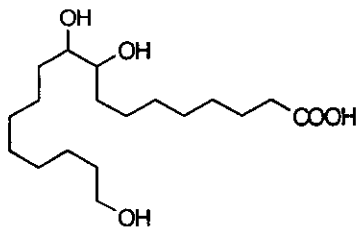


[化学名・別名]Acanthoside D. Eleutheroside E
[CAS No.]96038-87-8
[化合物分類]リグナン化合物(Simple furofuranoid lignan)
[構造式]
[分子式]$C_{34}H_{46}O_{18}$
[分子量]742.727
[正確な分子量]742.26842
[基原]次の植物から分離: シベリアのチョウセンニンジン(*Eleutherococcus* (*Acanthopanax*) *senticosu*), *Ligustrum japonicum*, *Liriodendron tulipifera*, *Albizzia julibrissin*, *Viscum album*
[性状]針状結晶
[融点]Mp 269-270 ℃
[比旋光度]:[α]$_D^{22}$ -18.5 (c, 0.54 in 50% EtOH 溶液)

----------文献----------

Vermes, B. et al., Phytochemistry, 1991, 30, 3087, (合成法, Acanthosides, 配糖体)

§ 9,10,18-Trihydroxyoctadecanoic acid; (9*S*,10*J*)-form



[化学名・別名]Phloionolic acid. Floionolic acid
[CAS No.]17705-68-9
[化合物分類]脂肪族化合物(Saturated unbranched carboxylic acid andlactone)
[構造式]
[基原]コルクやその他の植物, 例えば, *Olea europaea*, *Agave americana*, *Chamaepeuce afra*, *Ligustrum japonicum*, apple wax and also cutins
[性状]結晶(MeOH)

[融点]Mp 104-105 ℃
[比旋光度]:[α]$_{Hg}^{589}$ +22.75
[PKa 値]pK_{a1} 4.95

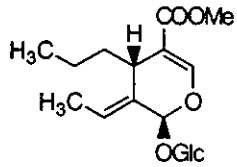
----------文献----------

Duhamel, L., Bull. Soc. Chim. Fr., 1965, 399, (構造決定)
Eglinton, G. et al., Phytochemistry, 1968, 7, 313, (Mas)
McGhie, J.F. et al., Chem. Ind. (London), 1972, 463, (stereochem)

§§モクセイ科トウネズミモチ(*Ligustrum lucidum* Aiton)の果実。

§ Nuezhengalaside

[CAS No.]206275-18-5
[化合物分類]テルペノイド(Secoiridoid monoterpenoid)
[構造式]



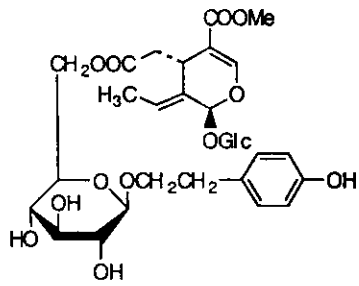
[分子式]$C_{18}H_{28}O_9$
[分子量]388.414
[正確な分子量]388.173335
[基原]*Ligustrum lucidum*
[性状]結晶
[融点]Mp 144-147 ℃

----------文献----------

Shi, L.F. et al., Yaoxue Xuebao, 1997, 32, 442; CA, 128, 292718, (分離, H-NMR, C13-NMR)

§ Nuezhenide

[CAS No.]39011-92-2
[化合物分類]テルペノイド(Secoiridoid monoterpenoid)
[構造式]



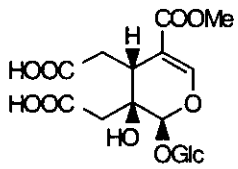
[分子式]$C_{31}H_{42}O_{17}$
[分子量]686.663
[正確な分子量]686.242205
[基原]次の植物の熟した果実から分離: *Ligustrum lucidum*, *Ligustrum japonicum*
[性状]結晶(EtOH)
[融点]Mp 125-127 ℃
[比旋光度]:[α]$_D^{17}$ -150 (c, 1 in MeOH)

----------文献----------

Inouye, H. et al., Tetrahedron, 1972, 28, 4231, (分離)
Lalonde, R.T. et al., J.A.C.S., 1976, 98, 3007, (分離)
Kikuchi, M. et al., CA, 1985, 102, 218342j, (Neonuezhenide)

§ Nuezhenidic acid

[CAS No.]183238-67-7
[化合物分類]テルペノイド(Iridoid monoterpenoid)
[構造式]

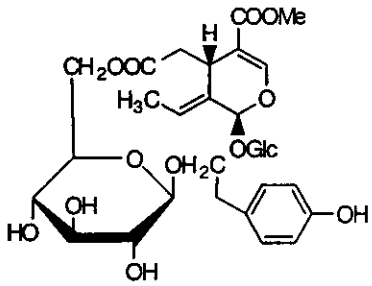


[分子式]$C_{17}H_{24}O_{14}$
[分子量]452.368
[正確な分子量]452.11661
[基原]*Ligustrum lucidum*
[性状]結晶
[融点]Mp 232-233 ℃
[UV]:[neutral] λ_{max} 232 (ε 12916) (EtOH)

----------文献----------

Wu, L. et al., Zhongguo Yaowu Huaxue Zazhi, 1996, 6, 117; CA, 125, 323033, (分離, H-NMR, C13-NMR)
Wu, L.-J. et al., Zhiwu Xuebao, 1998, 40, 83; CA, 130, 49824p, (分離, H-NMR, C13-NMR)

§ **Specnuezhenide**
[CAS No.]202586-63-8
[化合物分類]テルペノイド(Secoiridoid monoterpenoid)
[構造式]



[分子式]$C_{31}H_{42}O_{17}$
[分子量]686.663
[正確な分子量]686.242205
[基原]*Ligustrum lucidum*
[UV]:[neutral] λ_{max} 228; 238 (sh); 279; 285(MeOH)

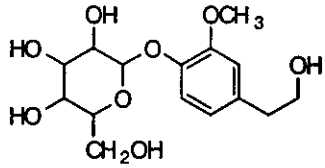
----------文献----------

Shi, L.F. et al., Yaoxue Xuebao, 1997, 32, 442, (分離, H-NMR, C13-NMR)
Shi, L.F. et al., Biomed. Chromatogr., 1998, 12, 27, (HPLC)

**********ネットル (Nettle) **********

§§イラクサ科セイヨウイラクサ(*Urtica dioica* L.)の葉。

§ **2-(3,4-Dihydroxyphenyl) ethanol; 3'-Me ether, 4'-*O*-β-D-glucopyranoside**
[CAS No.]104380-15-6
[化合物分類]単環芳香族(Simple phenol)
[構造式]

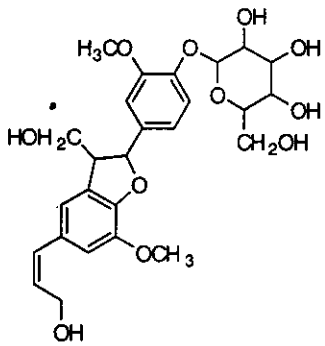


[分子式]$C_{15}H_{22}O_8$
[分子量]330.334
[正確な分子量]330.13147
[基原]*Cinnamomum reticulatum*, *Urtica dioica*

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Jimenez, C. et al., Nat. Prod. Rep., 1994, 591, (レビュー, 配糖体)

§ **4,7'-Epoxy-3,8'-bilign-7-ene-3',4',5,9,9'-pentol; (7'*S*,8'*R*)-form, 3',5-Di-Me ether, 4'-*O*-β-D-glucopyranoside**
[CAS No.]107870-88-2
[化合物分類]リグナン化合物(Neolignan)
[構造式]



[分子式]$C_{26}H_{32}O_{11}$
[分子量]520.532
[正確な分子量]520.194465
[基原]*Cistanche tubulosa*, *Urtica dioica*, *Vinca rosea*
[性状]粉末
[比旋光度]:$[\alpha]_D^{25}$ -56.4 (c, 1.1 in MeOH)

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Yoshizawa, F. et al., Chem. Pharm. Bull., 1990, 38, 1927, (配糖体)

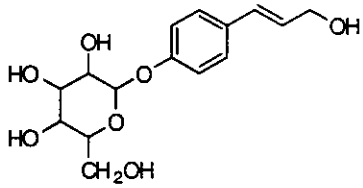
§ **3'-Hydroxyacetophenone(旧 CAS 名)**
[化学名・別名]1-(3-Hydroxyphenyl) ethanone(CAS 名). *m*-Acetylphenol. 3-Hydroxyphenyl methyl ketone
[CAS No.]121-71-1
[化合物分類]単環芳香族(Simple aryl ketone)
[構造式]構造式は次の化合物と類似: 2'-Hydroxyacetophenone
[分子式]$C_8H_8O_2$

[分子量]136.15
[正確な分子量]136.05243
[基原]*Dianthus caryophyllus*（ナデシコ科）, *Urtica dioica*（イラクサ科）
[性状]針状結晶
[融点]Mp 96 ℃
[沸点]Bp 296 ℃. Bp_5 153 ℃
[PKa 値]pK_{a1} -6.59（25 ℃, H_2SO_4 溶液） pK_a 9.25（25 ℃）
[化学物質毒性データ総覧(RTEC)登録番号]AM8754000

----------文献----------

Kraus, R. et al., Phytochemistry, 1990, 29, 1653,（分離, Mas）
Curir, P. et al., Phytochemistry, 1996, 41, 447,（分離, 活性）

§ 3-(4-Hydroxyphenyl)-2-propen-1-ol; (*E*)-form, 4'-*O*-β-D-Glucopyranoside
[化学名・別名]*p*-Coumaryl β-D-glucopyranoside
[CAS No.]120442-73-1
[その他の CAS No.]59092-89-6
[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]

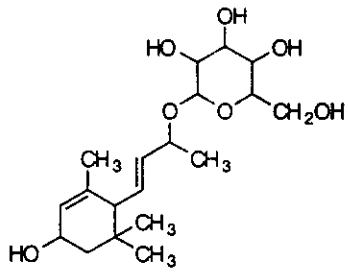


[分子式]$C_{15}H_{20}O_7$
[分子量]312.319
[正確な分子量]312.120905
[基原]*Arum italicum*, *Lilium cordatum*, *Millingtonia hortensis*, *Urtica dioica*
[性状]針状結晶
[融点]Mp 171-174 ℃
[比旋光度]:$[\alpha]_D^{17}$ -57.4 (c, 0.9 in MeOH)

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Thieme, H., Naturwissenschaften, 1963, 50, 571; 1964, 51, 217
Nakano, K. et al., Phytochemistry, 1989, 28, 301,（配糖体）

§ 4,7-Megastigmadiene-3,9-diol; (3ξ,7*E*,9ξ)-form, 9-*O*-β-D-Glucopyranoside
[化合物分類]テルペノイド(Megastigmane norterpenoid)
[構造式]

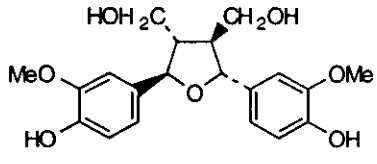


[分子式]$C_{19}H_{32}O_7$
[分子量]372.458
[正確な分子量]372.214805
[基原]*Urtica dioica*
[その他のデータ]光学異性体の混合物として分離

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
De Tommasi, N. et al., J. Nat. Prod., 1992, 55, 1025,（配糖体）
Neugebauer, W. et al., Nat. Prod. Lett., 1995, 6, 177,（配糖体）

§ Neoolivil
[化学名・別名]4,4',9,9'-Tetrahydroxy-3,3'-dimethoxy-7,7'-epoxylignan
[CAS No.]77790-55-7
[関連 CAS No.]486-02-2, 129065-76-5
[その他の CAS No.]129387-92-4, 129387-93-5
[化合物分類]リグナン化合物
(7,7'-Epoxytetrahydrofuranoid lignan)
[構造式]



Absolute Configuration

[分子式]$C_{20}H_{24}O_7$
[分子量]376.405

[正確な分子量]376.152205
[一般的性質]絶対構造は 1997 年に改正された
[基原]*Thymus longiflorus, Urtica dioica*
[性状]粉末
[比旋光度]:[α]$_D^{23}$ +49 (c, 0.16 in EtOH)

----------文献----------

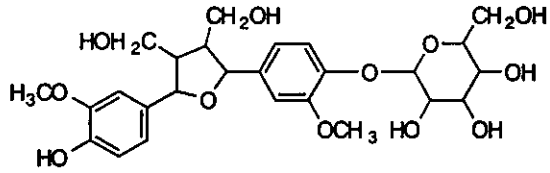
Hernandez, A. et al., Phytochemistry, 1981, 20, 181, (分離, C13-NMR, Mas)
Kraus, R. et al., Annalen, 1990, 1205, (配糖体)
Sugiyama, M. et al., Phytochemistry, 1993, 33, 1215, (9-glucoside)

§ Neoolivil; Tetra-Ac
[構造式]些細な誘導体. 有効な構造式はない.
[基原]*Thymus longiflorus, Urtica dioica*
[性状]無定型の塊
[比旋光度]:[α]$_D^{23}$ +17 (EtOH)

----------文献----------

Hernandez, A. et al., Phytochemistry, 1981, 20, 181, (分離, C13-NMR, Mas)
Kraus, R. et al., Annalen, 1990, 1205, (配糖体)
Sugiyama, M. et al., Phytochemistry, 1993, 33, 1215, (9-glucoside)
Schoettner, M. et al., Phytochemistry, 1997, 46, 1107, (分離, H-NMR, C13-NMR, Mass, 絶対構造)

§ Neoolivil; 4-*O*-β-D-Glucopyranoside
[CAS No.]104402-97-3
[化合物分類]リグナン化合物(7,7'-Epoxytetrahydrofuranoid lignan)
[構造式]

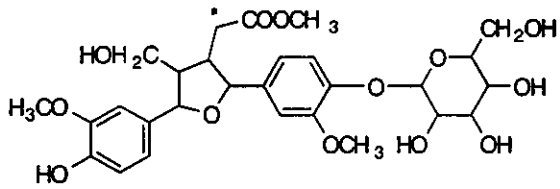


[分子式]$C_{26}H_{34}O_{12}$
[分子量]538.547
[正確な分子量]538.20503
[基原]*Urtica dioica*

----------文献----------

Hernandez, A. et al., Phytochemistry, 1981, 20, 181, (分離, C13-NMR, Mas)
Kraus, R. et al., Annalen, 1990, 1205, (配糖体)
Sugiyama, M. et al., Phytochemistry, 1993, 33, 1215, (9-glucoside)
Schoettner, M. et al., Phytochemistry, 1997, 46, 1107, (分離, H-NMR, C13-NMR, Mass, 絶対構造)

§ Neoolivil; 4-*O*-β-D-Glucopyranoside, 9-Ac
[CAS No.]104425-71-0
[化合物分類]リグナン化合物
(7,7'-Epoxytetrahydrofuranoid lignan)
[構造式]

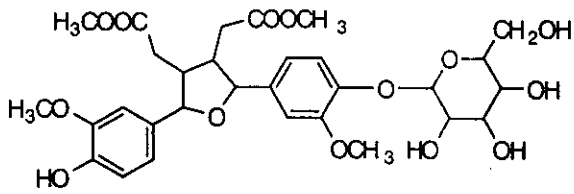


[分子式]$C_{28}H_{36}O_{13}$
[分子量]580.585
[正確な分子量]580.215595
[基原]*Urtica dioica*

----------文献----------

Hernandez, A. et al., Phytochemistry, 1981, 20, 181, (分離, C13-NMR, Mas)
Kraus, R. et al., Annalen, 1990, 1205, (配糖体)
Sugiyama, M. et al., Phytochemistry, 1993, 33, 1215, (9-glucoside)
Schoettner, M. et al., Phytochemistry, 1997, 46, 1107, (分離, H-NMR, C13-NMR, Mass, 絶対構造)

§ Neoolivil; 4-*O*-β-D-Glucopyranoside, 9,9'-di-Ac
[CAS No.]104380-18-9
[化合物分類]リグナン化合物(7,7'-Epoxytetrahydrofuranoid lignan)
[構造式]



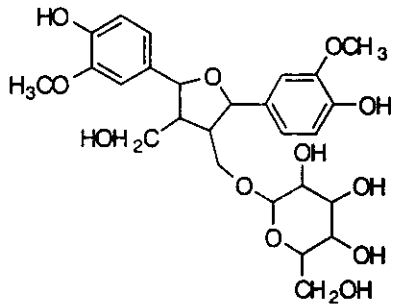
[分子式] $C_{30}H_{38}O_{14}$
[分子量] 622.622
[正確な分子量] 622.22616
[基原] *Urtica dioica*

---文献---

Hernandez, A. et al., Phytochemistry, 1981, 20, 181, (分離, C13-NMR, Mas)
Kraus, R. et al., Annalen, 1990, 1205, (配糖体)
Sugiyama, M. et al., Phytochemistry, 1993, 33, 1215, (9-glucoside)
Schoettner, M. et al., Phytochemistry, 1997, 46, 1107, (分離, H-NMR, C13-NMR, Mass, 絶対構造)

§ Neoolivil; 9-*O*-β-D-Glucopyranoside

[CAS No.] 129170-78-1
[化合物分類] リグナン化合物(7,7'-Epoxytetrahydrofuranoid lignan)
[構造式]



[分子式] $C_{26}H_{34}O_{12}$
[分子量] 538.547
[正確な分子量] 538.20503
[基原] 次の植物から分離: *Urtica dioica*

---文献---

Hernandez, A. et al., Phytochemistry, 1981, 20, 181, (分離, C13-NMR, Mas)
Kraus, R. et al., Annalen, 1990, 1205, (配糖体)
Sugiyama, M. et al., Phytochemistry, 1993, 33, 1215, (9-glucoside)
Schoettner, M. et al., Phytochemistry, 1997, 46, 1107, (分離, H-NMR, C13-NMR, Mass, 絶対構造)
Shen, Y.-C. et al., Phytochemistry, 1997, 46, 1111, (Taxumairin)

§ 14-Octacosanol

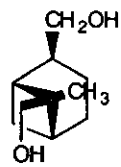
[CAS No.] 138967-02-9
[化合物分類] 脂肪族化合物(Saturated unbranched alcohol)
[構造式] $H_3C(CH_2)_{13}CH(OH)(CH_2)_{12}CH_3$
[分子式] $C_{28}H_{58}O$
[分子量] 410.766
[正確な分子量] 410.448765
[基原] *Urtica dioica* の根
[融点] Mp 79-80 ℃

---文献---

Gansser, D. et al., Planta Med., 1995, 61, 138, (分離, 合成法, IR, H-NMR, 性質)

§ 9,10-Pinanediol

[化合物分類] テルペノイド(Pinane monoterpenoid)
[構造式]



Relative configuration

[分子式] $C_{10}H_{18}O_2$
[分子量] 170.251
[正確な分子量] 170.13068
[基原] *Urtica dioica*
[性状] オイル

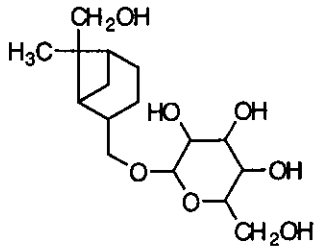
---文献---

Kraus, R. et al., Phytochemistry, 1991, 30, 1203, (分離, Mass, H-NMR, C13-NMR)

§ 9,10-Pinanediol; 10-*O*-β-D-Glucopyranoside

[CAS No.] 135378-06-2
[化合物分類] テルペノイド(Pinane monoterpenoid)

[構造式]

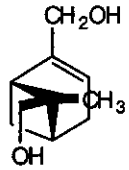


[分子式] $C_{16}H_{28}O_7$
[分子量] 332..393
[正確な分子量] 332.183505
[基原] *Urtica dioica*

----------文献----------

Kraus, R. et al., Phytochemistry, 1991, 30, 1203, (分離, Mass, H-NMR, C13-NMR)

§ 2-Pinene-9,10-diol
[CAS No.] 135378-04-0
[化合物分類] テルペノイド (Pinane monoterpenoid)
[構造式]



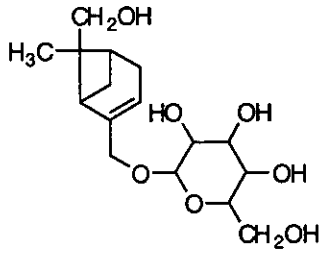
Relative configuration

[分子式] $C_{10}H_{16}O_2$
[分子量] 168.235
[正確な分子量] 168.11503
[基原] *Urtica dioica* の根
[性状] オイル

----------文献----------

Kraus, R. et al., Phytochemistry, 1991, 30, 1203, (分離, Mass, H-NMR, C13-NMR)

§ 2-Pinene-9,10-diol; 10-*O*-β-D-Glucopyranoside
[CAS No.] 135378-05-1
[化合物分類] テルペノイド (Pinane monoterpenoid)
[構造式]

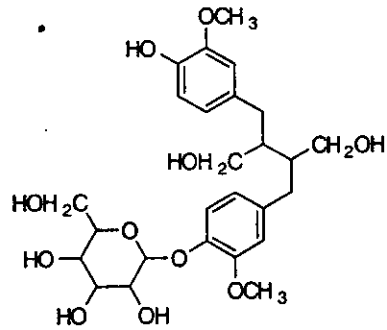


[分子式] $C_{16}H_{26}O_7$
[分子量] 330.377
[正確な分子量] 330.167855
[基原] *Urtica dioica*

----------文献----------

Kraus, R. et al., Phytochemistry, 1991, 30, 1203, (分離, Mass, H-NMR, C13-NMR)

§ Secoisolariciresinol; (8*R*,8'*R*)-form, 4-*O*-β-D-Glucopyranoside
[CAS No.] 129102-89-2
[化合物分類] リグナン化合物 (Side-chain oxygenated dibenzylbutane lignan)
[構造式]



[分子式] $C_{26}H_{36}O_{11}$
[分子量] 524.564
[正確な分子量] 524.225765
[基原] 次の植物から分離: *Urtica dioica*

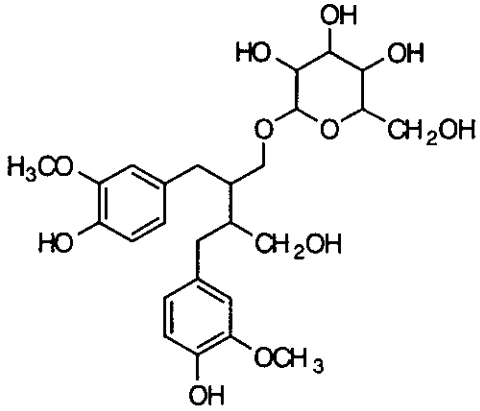
----------文献----------

Briggs, L.H. et al., Tet. Lett., 1959, No. 4, 14, (分離, 構造決定)
Freudenberg, K. et al., Tet. Lett., 1959, No. 17, 19, (分離)
Traveso, G., Gazz. Chim. Ital., 1962, 90, 792, (絶対構造)
Majumdar, R.B. et al., Indian J. Chem., 1972, 10, 677, (分離, 構造決定)
Andersson, R. et al., Acta Chem. Scand., Ser. B, 1975, 29, 835, (分離)
Fonseca, S.F. et al., Phytochemistry, 1978, 17, 499, (分離, C13-NMR)
Satyanarayana, P. et al., J. Nat. Prod., 1988, 51, 44, (誘導体)

Kraus, R. et al., Annalen, 1990, 1205, (4-glucoside)
Rodrigues Filho, E. et al., Phytochemistry, 1992, 31, 2115, (ester)
Das, B. et al., Phytochemistry, 1993, 33, 1489, (3-Demethylsecoisolariciresinol)
Fuchino, H. et al., Chem. Pharm. Bull., 1995, 43, 1937, (diferuloyl deriv)
Martinez V., J.C. et al., Phytochemistry, 1999, 50, 883, (Virola sebifera di-Ac)

§ Secoisolariciresinol; (8*R*,8'*R*)-form, 9-*O*-β-D-Glucopyranoside

[CAS No.]63320-67-2
[化合物分類]リグナン化合物(Side-chain oxygenated dibenzylbutane lignan)
[構造式]



Structure under review

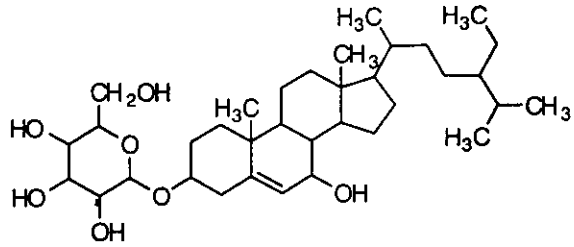
[分子式] $C_{26}H_{36}O_{11}$
[分子量] 524.564
[正確な分子量]524.225765
[基原] *Berchemia racemosa*, *Picea abies*, *Pinus massoniana*, *Pinus sylvestris*, *Urtica dioica*
[性状]無定型の粉末
[比旋光度]:[α]$_D$ -22.9 (c, 0.5 in EtOH)
[UV]:[neutral] λ $_{max}$ 223 (sh) (log ε 4.26); 282 (log ε 3.88) (EtOH)

----------文献----------

Kraus, R. et al., Annalen, 1990, 1205, (4-glucoside)

§ Stigmast-5-ene-3,7-diol; (3β,7α,24*R*)-form, 3-*O*-β-D-Glucopyranoside

[CAS No.]112137-81-2
[化合物分類]ステロイド(Stigmastane steroid). (C29).
[構造式]



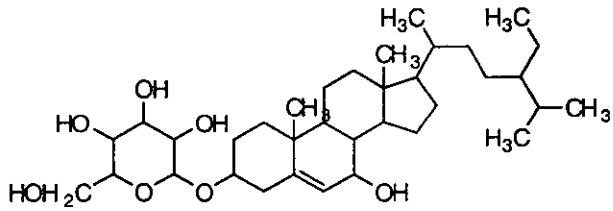
[分子式] $C_{35}H_{60}O_7$
[分子量]592.855
[正確な分子量]592.433905
[基原] *Urtica dioica*

----------文献----------

Chaurasia, N. et al., J. Nat. Prod., 1987, 50, 881, (分離, 3-glucoside)
Fukuyama, Y. et al., Planta Med., 1988, 54, 34, (分離, H-NMR, C13-NMR)

§ Stigmast-5-ene-3,7-diol; (3β,7β,24*R*)-form, 3-*O*-β-D-Glucopyranoside

[CAS No.]112137-80-1
[化合物分類]ステロイド(Stigmastane steroid).
(C29).
[構造式]



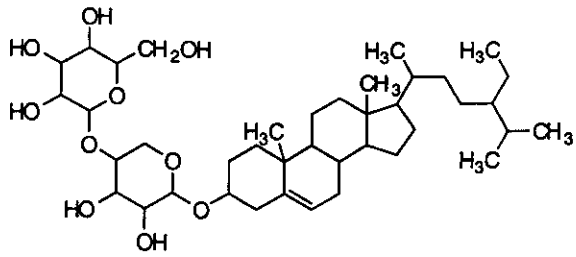
[分子量]592.855
[正確な分子量]592.433905
[基原] *Urtica dioica*

----------文献----------

Chaurasia, N. et al., J. Nat. Prod., 1987, 50, 881, (分離, 3-glucoside)

§ Stigmast-5-en-3-ol; (3β,24*R*)-form, 3-*O*-[β-D-Glucopyranosyl-(1→4)-α-L-arabinopyranoside]

[CAS No.]253670-59-6
[化合物分類]ステロイド(Stigmastane steroid). (C29).
[構造式]



[分子式]$C_{40}H_{68}O_{10}$
[分子量]708.971
[正確な分子量]708.48125
[基原]*Urtica dioica*

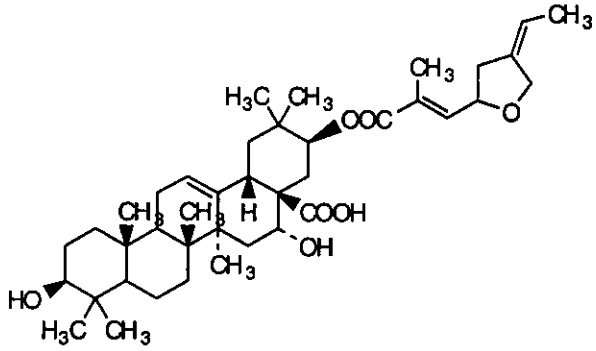
----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2071, (生育)
Tiwari, K.P. et al., Phytochemistry, 1979, 18, 2044, (配糖体)
Iribarren, A.M. et al., Phytochemistry, 1984, 23, 2087; 1985, 24, 360; 1987, 26, 857, (配糖体)

*********ネムノキ (Nemunoki, Silk tree) *********

§§マメ科ネムノキ(*Albizzia julibrissin* Durazzini)の樹皮。

§ Acacigenin B
[CAS No.]71545-18-1
[化合物分類]テルペノイド(Oleanane triterpenoid)
[構造式]

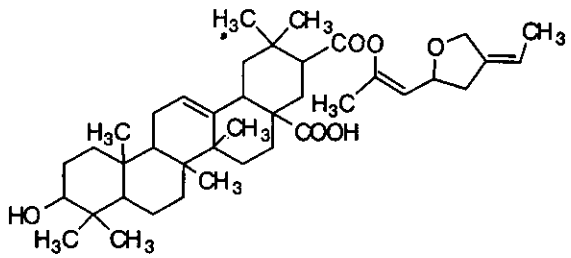


[分子式]$C_{40}H_{60}O_7$
[分子量]652.91
[正確な分子量]652.433905
[基原]*Acacia concinna, Albizzia julibrissin*
[性状]無定型の粉末 (EtOH)
[融点]Mp 265-270 ℃
[比旋光度]:$[\alpha]_D$ +55 (c, 1 in $CHCl_3$)

----------文献----------

Anjaneyulu, A.S.R. et al., Phytochemistry, 1979, 18, 463, (分離)
Woo, W.S. et al., J. Nat. Prod., 1984, 47, 547, (誘導体)

§ Acacigenin B; 16-Deoxy
[化学名・別名]16-Deoxyacacigenin
[CAS No.]91452-89-0
[化合物分類]テルペノイド(Oleanane triterpenoid)
[構造式]

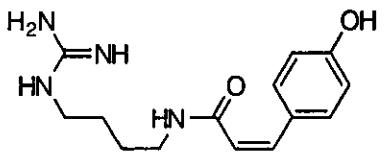


[分子式]$C_{40}H_{60}O_6$
[分子量]636.91
[正確な分子量]636.43899
[基原]次の植物から分離: *Albizzia julibrissin*
[融点]Mp 258-262 ℃

----------文献----------

Anjaneyulu, A.S.R. et al., Phytochemistry, 1979, 18, 463, (分離)
Woo, W.S. et al., J. Nat. Prod., 1984, 47, 547, (誘導体)

§ (4-Aminobutyl)guanidine; N^1-(4-Hydroxycinnamoyl) (Z-)
[化学名・別名]N^1-*cis*-*p*-Coumaroylagmatine
[化合物分類]アルカロイド化合物(Cinnamic acid amide), アルカロイド化合物(Putrescine alkaloid)
[構造式]



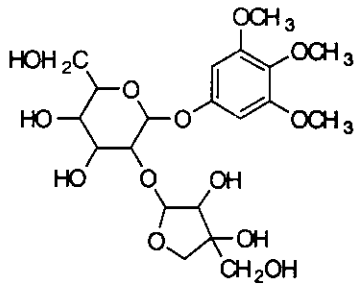
[分子式]$C_{14}H_{20}N_4O_2$

[分子量]276.338
[正確な分子量]276.158626
[基原]*Albizzia julibrissin*
[性状]シロップもしくは粉末
[UV]:[neutral] λ_{max} 278 (ε 2000) (H_2O)

---文献---

Kossel, A., Hoppe Seyler's Z. Physiol. Chem., 1910, 66, 257; 68, 170, (分離, 構造決定, 合成法)
Heyl, F.W., J.A.C.S., 1919, 41, 681, (分離)
Stoessl, A. et al., Phytochemistry, 1965, 4, 973, (分離, UV, 構造決定, 合成法, *N*-coumaroyl)
Smith, T.A. et al., Phytochemistry, 1978, 17, 1093, (生育, *N*-coumaroyl)
Bird, C.R. et al., Phytochemistry, 1981, 20, 2345, (生合成, *N*-coumaroyl)
Reis, D.J. et al., Ann. N.Y. Acad. Sci., 1999, 881, 65, (レビュー, 活性)

§ 1,2,3,5-Benzenetetrol; 1,2,3-Tri-Me ether, 5-*O*-[β-D-apiofuranosyl-(1 → 2)-β-D-glucopyranoside]
[CAS No.]142542-79-8
[化合物分類]単環芳香族(Simple phenol), 炭水化物(Disaccharide)
[構造式]

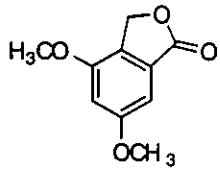


[分子式]$C_{20}H_{30}O_{13}$
[分子量]478.449
[正確な分子量]478.168645
[基原]次の植物から分離: *Albizzia julibrissin* の茎皮
[性状]粉末
[比旋光度]:[α]$_D^{25}$ -89.5 (c, 0.1 in MeOH)

---文献---

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Fuchino, H. et al., Chem. Pharm. Bull., 1995, 43, 1937, (tri-Me apiosylglucoside)

§ 4,6-Dihydroxy-1(3*H*)-isobenzofuranone; Di-Me ether
[化学名・別名]4,6-Dimethoxy-1(3*H*)-isobenzofuranone. 4,6-Dimethoxyphthalide
[CAS No.]58545-97-4
[化合物分類]ベンゾフラノイド(Isobenzofuran)
[構造式]

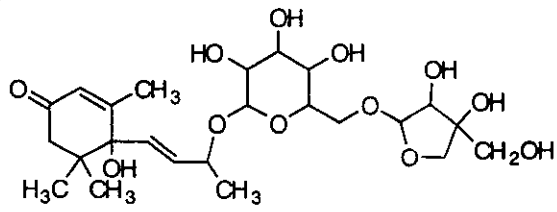


[分子式]$C_{10}H_{10}O_4$
[分子量]194.187
[正確な分子量]194.05791
[基原]次の植物から分離: *Albizzia julibrissin* の心材
[融点]Mp 164 ℃

---文献---

Brockmann, H. et al., Chem. Ber., 1957, 90, 2302, (合成法)
Nakano, Y. et al., Mokuzai Gakkaishi, 1975, 21, 577; CA, 84, 102290w

§ 6,9-Dihydroxy-4,7-megastigmadien-3-one; (6*S*,7*E*,9*R*)-form, 9-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]
[化合物分類]テルペノイド(Megastigmane norterpenoid)
[構造式]



[分子式]$C_{24}H_{38}O_{12}$
[分子量]518.557
[正確な分子量]518.23633
[基原]次の植物の茎皮から分離: *Albizzia julibrissin*, *Eriobotrya japonica*
[性状]粉末
[比旋光度]:[α]$_D^{25}$ +15 (c, 0.14 in MeOH)

---文献---

Higuchi, H. et al., Chem. Pharm. Bull., 1992, 40, 534, (9-apiosylglucoside)
De Tommasi, N. et al., J. Nat. Prod., 1992, 55, 1025, (9-apiosylglucoside)