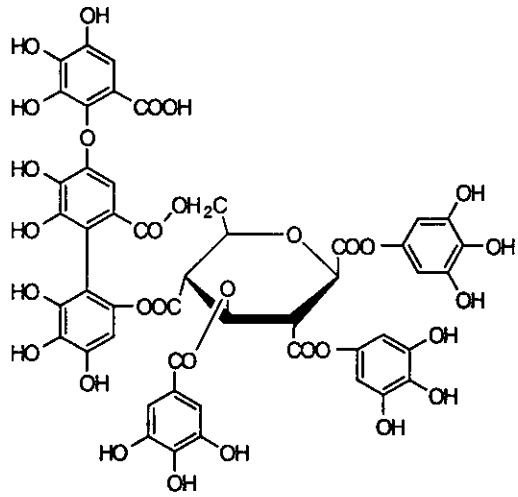
§ Rugosin A

[化学名・別名]1,2,3-Tri-*O*-galloyl-4,6-valoneoyl-β-D-glucopyranose

[CAS No.]84744-48-9

[化合物分類]タンニン化合物(Valoneoyl ester tannins)

[構造式]



[分子式]$C_{48}H_{34}O_{31}$

[分子量]1106.778

[正確な分子量]1106.108415

[基原]次の植物から得られるタンニン: *Stachyurus praecox*, *Rosa rugosa*, *Coriaria japonica*

[性状]淡褐色の無定型の粉末・五水和物

[比旋光度]:[α]$_D$ +110 (c, 1 in Me_2CO)

----------文献----------

Okuda, T. et al., Chem. Pharm. Bull., 1982, 30, 4230

Hatano, T. et al., Chem. Pharm. Bull., 1986, 34, 4533; 1989, 36, 3920; 1990, 38, 3308, (UV, CD, H-NMR, C13-NMR, 構造決定)

Lee, M.W. et al., Phytochemistry, 1992, 31, 2835

Yoshida, T. et al., Phytochemistry, 1993, 32, 1287, (Loropetalin A)

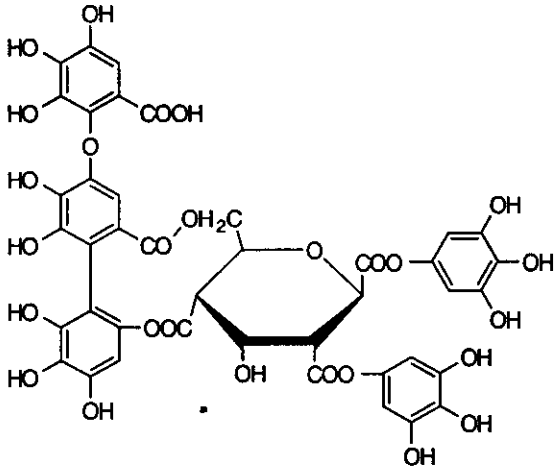
§ Rugosin A; 1-*O*-Degalloyl

[化学名・別名]Rugosin B

[CAS No.]84744-49-0

[化合物分類]タンニン化合物(Valoneoyl ester tannins)

[構造式]



[分子式]$C_{41}H_{30}O_{27}$

[分子量]954.672

[正確な分子量]954.097455

[基原]*Stachyurus praecox*, *Rosa rugosa*

[性状]淡褐色の無定型の粉末・四水和物

[比旋光度]:[α]$_D$ +124 (c, 1 in EtOH)

----------文献----------

Okuda, T. et al., Chem. Pharm. Bull., 1982, 30, 4230

Hatano, T. et al., Chem. Pharm. Bull., 1986, 34, 4533; 1989, 36, 3920; 1990, 38, 3308, (UV, CD, H-NMR, C13-NMR, 構造決定)

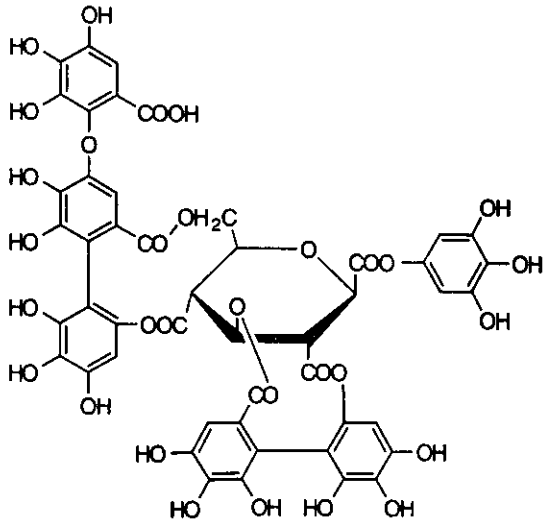
Lee, M.W. et al., Phytochemistry, 1992, 31, 2835

Yoshida, T. et al., Phytochemistry, 1993, 32, 1287, (Loropetalin A)

§ Rugosin C

[化学名・別名]1-*O*-Galloyl-2,3-(*S*)-hexahydroxydiphenoyl-4,6-(*S*)-valoneoyl-β-D-glucopyranose

[CAS No.]84744-50-3
[化合物分類]タンニン化合物(Valoneoyl ester tannins)
[構造式]



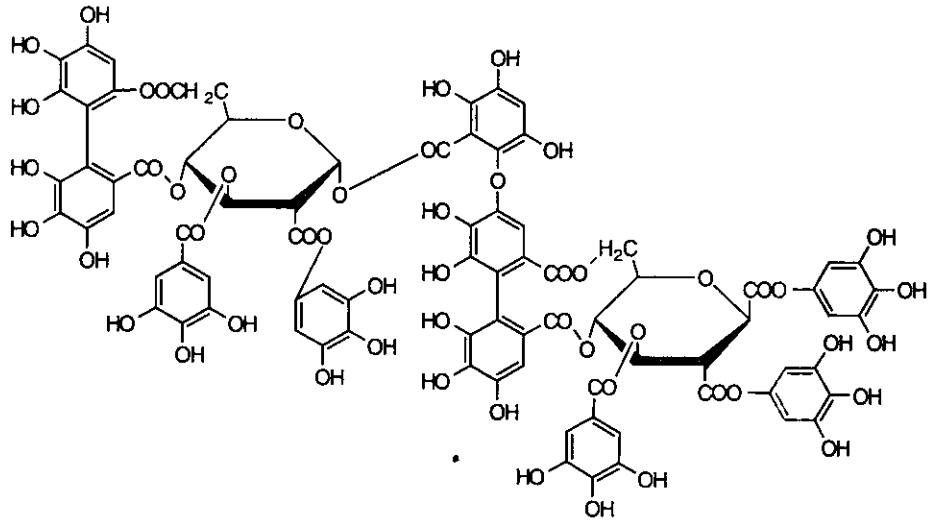
[分子式]$C_{48}H_{32}O_{31}$
[分子量]1104.762
[正確な分子量]1104.092765
[基原]次の植物から分離: *Rosa rugosa*, *Stachyurus praecox*
[性状]淡褐色の無定型の粉末・七水和物
[比旋光度]:[α]$_D$ +90 (c, 1 in Me_2CO)

----------文献----------

Okuda, T. et al., Chem. Pharm. Bull., 1982, 30, 4230
Hatano, T. et al., Chem. Pharm. Bull., 1990, 38, 3308; 1991, 39, 1689, (CD, UV, H-NMR, C13-NMR)
Hatano, T. et al., Heterocycles, 1990, 31, 1221, (C13-NMR)
Tanaka, T. et al., Chem. Pharm. Bull., 1991, 39, 60, (Calamanin A)
Lee, M.W. et al., Phytochemistry, 1992, 31, 2835, (H-NMR, 誘導体)

§ Rugosin D

[CAS No.]84754-11-0
[化合物分類]タンニン化合物(Valoneoyl ester tannins), タンニン化合物(Hexahydroxydiphenoyl ester tannins)
[構造式]



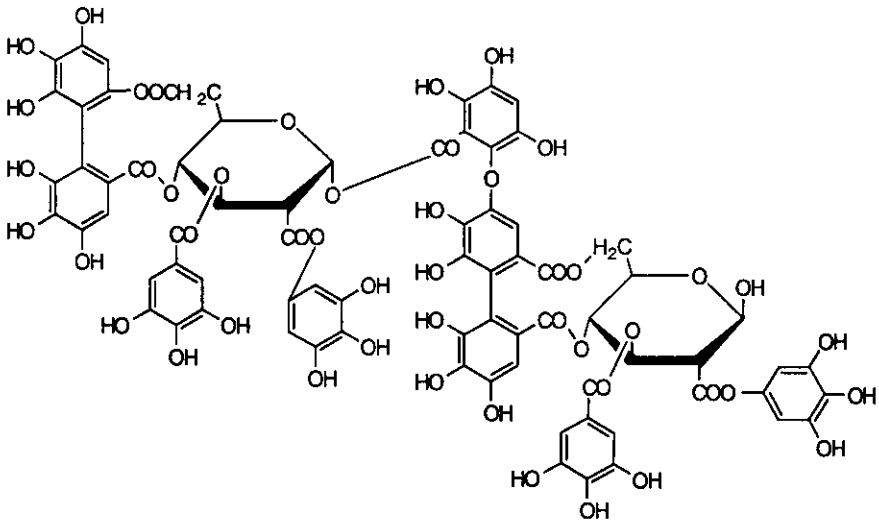
[分子式]$C_{82}H_{58}O_{52}$
[分子量]1875.329
[正確な分子量]1874.18943
[基原]次の植物から得られるタンニン: *Rosa rugosa*, *Coriaria japonica*
[用途]*in vivo* で強い抗腫瘍活性を有する
[性状]無定型の粉末・九水和物
[比旋光度]:[α]$_D$ +118 (c, 1 in Me_2CO)
[UV]:[neutral] λ_{max} 219 (ε 147900); 277 (ε 69200) (MeOH)

----------文献----------

Okuda, T. et al., Chem. Pharm. Bull., 1982, 30, 4234
Hatano, T. et al., Chem. Pharm. Bull., 1986, 34, 4533, (Coriarin E)
Miyamoto, K. et al., Chem. Pharm. Bull., 1987, 35, 814, (薬理)
Hatano, T. et al., Chem. Pharm. Bull., 1987, 38, 3341, (CD, H-NMR, C13-NMR)

§ Rugosin D; 1-De-*O*-galloyl

[化学名・別名]Rugosin E
[CAS No.]84744-51-4
[化合物分類]タンニン化合物(Valoneoyl ester tannins), タンニン化合物(Hexahydroxydiphenoyl ester tannins)
[構造式]

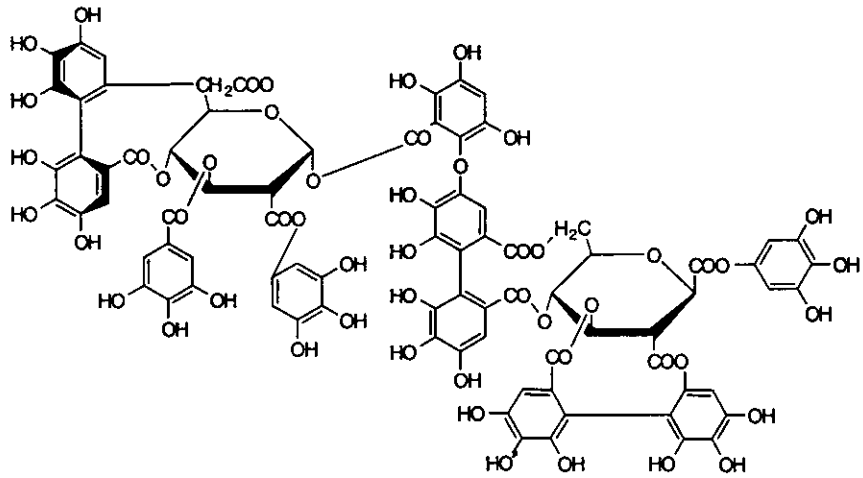


[分子式]$C_{75}H_{54}O_{48}$
[分子量]1723.223
[正確な分子量]1722.17847
[基原]*Rosa rugosa*
[用途]強い抗腫瘍活性を有する
[性状]淡褐色の無定型の粉末・五水和物
[比旋光度]:[α]$_D$ +140 (c, 1 in Me_2CO)
[UV]:[neutral] λ $_{max}$ 220 (ε 154000); 275 (ε 74000) (MeOH)

----------文献----------

Okuda, T. et al., Chem. Pharm. Bull., 1982, 30, 4234
Hatano, T. et al., Chem. Pharm. Bull., 1986, 34, 4533, (Coriarin E)
Miyamoto, K. et al., Chem. Pharm. Bull., 1987, 35, 814, (薬理)
Hatano, T. et al., Chem. Pharm. Bull., 1987, 38, 3341, (CD, H-NMR, C13-NMR)

§ Rugosin F
[CAS No.]84744-52-5
[化合物分類]タンニン化合物(Valoneoyl ester tannins)
[構造式]



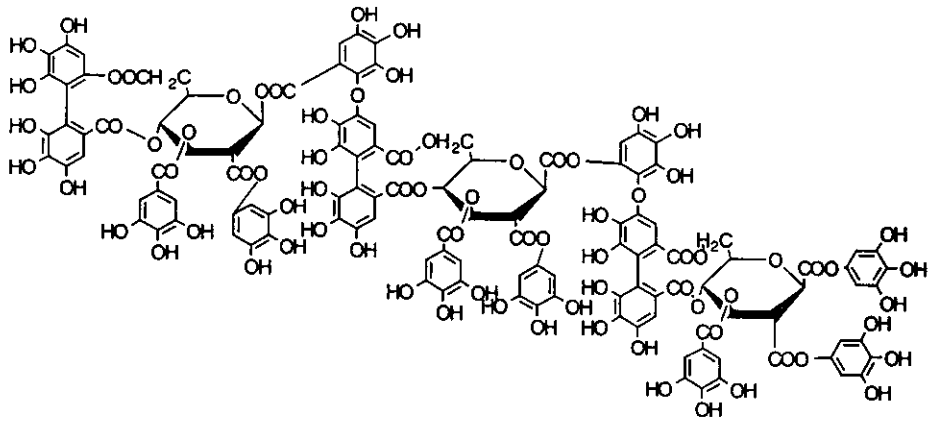
[分子式]$C_{82}H_{56}O_{52}$
[分子量]1873.313
[正確な分子量]1872.17378
[基原]次の植物から得られるタンニン: *Rosa rugosa*
[性状]淡褐色の無定型の粉末・十二水和物
[比旋光度]:[α]$_D$ +88 (c, 1 in Me_2CO)

----------文献----------

Okuda, T. et al., Chem. Pharm. Bull., 1982, 30, 4234
Hatano, T. et al., Chem. Pharm. Bull., 1990, 30, 3341, (H-NMR, C13-NMR, CD)
Yoshida, T. et al., Chem. Pharm. Bull., 1991, 39, 49, (Degalloylrugosin F)
Tanaka, T. et al., Chem. Pharm. Bull., 1991, 39, 60, (Calamanin B)
Yoshida, T. et al., Phytochemistry, 1991, 30, 2747, (Davuricin D_1)
Lee, M.W. et al., Phytochemistry, 1992, 31, 2835, (Alnusjaponin A)
Jin, Z.X. et al., Phytochemistry, 1998, 48, 333, (Heterophylliin F)

§ Rugosin G
[CAS No.]84754-12-1
[化合物分類]タンニン化合物(Valoneoyl ester tannins)
[構造式]

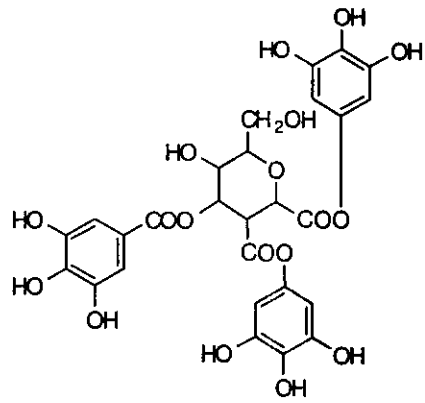
[分子式]$C_{123}H_{86}O_{78}$
[分子量]2811.986
[正確な分子量]
2810.27632
[基原]次の植物から得られるタンニン:
Rosa rugosa
[性状]淡褐色の無定型の粉末・十八水和物
[比旋光度]:[α]$_D$
+109 (c, 1 in Me_2CO)



---文献---

Okuda, T. et al., Chem. Pharm. Bull., 1982, 30, 4234
Hatano, T. et al., Chem. Pharm. Bull., 1990, 38, 3341, (CD, H-NMR, C13-NMR)

§ 1,2,3-Trigalloylglucose; β -D-Pyranose-form
[CAS No.]84415-91-8
[化合物分類]タンニン化合物(Simple gallate ester tannins)
[構造式]

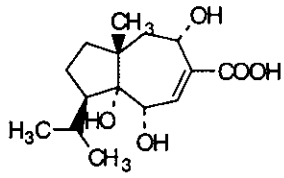


[分子量]636.476
[基原]次の植物から分離: *Euphorbia thymifolia, Coriaria japonica, Rosa rugosa, Cornus officinalis*
[性状]淡褐色の無定型粉末
[比旋光度]:[α]$_D^{20}$ +28.6 (c, 0.7 in Me_2CO)
[UV]:[neutral] λ $_{max}$ 278 (ε 34852) (MeOH)

---文献---

Okuda, T. et al., Chem. Pharm. Bull., 1982, 30, 4230, (分離)
Nishizawa, K. et al., Phytochemistry, 1990, 29, 2491, (UV, IR, H-NMR, C13-NMR)
Lee, S.-H. et al., Phytochemistry, 1990, 29, 3621, (H-NMR)
Xu, H.-X. et al., Heterocycles, 1994, 38, 167, (Geponin)
Nawwar, M.A.M. et al., Phytochemistry, 1994, 36, 793, (分離, H-NMR, C13-NMR)

§ 5,6,9-Trihydroxy-7-daucen-14-oic acid
[化学名・別名]Rugosic acid C
[CAS No.]135404-55-6
[化合物分類]テルペノイド(Daucane sesquiterpenoids)
[構造式]



[分子式]$C_{15}H_{24}O_5$
[分子量]284.352
[正確な分子量]284.162375
[基原]*Rosa rugosa*
[性状]シロップ

---文献---

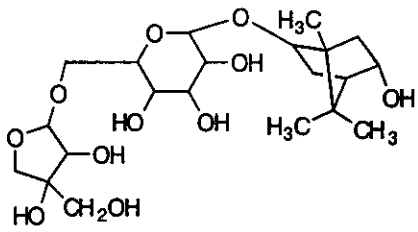
Hashidoko, Y. et al., Agric. Biol. Chem., 1991, 55, 1049, (分離, H-NMR)

***********ハマボウフウ (Hamabofu) ***********

§§ セリ科ハマボウフウ(*Glehnia littoralis* Fr. Schmidt)の根および根茎。

§ 2,5-Bornanediol; (1*S*,2*R*,5*S*)-form, 2-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]

[CAS No.]217969-13-6
[化合物分類]テルペノイド(Camphane monoterpenoids)
[構造式]



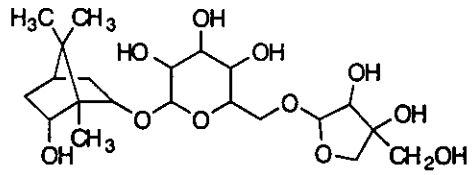
[分子式]$C_{21}H_{36}O_{11}$
[分子量]464.509
[正確な分子量]464.225765
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:$[\alpha]_D^{22}$ -49 (c, 1.7 in MeOH)

----------文献----------

Marquet, A. et al., Bull. Soc. Chim. Fr., 1967, 128, (合成法)
Allen, M.S. et al., Can. J. Chem., 1979, 57, 733, (合成法)
Mahmood, U. et al., Phytochemistry, 1983, 22, 774, (分離)
Gunawardana, Y.A.G.P. et al., J. Nat. Prod., 1988, 51, 142, (分離, C13-NMR, H-NMR)
Inoshiri, S. et al., Phytochemistry, 1988, 27, 2869, (分離, H-NMR, C13-NMR)
Ahmed, A.A. et al., Phytochemistry, 1991, 30, 1207, (分離)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1595, (配糖体)

§ 2,6-Bornanediol; (2*R*,6*S*)-form, 2-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]

[CAS No.]217969-20-5
[化合物分類]テルペノイド(Camphane monoterpenoids)
[構造式]



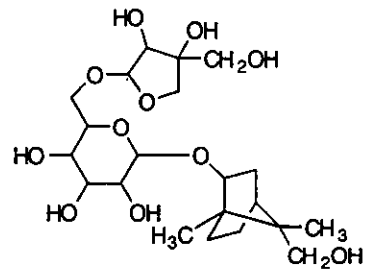
[分子式]$C_{21}H_{36}O_{11}$
[分子量]464.509
[正確な分子量]464.225765
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:$[\alpha]_D^{22}$ -82.2 (c, 0.4 in MeOH)

----------文献----------

Allen, M.S. et al., Can. J. Chem., 1979, 57, 733, (合成法, IR, H-NMR, Mass)
Darby, N. et al., Can. J. Chem., 1979, 57, 742, (合成法)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1595, (配糖体)
Kuo, Y.H. et al., Chem. Pharm. Bull., 2000, 48, 766, (Platydiol)

§ 2,9-Bornanediol; 2-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]

[CAS No.]217969-26-1
[化合物分類]テルペノイド(Camphane monoterpenoids)
[構造式]



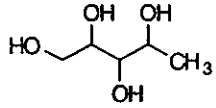
[分子式]$C_{21}H_{36}O_{11}$
[分子量]464.509
[正確な分子量]464.225765
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:$[\alpha]_D^{22}$ -61.9 (c, 1.2 in MeOH)

----------文献----------

Vasanth, S. et al., J. Nat. Prod., 1990, 53, 354, (分離, H-NMR, C13-NMR, 結晶構造)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1595, (配糖体)

§ 5-Deoxyarabinitol: D-form

[CAS No.]67968-44-9
[化合物分類]炭水化物(Pentitols), 炭水化物(5-Deoxy sugars)
[構造式]



基原]*Glehnia littoralis* の果実

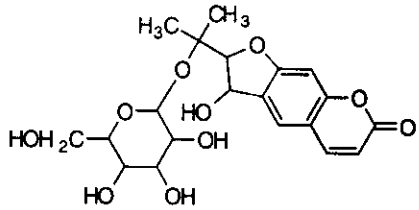
[性状]シロップ
[比旋光度]:[α]$_D^{24}$ -23 (c, 1.1 in MeOH)

----------文献----------

Zissis, E. et al., J.A.C.S., 1954, 76, 5515-5522, (合成法)
Takai, K. et al., J.O.C., 1985, 50, 3247-3251, (合成法)
Wiesler, W.T. et al., J.A.C.S., 1989, 111, 9205-9213, (CD, 絶対構造)
Andrews, M.A. et al., J.O.C., 1989, 54, 5257-5264, (合成法, H-NMR, C13-NMR)
Ishikawa, T. et al., Chem. Pharm. Bull., 2001, 49, 584-588, (分離, H-NMR, C13-NMR)

§ 2,3-Dihydro-3-hydroxy-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one; (2*S*,3*R*)-form, 1'-*O*-β-D-Glucopyranoside

[CAS No.]87592-77-6
[化合物分類]ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted), ベンゾピラノイド(Dihydrofuranocoumarins)
[構造式]



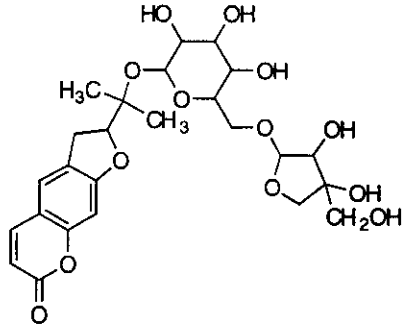
[分子式]$C_{20}H_{24}O_{10}$
[分子量]424.404
[正確な分子量]424.13695
[基原]*Angelica archangelica*, *Cnidium monnieri*, *Glehnia littoralis*
[性状]針状結晶 (MeOH)
[融点]Mp 267-269 ℃
[比旋光度]:[α]$_D^{22}$ -18 (c, 0.8 in Py)

----------文献----------

Savina, A.A. et al., Khim. Prir. Soedin., 1970, 6, 185; Chem. Nat. Compd. (Engl. Transl.), 1970, 6, 182, (Smyrnioridin)
Perel'son, M.E. et al., Khim. Prir. Soedin., 1971, 7, 712; Chem. Nat. Compd. (Engl. Transl.), 1971, 7, 692, (H-NMR, 誘導体)
Ishii, H. et al., Chem. Pharm. Bull., 1973, 21, 2346, (Xanthoarnol)
Lemmich, J. et al., Phytochemistry, 1983, 22, 553, (誘導体)
Asahara, T. et al., Planta Med., 1984, 50, 488, (Decuroside V)
Vilegas, W. et al., J. Nat. Prod., 1993, 56, 416, (分離)
Lemmich, J., Phytochemistry, 1995, 38, 427, (1'-glucoside)
Jimenez, B. et al., Phytochemistry, 2000, 53, 1025, (Senecioyloxymarmesin, 3-Hydroxyprantschimgin)

§ 2,3-Dihydro-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one; (*S*)-form, *O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]

[化合物分類]ベンゾピラノイド(Dihydrofuranocoumarins), ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted)
[構造式]



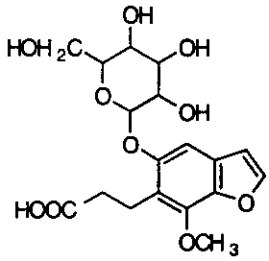
[分子式]$C_{25}H_{32}O_{13}$
[分子量]540.52
[正確な分子量]540.184295
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:[α]$_D^{22}$ -45.8 (c, 0.5 in MeOH)

----------文献----------

Abu-Mustafa, E.A. et al., J.O.C., 1961, 26, 161, (分離, UV, 誘導体)
Ognyanov, I. et al., Z. Naturforsch., B, 1967, 22, 1231, (分離)
Nielsen, B.E. et al., Acta Chem. Scand., 1970, 24, 2863, (分離)
(Seseliflorin)
成法)
Molho, D. et al., Bull. Soc. Chim. Fr., 1972, 208, (分離)
Abyshev, A.Z. et al., Khim. Prir. Soedin., 1972, 8, 114; Chem. Nat. Compd. (Engl. Transl.), 1972, 8, 107,

(分離, IR, UV, H-NMR)
Aminov, A.M. et al., Khim. Prir. Soedin., 1972, 8, 799; 1973, 9, 487; Chem. Nat. Compd. (Engl. Transl.), 1972, 8, 779; 1973, 9, 459, (分離)
Dukhovlinova, L.J. et al., Khim. Prir. Soedin., 1973, 9, 663; 1974, 10, 785; Chem. Nat. Compd. (Engl. Transl.), 1973, 9, 626; 1974, 10, 806, (分離)
Talapatra, S.K. et al., Phytochemistry, 1973, 12, 2312, (分離)
De Pascual Teresa, J. et al., An. Quim., 1979, 75, 175, (分離)
Burke, B.A. et al., Heterocycles, 1981, 16, 897, (分離)
Murray, R.D.H. et al., The Natural Coumarins, J. Wiley, 1982, (専門書)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1404, (Marmesin apiosylglucoside)

§ 5,7-Dihydroxy-6-benzofuranpropanoic acid; 7-Me ether, 5-*O*-β-D-glucopyranoside
[化合物分類]ベンゾフラノイド(Benzofurans), 単環芳香族(Simple phenylpropanoids)
[構造式]

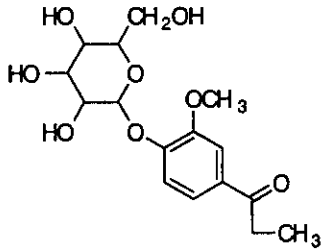


[分子式]$C_{18}H_{22}O_{10}$
[分子量]398.366
[正確な分子量]398.1213
[基原]*Glehnia littoralis* の果実
[性状]無定型の粉末
[比旋光度]:[α]$_D^{21}$ -60 (c, 1.8 in H_2O)

----------文献----------

Ishikawa, T. et al., Chem. Pharm. Bull., 2001, 49, 584-588

§ 1-(3,4-Dihydroxyphenyl)-1-propanone; 3-Me ether, 4-*O*-β-D-glucopyranoside
[化学名・別名]Baihuaqianhuoside
[CAS No.]155969-61-2
[化合物分類]単環芳香族(Simple aryl ketones), 単環芳香族(Simple phenylpropanoids)
[構造式]

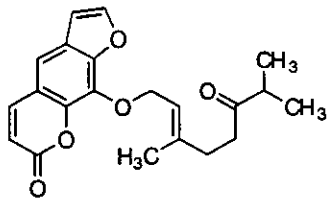


[分子式]$C_{16}H_{22}O_8$
[分子量]342.345
[正確な分子量]342.13147
[基原]*Peucedanum praeruptorum, Glehnia littoralis*
[性状]結晶($CHCl_3$/MeOH)
[融点]Mp 165.5-167.5 ℃ (149-151 ℃)
[比旋光度]:[α]$_D^{22}$ -66 (c, 0.3 in MeOH)

----------文献----------

Kong, L.Y. et al., Yaoxue Xuebao, 1994, 29, 276, (Baihuaqianhuoside)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1939, (Baihuaqianhuoside)

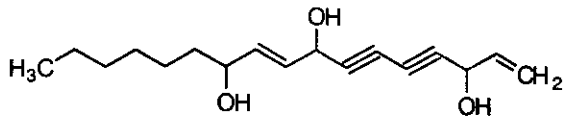
§ 8-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one; 6',7'-Dihydro, 6'-oxo
[化学名・別名]8-(3,7-Dimethyl-6-oxo-2-octenyloxy) psoralen
[化合物分類]ベンゾピラノイド(Furanocoumarins), ベンゾピラノイド(7,8-Dioxygenated coumarins)
[構造式]



[分子式]$C_{21}H_{22}O_5$
[分子量]354.402
[正確な分子量]354.146725
[基原]*Glehnia littoralis*
[性状]ガム
[比旋光度]:[α]$_D^{22}$ -23 (c, 0.5 in $CHCl_3$)

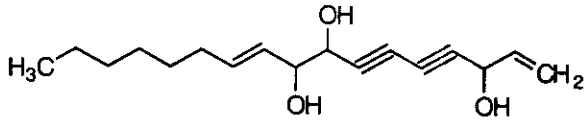
----------文献----------

Sharma, Y.N. et al., Tetrahedron, 1966, 22, 3221, (Geranyloxypsoralen)
Rashid, M.A. et al., J. Nat. Prod., 1992, 55, 851, (誘導体)
Ito, C. et al., Chem. Pharm. Bull., 1998, 46, 341, (Lansiumarins)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1939, (Dimethyloxooctenyloxypsoralen)

§ **1,9-Heptadecadiene-4,6-diyne-3,8,11-triol; (+)-(*Z*)-form**
[CAS No.] 181638-07-3
[化合物分類] 脂肪族化合物 (Acetylenic alcohols)
[構造式]

[基原] *Glehnia littoralis* spp. *leiocarpa*
[性状] 青白い黄色のオイル
[比旋光度]: $[\alpha]_D^{24}$ +83.7 (c, 0.09 in $CHCl_3$)

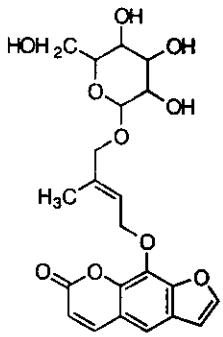
----------文献----------

Matsuura, H. et al., Planta Med., 1996, 62, 256, (分離, IR, H-NMR, Mass)

§ **1,10-Heptadecadiene-4,6-diyne-3,8,9-triol; (-)-(*E*)-form**
[CAS No.] 181638-08-4
[化合物分類] 脂肪族化合物 (Acetylenic alcohols)
[構造式]

[基原] *Glehnia littoralis* ssp. *leiocarpa*
[性状] 青白い黄色のオイル
[比旋光度]: $[\alpha]_D^{24}$ -19 (c, 0.06 in $CHCl_3$)

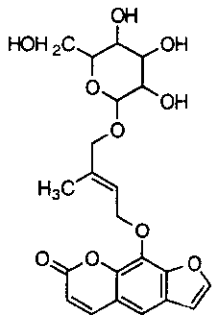
----------文献----------

Matsuura, H. et al., Planta Med., 1996, 62, 256, (分離, IR, H-NMR, Mass)

§ **Imperatorin; 4'-β-D-Glucopyranosyloxy (*E*-)**
[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] $C_{22}H_{24}O_{10}$
[分子量] 448.426
[正確な分子量] 448.13695
[基原] *Glehnia littoralis*
[性状] 無定型の粉末
[比旋光度]: $[\alpha]_D^{22}$ -42.3 (c, 0.5 in MeOH)

----------文献----------

Govindachari, T.R. et al., Tetrahedron, 1968, 24, 753, (分離)
Basa, S.C. et al., Chem. Ind. (London), 1970, 746, (分離, UV, IR, NMR)
Booer, M. et al., Ghana J. Sci., 1970, 10, 82, (薬理)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1377, (生育)
Murray, R.D.H. et al., The Natural Coumarins, J. Wiley, 1982, (生育, 毒性)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1404, (4'-glucosyloxy derivs)
Masuda, T. et al., Phytochemistry, 1998, 47, 13, (分離, UV, H-NMR, C13-NMR)

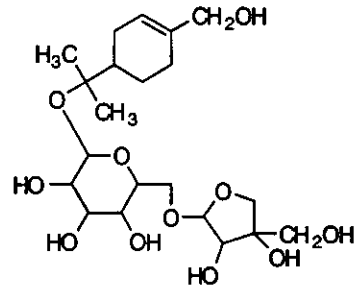
§ **Imperatorin; 4'-β-D-Glucopyranosyloxy (*Z*-)**
[化合物分類] ベンゾピラノイド (Furanocoumarins), ベンゾピラノイド (7,8-Dioxygenated coumarins)
[構造式]

[分子量] 448.426
[正確な分子量] 448.13695
[基原] *Glehnia littoralis*
[性状] 無定型の粉末
[比旋光度]: $[\alpha]_D^{22}$ -46.9 (c, 0.2 in MeOH)

----------文献----------

Govindachari, T.R. et al., Tetrahedron, 1968, 24, 753, (分離)
Basa, S.C. et al., Chem. Ind. (London), 1970, 746, (分離, UV, IR, NMR)
Booer, M. et al., Ghana J. Sci., 1970, 10, 82, (薬理)

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1377, (生育)
Murray, R.D.H. et al., The Natural Coumarins, J. Wiley, 1982, (生育, 毒性)
Masuda, T. et al., Phytochemistry, 1998, 47, 13, (分離, UV, H-NMR, C13-NMR)

§ *p*-Menth-1-ene-7,8-diol; (*R*)-form, 8-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]
[CAS No.]217969-33-0
[化合物分類]テルペノイド(p-Menthane monoterpenoids)
[構造式]

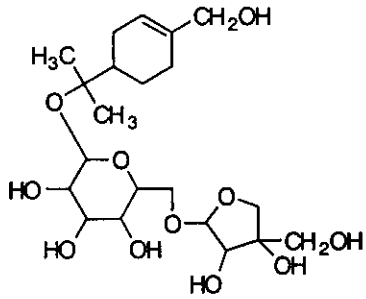


[分子式]$C_{21}H_{36}O_{11}$
[分子量]464.509
[正確な分子量]464.225765
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:$[\alpha]_D^{22}$ -22.8 (c, 0.4 in MeOH)

----------文献----------

Sato, T., Nippon Kagaku Zasshi, 1965, 86, 252; 1967, 88, 1005, (合成法)
Tan, R.X. et al., Phytochemistry, 1991, 30, 583, (分離, H-NMR, C13-NMR)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1595; 1999, 47, 639, (配糖体)
Ishikawa, T. et al., Chem. Pharm. Bull., 1998, 46, 1603, (配糖体)

§ *p*-Menth-1-ene-7,8-diol; (*S*)-form, 8-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]
[化合物分類]テルペノイド(p-Menthane monoterpenoids)
[構造式]

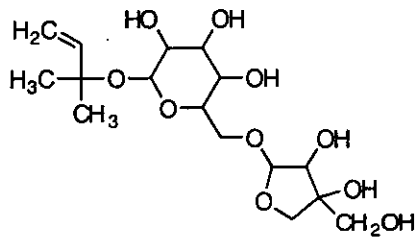


[分子量]464.509
[正確な分子量]464.225765
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:$[\alpha]_D^{22}$ -35.7 (c, 0.5 in MeOH)

----------文献----------

Sato, T., Nippon Kagaku Zasshi, 1965, 86, 252; 1967, 88, 1005, (合成法)
Tan, R.X. et al., Phytochemistry, 1991, 30, 583, (分離, H-NMR, C13-NMR)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1595; 1999, 47, 639, (配糖体)
Ishikawa, T. et al., Chem. Pharm. Bull., 1998, 46, 1603, (配糖体)

§ 2-Methyl-3-buten-2-ol; *O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]
[化合物分類]テルペノイド(Hemiterpenoids)
[構造式]



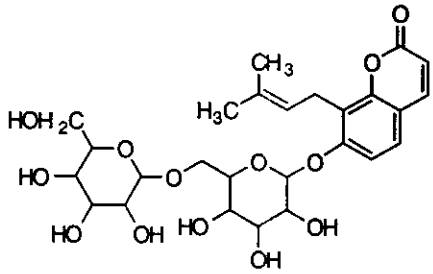
[分子式]$C_{16}H_{28}O_{10}$
[分子量]380.391
[正確な分子量]380.16825
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:$[\alpha]_D^{22}$ -84 (c, 0.2 in MeOH)

----------文献----------

Naves, Y.-R. et al., Bull. Soc. Chim. Fr., 1971, 886, (分離)
Pinar, M.M. et al., Phytochemistry, 1977, 16, 281, (配糖体)
Ahmed, A.A. et al., J. Nat. Prod., 1996, 59, 1171, (配糖体)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1939, (apiosylglucoside)
Vani, P.V.S.N. et al., Synth. Commun., 2000, 31, 219, (合成法, H-NMR)

§ Osthenol; *O*-[β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranoside

[化学名・別名] β-Gentiobiosylosthenol
[化合物分類] ベンゾピラノイド(7-Oxygenated coumarins, 8-substituted)
[構造式]

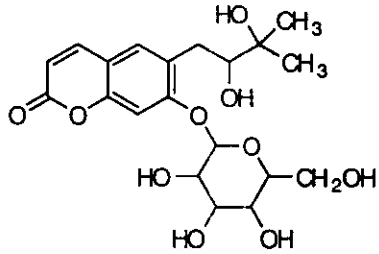


[分子式] $C_{26}H_{34}O_{13}$
[分子量] 554.547
[正確な分子量] 554.19945
[基原] *Glehnia littoralis*
[性状] 針状結晶 (H_2O)
[比旋光度]: $[\alpha]_D^{26}$ 0 (c, 0.337 in MeOH)

----------文献----------

Sasaki, H. et al., Chem. Pharm. Bull., 1980, 28, 1847, (β-Gentiobiosylosthenol)

§ Peucedanol; (*S*)-form, 7-*O*-β-D-Glucopyranoside
[化合物分類] ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted)
[構造式]

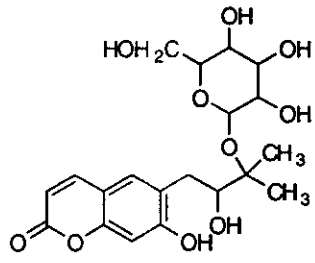


[分子式] $C_{20}H_{26}O_{10}$
[分子量] 426.419
[正確な分子量] 426.1526
[基原] *Glehnia littoralis*
[性状] 無定型の粉末
[比旋光度]: $[\alpha]_D^{22}$ -91.9 (c, 2.4 in MeOH)

----------文献----------

Desai, P.D. et al., Indian J. Chem., 1967, 5, 41, (分離, 誘導体)
Abyshev, A.Z. et al., Khim. Prir. Soedin., 1968, 4, 378; 1970, 6, 300; Chem. Nat. Compd. (Engl. Transl.), 1968, 4, 320; 1970, 6, 301, (分離)
Rondest, J. et al., Phytochemistry, 1968, 7, 1019, (分離, 合成法, Mass, H-NMR, UV)
Hata, K. et al., Yakugaku Zasshi, 1968, 88, 513; CA, 69, 96521, (分離)
Dreyer, D.L. et al., Phytochemistry, 1972, 11, 702, (分離, 合成法)
Joshi, P.P. et al., Indian J. Chem., Sect. B, 1975, 13, 772, (分離)
Lemmich, J. et al., Phytochemistry, 1978, 17, 139, (分離)
Gantimur, D. et al., Khim. Prir. Soedin., 1985, 21, 190; Chem. Nat. Compd. (Engl. Transl.), 1985, 21, 177, (配糖体)
Ikeshiro, Y. et al., Phytochemistry, 1994, 35, 1339, (Peujaponiside)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1404, (S-form glycosides)

§ Peucedanol; (*S*)-form, 3'-*O*-β-D-Glucopyranoside
[化合物分類] ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted)
[構造式]



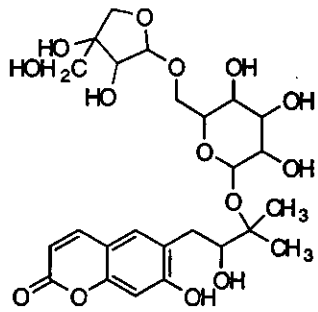
[分子量] 426.419
[正確な分子量] 426.1526
[基原] *Glehnia littoralis*
[性状] 無定型の粉末
[比旋光度]: $[\alpha]_D^{22}$ -22.4 (c, 0.5 in MeOH)

----------文献----------

Desai, P.D. et al., Indian J. Chem., 1967, 5, 41, (分離, 誘導体)
Abyshev, A.Z. et al., Khim. Prir. Soedin., 1968, 4, 378; 1970, 6, 300; Chem. Nat. Compd. (Engl. Transl.), 1968, 4, 320; 1970, 6, 301, (分離)
Rondest, J. et al., Phytochemistry, 1968, 7, 1019, (分離, 合成法, Mass, H-NMR, UV)
Hata, K. et al., Yakugaku Zasshi, 1968, 88, 513; CA, 69, 96521, (分離)
Dreyer, D.L. et al., Phytochemistry, 1972, 11, 702, (分離, 合成法)
Joshi, P.P. et al., Indian J. Chem., Sect. B, 1975, 13, 772, (分離)
Lemmich, J. et al., Phytochemistry, 1978, 17, 139, (分離)

Ikeshiro, Y. et al., Phytochemistry, 1994, 35, 1339, (Peujaponiside)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1404, (S-form glycosides)

§ Peucedanol; (*S*)-form, 3'-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]
[化合物分類]ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted)
[構造式]

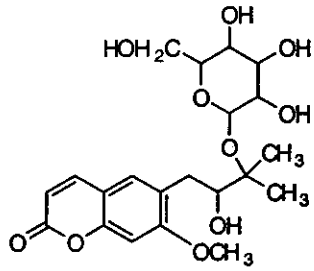


[分子式]$C_{25}H_{34}O_{14}$
[分子量]558.535
[正確な分子量]558.19486
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:$[\alpha]_D^{22}$ -37.6 (c, 0.8 in MeOH)

----------文献----------

Desai, P.D. et al., Indian J. Chem., 1967, 5, 41, (分離, 誘導体)
Abyshev, A.Z. et al., Khim. Prir. Soedin., 1968, 4, 378; 1970, 6, 300; Chem. Nat. Compd. (Engl. Transl.), 1968, 4, 320; 1970, 6, 301, (分離)
Rondest, J. et al., Phytochemistry, 1968, 7, 1019, (分離, 合成法, Mass, H-NMR, UV)
Hata, K. et al., Yakugaku Zasshi, 1968, 88, 513; CA, 69, 96521, (分離)
Dreyer, D.L. et al., Phytochemistry, 1972, 11, 702, (分離, 合成法)
Joshi, P.P. et al., Indian J. Chem., Sect. B, 1975, 13, 772, (分離)
Lemmich, J. et al., Phytochemistry, 1978, 17, 139, (分離)
Gantimur, D. et al., Khim. Prir. Soedin., 1985, 21, 190; Chem. Nat. Compd. (Engl. Transl.), 1985, 21, 177, (配糖体)
Ikeshiro, Y. et al., Phytochemistry, 1994, 35, 1339, (Peujaponiside)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1404, (S-form glycosides)

§ Peucedanol; (*S*)-form, 7-Me ether, 3'-*O*-β-D-glucopyranoside
[化合物分類]ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted)
[構造式]

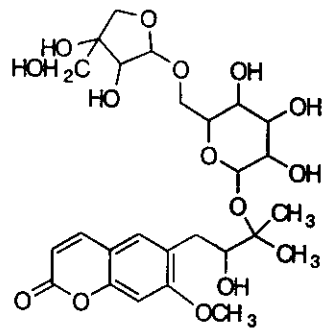


[分子式]$C_{21}H_{28}O_{10}$
[分子量]440.446
[正確な分子量]440.16825
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:$[\alpha]_D^{22}$ -43.8 (c, 0.8 in MeOH)

----------文献----------

Desai, P.D. et al., Indian J. Chem., 1967, 5, 41, (分離, 誘導体)
Abyshev, A.Z. et al., Khim. Prir. Soedin., 1968, 4, 378; 1970, 6, 300; Chem. Nat. Compd. (Engl. Transl.), 1968, 4, 320; 1970, 6, 301, (分離)
Rondest, J. et al., Phytochemistry, 1968, 7, 1019, (分離, 合成法, Mass, H-NMR, UV)
Hata, K. et al., Yakugaku Zasshi, 1968, 88, 513; CA, 69, 96521, (分離)
Dreyer, D.L. et al., Phytochemistry, 1972, 11, 702, (分離, 合成法)
Joshi, P.P. et al., Indian J. Chem., Sect. B, 1975, 13, 772, (分離)
Lemmich, J. et al., Phytochemistry, 1978, 17, 139, (分離)
Gantimur, D. et al., Khim. Prir. Soedin., 1985, 21, 190; Chem. Nat. Compd. (Engl. Transl.), 1985, 21, 177, (配糖体)
Ikeshiro, Y. et al., Phytochemistry, 1994, 35, 1339, (Peujaponiside)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1404, (S-form glycosides)

§ Peucedanol; (*S*)-form, 7-Me ether, 3'-*O*-[β-D-apiofuranosyl-(1 → 6)-β-D-glucopyranoside]
[化合物分類]ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted)
[構造式]



[分子式]$C_{26}H_{36}O_{14}$
[分子量]572.562
[正確な分子量]572.21051
[基原]*Glehnia littoralis*
[性状]無定型の粉末
[比旋光度]:$[\alpha]_D^{22}$ -61.9 (c, 1.2 in MeOH)

----------文献----------

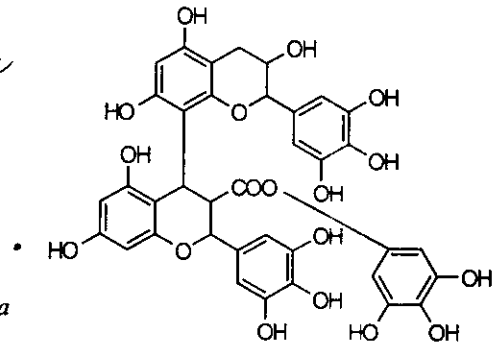
Rondest, J. et al., Phytochemistry, 1968, 7, 1019, (分離, 合成法, Mass, H-NMR, UV)
Hata, K. et al., Yakugaku Zasshi, 1968, 88, 513; CA, 69, 96521, (分離)
Dreyer, D.L. et al., Phytochemistry, 1972, 11, 702, (分離, 合成法)
Joshi, P.P. et al., Indian J. Chem., Sect. B, 1975, 13, 772, (分離)
Lemmich, J. et al., Phytochemistry, 1978, 17, 139, (分離)
Gantimur, D. et al., Khim. Prir. Soedin., 1985, 21, 190; Chem. Nat. Compd. (Engl. Transl.), 1985, 21, 177, (配糖体)
Ikeshiro, Y. et al., Phytochemistry, 1994, 35, 1339, (Peujaponiside)
Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1404, (S-form glycosides)

**********ハマメリス (Winter bloom) **********

§§ マンサク科アメリカマンサク(*Hamamelis virginiana* L.)の葉または樹皮。

§ 3,3',4',5,5',7-Hexahydroxyflavan-(4 → 8)-3,3',4',5,5',7-hexahydroxyflavan; (2*R*,2'*R*,3*R*,3'*S*,4*R*)-form, 3-*O*-(3,4,5-Trihydroxybenzoyl)

[化学名・別名]3-Galloylprodelphinidin B_1
[CAS No.]152100-01-1
[化合物分類]フラボノイド(Proanthocyanidin flavonoids), タンニン化合物(Simple gallate ester tannins)
[構造式]



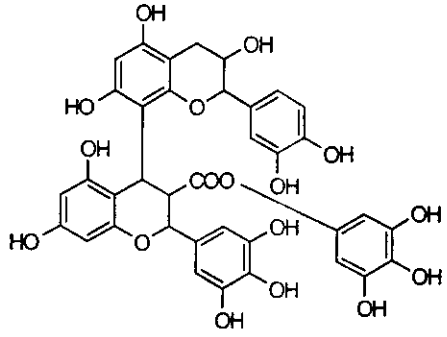
[分子式]$C_{37}H_{30}O_{18}$
[分子量]762.633
[正確な分子量]762.14322
[基原]次の植物から分離: *Cistus incanus*, *Hamamelis virginiana*

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002

§ 3,3',4',5,5',7-Hexahydroxyflavan-(4 → 8)-3,3',4',5,5',7-hexahydroxyflavan; (2*R*,2'*R*,3*R*,3'*S*,4*R*)-form, 3'''-Deoxy, 3-*O*-(3,4,5-trihydroxybenzoyl)

[化合物分類]フラボノイド(Proanthocyanidin flavonoids), タンニン化合物(Simple gallate ester tannins)
[構造式]

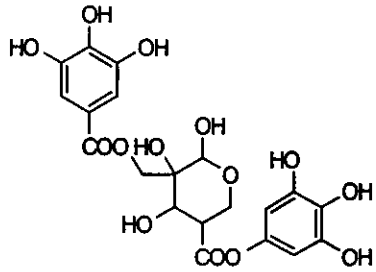


[分子式]$C_{37}H_{30}O_{17}$
[分子量]746.634
[正確な分子量]746.148305
[基原]*Hamamelis virginiana* (マンサク科)

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002

§ 2-*C*-Hydroxymethylribose; D-Pyranose-form, 2',4-Bis(3,4,5-trihydroxybenzoyl)
[化学名・別名]2',4-Di-*O*-galloyl-D-hamamelopyranose
[化合物分類]タンニン化合物(Simple gallate ester tannins)
[構造式]

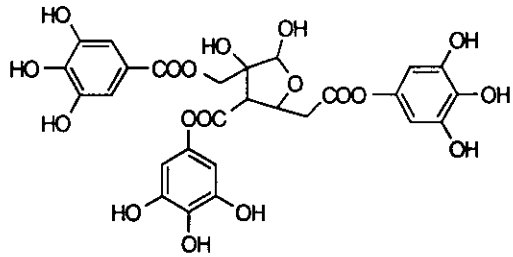


[分子式]$C_{20}H_{20}O_{14}$
[分子量]484.37
[正確な分子量]484.08531
[基原]*Hamamelis virginiana*（マンサク科）

----------文献----------

Shafizadeh, F., Adv. Carbohydr. Chem., 1956, 11, 263,（レビュー）
Nonaka, G. et al., Chem. Pharm. Bull., 1984, 32, 483,（gallates）
Haberland, C. et al., Phytochemistry, 1994, 60, 464,（gallates）
Hartisch, C. et al., Phytochemistry, 1996, 42, 191,（gallates）

§ 2-*C*-Hydroxymethylribose; α-D-Furanose-form, 2',3,5-Tris(3,4,5-trihydroxybenzoyl)
[化学名・別名]2',3,5-Tri-*O*-galloyl-α-D-hamamelofuranose
[化合物分類]タンニン化合物(Simple gallate ester tannins)
[構造式]

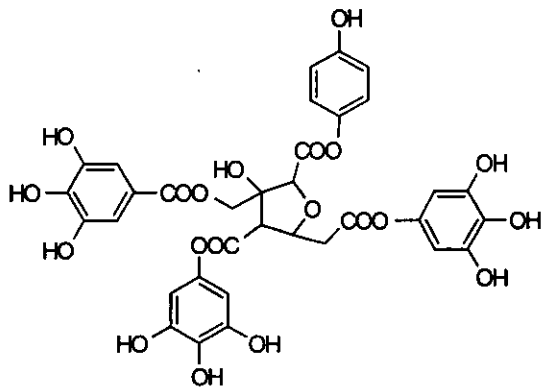


[分子式]$C_{27}H_{24}O_{18}$
[分子量]636.476
[正確な分子量]636.09627
[基原]*Hamamelis virginiana*（マンサク科）

----------文献----------

Shafizadeh, F., Adv. Carbohydr. Chem., 1956, 11, 263,（レビュー）
C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Mayer, W., Annalen, 1965, 688, 232,（構造決定, Hamamelitannin）
Ezekiel, A.D. et al., Carbohydr. Res., 1969, 11, 233,（合成法, Hamamelitannin）

§ 2-*C*-Hydroxymethylribose; α-D-Furanose-form, 4-Hydroxybenzoyl glycoside, 2',3,5-tris (3,4,5-trihydroxybenzoyl)
[化合物分類]タンニン化合物(Simple gallate ester tannins)
[構造式]

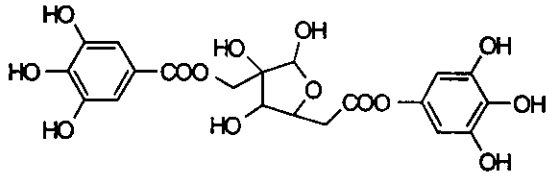


[分子式]$C_{34}H_{28}O_{20}$
[分子量]756.583
[正確な分子量]756.1174
[基原]*Hamamelis virginiana*（マンサク科）

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Shafizadeh, F., Adv. Carbohydr. Chem., 1956, 11, 263,（レビュー）
Mayer, W., Annalen, 1965, 688, 232,（構造決定, Hamamelitannin）
Ezekiel, A.D. et al., Carbohydr. Res., 1969, 11, 233,（合成法, Hamamelitannin）

§ 2-*C*-Hydroxymethylribose; β-D-Furanose-form, 2',5-Bis(3,4,5-trihydroxybenzoyl)
[化学名・別名]2',5-Digalloylhamamelofuranose. Hamamelitannin
[CAS No.]469-32-9
[化合物分類]炭水化物(Branched chain sugars), タンニン化合物(Simple gallate ester tannins)
[構造式]

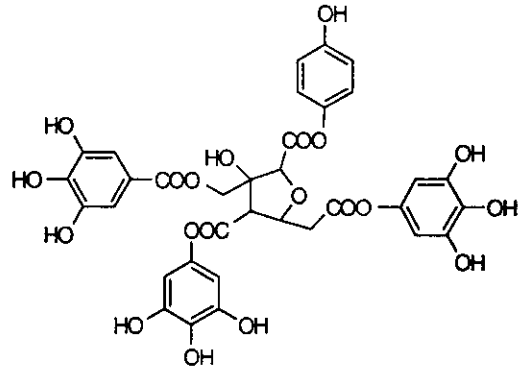


[分子式]$C_{20}H_{20}O_{14}$
[分子量]484.37
[正確な分子量]484.08531
[基原]次の植物から得られるタンニン: アメリカマンサク *Hamamelis virginiana*. *Quercus rubra*, *Castanea sativa* からも得られる
[性状]プリズム結晶もしくは針状結晶 + 1/2H_2O(H_2O)
[融点]Mp 146-147 ℃
[比旋光度]:[α]$_D^{19}$ +33 (c, 1.24 in H_2O)

----------文献----------

Mayer, W., Annalen, 1965, 688, 232, (構造決定, Hamamelitannin)
Ezekiel, A.D. et al., Carbohydr. Res., 1969, 11, 233, (合成法, Hamamelitannin)

§ 2-*C*-Hydroxymethylribose; β-D-Furanose-form, 4-Hydroxybenzoyl glycoside, 2',3,5-tris (3,4,5-trihydroxybenzoyl)
[化合物分類]タンニン化合物(Simple gallate ester tannins)
[構造式]

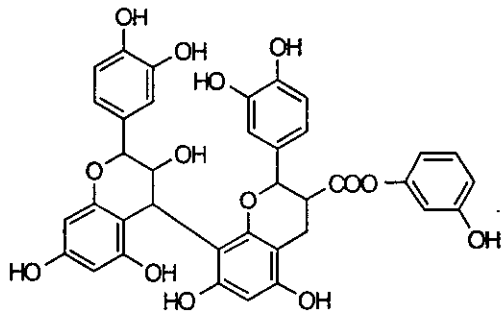


[分子式]$C_{34}H_{28}O_{20}$
[分子量]756.583
[正確な分子量]756.1174
[基原]*Hamamelis virginiana* (マンサク科)

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Shafizadeh, F., Adv. Carbohydr. Chem., 1956, 11, 263, (レビュー)
Mayer, W., Annalen, 1965, 688, 232, (構造決定, Hamamelitannin)
Ezekiel, A.D. et al., Carbohydr. Res., 1969, 11, 233, (合成法, Hamamelitannin)
Hartisch, C. et al., Phytochemistry, 1996, 42, 191, (gallates)

§ 3,3',4',5,7-Pentahydroxyflavan(4 → 8)-3,3',4',5,7-pentahydroxyflavan; (2*R*,2'*R*,3*R*,3'*S*,4*R*)-form, 3'-*O*-(4-Hydroxybenzoyl)
[化学名・別名]3'-(4-Hydroxybenzoyl) procyanidin B_1
[化合物分類]フラボノイド(Proanthocyanidin flavonoids)
[構造式]



[分子式]$C_{37}H_{30}O_{14}$
[分子量]698.636
[正確な分子量]698.16356
[基原]*Hamamelis virginiana* (マンサク科)

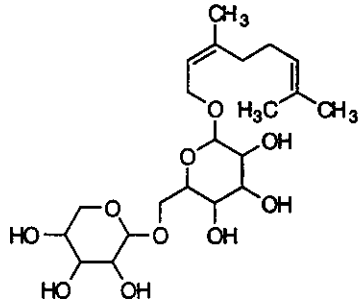
----------文献----------

Tanaka, T. et al., Phytochemistry, 1983, 22, 2575, (3-Galloylprocyanidin B_3)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Bae, Y.-S. et al., Phytochemistry, 1994, 35, 473, (Procyanidin B_3 3-glucoside)

Hartisch, C. et al., Phytochemistry, 1996, 42, 191, (4-Hydroxybenzoylprocyanidin B_1)

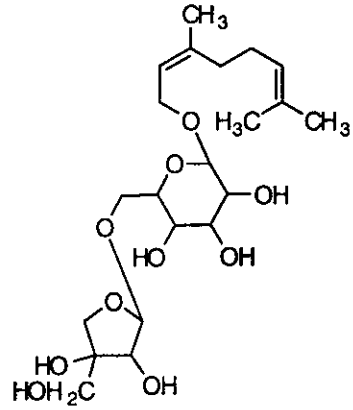
**********バラ (Rose) **********

§§ バラ科ダマスクバラ(*Rosa damascena* Miller)の花または果実。

§ 3,7-Dimethyl-2,6-octadien-1-ol; (*E*)-form, *O*-[α-L-Arabinopyranosyl-(1 → 6)-β-D-glucopyranoside]
[化学名・別名]Kenposide A
[CAS No.]152520-94-0
[化合物分類]テルペノイド(Acyclic monoterpenoids)
[構造式]

[分子式]$C_{21}H_{36}O_{10}$
[分子量]448.509
[正確な分子量]448.23085
[基原]*Hovenia dulcis*, *Rosa damascena* var. *bulgaria*
[性状]オイル
[比旋光度]:$[\alpha]_D^{22}$ -50 (c, 4 in MeOH)

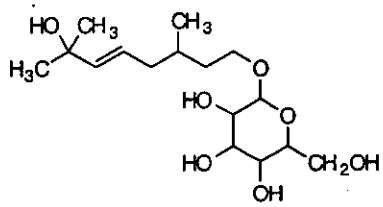
----------文献----------

Yoshikawa, K. et al., Phytochemistry, 1993, 34, 1431, (Kenposide A)

§ 3,7-Dimethyl-2,6-octadien-1-ol; (*E*)-form, *O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]
[化学名・別名]Acuminoside
[CAS No.]120163-17-9
[化合物分類]テルペノイド(Acyclic monoterpenoids)
[構造式]

[分子式]$C_{21}H_{36}O_{10}$
[分子量]448.509
[正確な分子量]448.23085
[基原]*Hypoxis acuminata*, *Hypoxis obtusa*, *Rosa damascena*, ブドウ(*Vitis vinefera*)
[性状]無定型
[融点]Mp 39-41 ℃
[比旋光度]:$[\alpha]_D^{19}$ -94.6 (c, 0.9 in MeOH)

----------文献----------

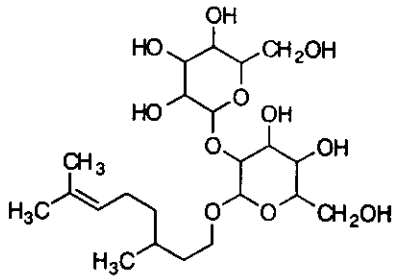
Bredenkamp, M.W. et al., Phytochemistry, 1988, 28, 263, (Acuminoside)
Lewis, R.J., Food Additives Handbook, Van Nostrand Reinhold International, New York, 1989, DTD000; DTD200; DTD800

§ 3,7-Dimethyl-5-octene-1,7-diol; (3*R*,5*E*)-form, 1-*O*-β-D-Glucopyranoside
[化合物分類]テルペノイド(Acyclic monoterpenoids)
[構造式]

[分子式]$C_{16}H_{30}O_7$
[分子量]334.409
[正確な分子量]334.199155
[基原]*Rosa damascena*
[比旋光度]:$[\alpha]_D^{22}$ -12.2 (c, 0.1 in H_2O)

----------文献----------

Watanabe, N. et al., Nat. Prod. Lett., 1998, 12, 5, (分離, H-NMR, C13-NMR, 合成法)

§ 3,7-Dimethyl-6-octen-1-ol; (ξ)-form, 1-*O*-[β-D-Glucopyranosyl-(1 → 2)-β-D-glucopyranoside]
[化学名・別名]Citronellyl β-sophoroside
[CAS No.]209681-41-4
[化合物分類]テルペノイド(Acyclic monoterpenoids)
[構造式]



[分子式] $C_{22}H_{40}O_{11}$
[分子量] 480.551
[正確な分子量] 480.257065
[基原] *Rosa damascena* var. *bulgaria* の花
[比旋光度]: $[\alpha]_D^{22}$ -16 (c, 0.1 in H_2O)

----------文献----------

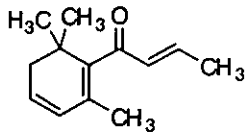
Oka, N. et al., Phytochemistry, 1998, 47, 1527, (Citronellyl β-sophoroside)

§ 10-Eicosene
[化学名・別名] 10-Icosene
[CAS No.] 66587-45-9
[関連 CAS No.] 78999-41-4, 78999-42-5
[化合物分類] 脂肪族化合物 (Unbranched alkenic alcohols)
[構造式] $H_3C(CH_2)_8CH=CH(CH_2)_8CH_3$
[分子式] $C_{20}H_{40}$
[分子量] 280.536
[正確な分子量] 280.313
[基原] 次の植物から分離: *Rosa damascena* (ブルガリアローズオイル)
[性状] オイル

----------文献----------

Kovats, E., J. Chromatogr., 1987, 406, 185, (分離)
Collazo, L.R. et al., J.O.C., 1993, 58, 43, (合成法, IR, Mass, H-NMR, C13-NMR)

§ 3,5,8-Megastigmatrien-7-one
[化学名・別名] 1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one. Damascenone. β-Damascenone
[CAS No.] 23726-93-4
[化合物分類] テルペノイド (Megastigmane norterpenoids)
[構造式]

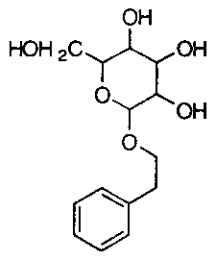


[分子式] $C_{13}H_{18}O$
[分子量] 190.285
[正確な分子量] 190.135765
[基原] *Rosa damascena*, その他多くの基原
[用途] 香水成分
[性状] オイル
[沸点] Bp_{13} 116-118 ℃

----------文献----------

Sarandeses, L.A. et al., J.O.C., 1992, 57, 2757, (合成法, β-Damascone)
Unnikrishnan, P.A., Org. Prep. Proced. Int., 1993, 25, 687, (合成法, β-Damascone)

§ 2-Phenylethanol; *O*-α-D-Glucopyranoside
[化学名・別名] 2-Phenylethyl α-D-glucopyranoside. Phenethyl α-D-glucoside
[CAS No.] 105088-18-4
[化合物分類] 単環芳香族 (Phenylacetic acid derivatives)
[構造式]

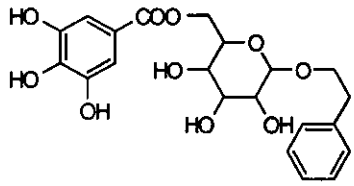


[分子式] $C_{14}H_{20}O_6$
[分子量] 284.308
[正確な分子量] 284.12599
[基原] *Rosa damascena bulgaria*, *Vitis vinifera* cv. Riesling

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 251, (生育)
Kozawa, M. et al., Chem. Pharm. Bull., 1983, 31, 2712, (Phenethyl ferulate)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. et al), American Pharmaceutical Association/Pharmaceutical Press, 1994, 340

§ 2-Phenylethanol; *O*-[3,4,5-Trihydroxybenzoyl-(→ 6)-β-D-glucopyranoside]
[化学名・別名]Phenethyl 6-galloylglucoside
[化合物分類]単環芳香族(Phenylacetic acid derivatives), タンニン化合物(Simple gallate ester tannins)
[構造式]

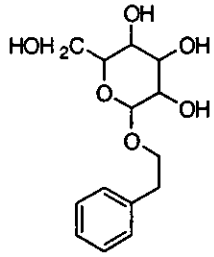


[分子式]$C_{21}H_{24}O_{10}$
[分子量]436.415
[正確な分子量]436.13695
[基原]次の植物から分離: *Rosa damascena*
[用途]Inhibitor of reverse transcriptase

----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 251, (生育)
Mel'nikov, V.N. et al., Khim. Prir. Soedin., 1976, 11, 807; Chem. Nat. Compd. (Engl. Transl.), 1976, 11, 822, (配糖体)
Kozawa, M. et al., Chem. Pharm. Bull., 1983, 31, 2712, (Phenethyl ferulate)
Lewis, R.J., Food Additives Handbook, Van Nostrand Reinhold International, New York, 1989, PDD750

§ 2-Phenylethanol; *O*-β-D-Galactopyranoside
[化学名・別名]2-Phenylethyl galactopyranoside. Phenethyl galactoside
[CAS No.]14861-16-6
[その他の CAS No.]55520-11-1
[化合物分類]単環芳香族(Phenylacetic acid derivatives)
[構造式]



[分子式]$C_{14}H_{20}O_6$
[分子量]284.308
[正確な分子量]284.12599
[基原]*Rosa damascena bulgaria*, *Vitis vinifera* cv. Riesling

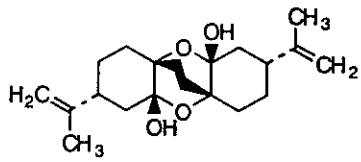
----------文献----------

C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 251, (生育)
Mel'nikov, V.N. et al., Khim. Prir. Soedin., 1976, 11, 807; Chem. Nat. Compd. (Engl. Transl.), 1976, 11, 822, (配糖体)
Kozawa, M. et al., Chem. Pharm. Bull., 1983, 31, 2712, (Phenethyl ferulate)

*********パルマローザ (Palmarosa) *********

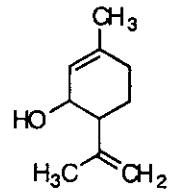
§§イネ科パルマローザ(*Cymbopogon martini* Stapf)の茎葉または全草。

§ Cymbodiacetal

[CAS No.] 111534-64-6
[化合物分類] テルペノイド (Miscellaneous bicyclic diterpenoids), テルペノイド (p-Menthane monoterpenoids)
[構造式]

[分子式] $C_{20}H_{30}O_4$
[分子量] 334.455
[正確な分子量] 334.21441
[基原] *Cymbopogon martini* の精油
[性状] 結晶 ($CHCl_3$)
[融点] Mp 206-207 ℃
[比旋光度]: $[\alpha]_D^{25}$ +26 (c, 0.12 in $CHCl_3$)

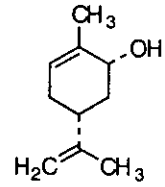
----------文献----------

Bottini, A.T. et al., Phytochemistry, 1987, 26, 2301, (分離, 結晶構造)

§ *p*-Mentha-1,8-dien-3-ol
[化学名・別名] 3-Methyl-6-(1-methylethenyl)-2-cyclohexen-1-ol (CAS 名).
6-Isopropenyl-3-methyl-2-cyclohexen-1-ol. Isopiperitenol
[CAS No.] 491-05-4
[関連 CAS No.] 4017-76-9, 65733-29-1, 65733-30-4, 74410-00-7, 96555-02-1
[化合物分類] テルペノイド (p-Menthane monoterpenoids)
[構造式]

[分子式] $C_{10}H_{16}O$
[分子量] 152.236
[正確な分子量] 152.120115
[基原] *Cymbopogon martini* と *Cymbopogon densiflorus* のオイル, 又は柑橘類オイルに存在する.
[沸点] $Bp_{0.9}$ 98 ℃

----------文献----------

Schenk, G.O. et al., Annalen, 1965, 687, 26, (合成法)
Nakamura, H. et al., Bull. Chem. Soc. Jpn., 1992, 65, 929, (合成法)

§ *p*-Mentha-1,8-dien-6-ol
[化学名・別名] 2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-ol. 5-Isopropenyl-2-methyl-2-cyclohexen-1-ol. Carveol. FEMA 2247
[CAS No.] 99-48-9
[関連 CAS No.] 1197-06-4, 1197-07-5
[化合物分類] テルペノイド (p-Menthane monoterpenoids)
[構造式]

(4*R*,6*R*)-form
[分子式] $C_{10}H_{16}O$
[分子量] 152.236
[正確な分子量] 152.120115
[基原] 次の植物のオイルに存在: グレープフルーツ (*Citrus paradisi*), マンダリン (*Citrus reticulata*), *Heracleum canescens*, *Cymbopogon martini*, また, クロフサスグリの液果, セロリ, ブラックティ, イノンド, キャラウェイの種子に存在する
[用途] 香水に用いられる. 香気成分
[傷害・毒性] 50 %致死量 (LD_{50}) (ラット, 経口) 3000 mg/kg
[化学物質毒性データ総覧 (RTECS) 登録番号] OS8400000

----------文献----------

Opdyke, D.L.J., Food Cosmet. Toxicol., 1973, 11, 1055, (レビュー, 毒性)
Grandi, R. et al., Tetrahedron, 1974, 30, 4037, (合成法)
Voisin, D. et al., Bull. Soc. Chim. Fr., 1975, 375, (合成法)
Ackermann, I.E. et al., Annalen, 1989, 79, (合成法, 配糖体)
Shimizu, S. et al., J. Essent. Oil Res., 1990, 2, 81, (配糖体)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 107, (レビュー)
Bouwmeester, H.J. et al., Phytochemistry, 1999, 50, 243, (生合成)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, MKY250

RTECS（化学物質毒性データ）

生体影響物質　　:天然物. 一時刺激物質.

健康障害に関するデータ

皮膚/眼の刺激に関するデータ

〈〈試験方法〉〉 標準ドライズ試験.
曝露経路　　：皮膚への塗布
被験動物　　：げっ歯類-ウサギ.
投与量・期間：500 mg/24 時間
参照文献

FCTXAV Food and Cosmetics Toxicology. (London, UK) V.1-19, 1963-81. For publisher information, see FCTOD7. [Vol.,頁,年(19-)]11,1055,1973

急性毒性に関するデータ

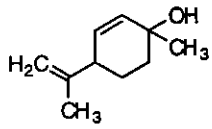
〈〈試験方法〉〉 LD50 試験(50%致死量試験).
曝露経路　　：経口投与.
被験動物　　：げっ歯類-ラット.
投与量・期間：3 gm/kg
毒性影響　　：致死量以外に毒性影響に関する報告はない.
参照文献

FCTXAV Food and Cosmetics Toxicology. (London, UK) V.1-19, 1963-81. For publisher information, see FCTOD7. [Vol.,頁,年(19-)]11,1055,1973

米国に於ける状況

EPA TSCA Section 8(b) CHEMICAL INVENTORY

§ *p*-Mentha-2,8-dien-1-ol; (1*R*,4*R*)-form

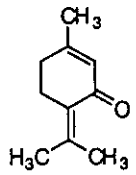


[CAS No.]52154-82-2
[化合物分類]テルペノイド(p-Menthane monoterpenoids), 脂肪族化合物(Simple heteroalicyclics (2 × O))
[構造式]
[基原]次の植物から分離: ジンジャーグラスのオイル(*Cymbopogon martini*), 種々の柑橘類オイル. 代謝と酸化でリモネンより製造
[沸点]$Bp_{6.5}$ 86.5 ℃
[屈折率]n^{20}_{D} 1.4881

----------文献----------

Naves, Y.R. et al., Bull. Soc. Chim. Fr., 1960, 37, (分離)
Schenk, G.O. et al., Annalen, 1964, 674, 93, (合成法)
Wang, W. et al., J. Chem. Res., Synop., 1998, 42, (合成法, H-NMR, C13-NMR)

§ *p*-Mentha-1,4(8)-dien-3-one

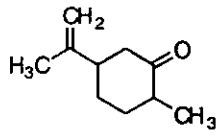


[化学名・別名]3-Methyl-6-(1-methylethylidene)-2-cyclohexen-1-one(CAS 名).
6-Isopropylidene-3-methyl-2-cyclohexenone. Piperitenone. Pulespenone. 3-Terpinolenone
[CAS No.]491-09-8
[化合物分類]テルペノイド(p-Menthane monoterpenoids)
[構造式]
[分子式]$C_{10}H_{14}O$
[分子量]150.22
[正確な分子量]150.104465
[基原]*Lippia*, *Mentha* spp., *Cymbopogon martini* のオイル
[性状]オイル
[沸点]Bp_{14} 120-122 ℃

----------文献----------

Naves, Y.R., Bull. Soc. Chim. Fr., 1963, 681, (分離)
Nigam, M.C. et al., Can. J. Chem., 1965, 43, 521, (分離)
Beereboom, J.J. et al., J.O.C., 1966, 31, 2026, (合成法)

Bohlmann, F. et al., Org. Magn. Reson., 1975, 7, 426, (C13-NMR)
Naves, Y.R., Riv. Ital. Essenze, Profumi, Piante Off., Aromi, Saponi, Cosmet., Aerosol, 1976, 58, 136, (レビュー)
Tanowitz, B.D. et al., J. Nat. Prod., 1984, 47, 739, (分離, H-NMR)

§ ***p*-Menth-8-en-2-one; (1*S*,4*S*)-form**
[CAS No.]6909-25-7
[化合物分類]テルペノイド(p-Menthane monoterpenoids)
[構造式]

[基原]キャラウェイのオイル. また, *Anathum sowa* (dill), *Lippia alba*, *Mentha* spp., *Cymbopogon martini* のようなその他のオイルからも得られる
[性状]オイル
[沸点]Bp 220-221 ℃
[比旋光度]:[α]$_D$ -19

----------文献----------

Nigam, M.C. et al., Can. J. Chem., 1965, 43, 521, (分離)
Opdyke, D.L.J., Food Cosmet. Toxicol., 1980, 18, 665, (レビュー, 毒性)
Verghese, J., Perfum. Flavor., 1980, 5, 23, (レビュー)
Jirovetz, L. et al., Ernaehrungsforschung, 1994, 18, 534; CA, 123, 168090m, (生育)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 163, (レビュー)
Tumen, G. et al., J. Essent. Oil Res., 1995, 7, 175; 177, (生育)
Gabriels, S. et al., Eur. J. Org. Chem., 1999, 1803, (1R,4R-form, 合成法, IR, H-NMR, C13-NMR, Mass)

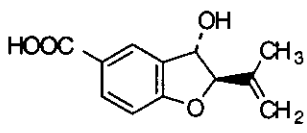
§§ **イネ科(*Cymbopogon martini* (Roxburgh) W. Watson var. *motia*)の茎葉または全草。**
該当物質なし

§§ **イネ科ジンジャーグラス(*Cymbopogon martini* Stapf var. *sofia*)の茎葉または全草。**
該当物質なし

**********パンダナ (Pandanus) **********

§§ **タコノキ科タコノキ(*Pandanus boninensis* Warburg)の枝葉または花。**
該当物質なし

§§ **タコノキ科アダン(*Pandanus odoratissimus* Linne f., non. illeg)の枝葉または花。**

§ **2,3-Dihydro-3-hydroxy-2-isopropenyl-5-benzofurancarboxylic acid; (2*R**,3*S**)-form, Me ester**
[化合物分類]ベンゾフラノイド(Benzofurans)
[構造式]

(2*R**,3*S**)-*form*
[分子式]$C_{13}H_{14}O_4$
[分子量]234.251
[正確な分子量]234.08921
[基原]*Pandanus odoratissimus*
[性状]オイル
[UV]:[neutral] λ $_{max}$ 220 (sh) (); 258 (); 290 (sh) () (溶媒の報告はない)

----------文献----------

Jong, T.-T. et al., Phytochemistry, 1998, 49, 2145, (分離, UV, H-NMR, C13-NMR)

§ **4-Hydroxy-3-(3-methyl-2-butenyl) benzoic acid; 2',3'-Dihydro, 2',3'-dihydroxy, Me ester**