

[比旋光度]:  $[\alpha]_D^{20} -166$  (c, 0.43 in MeOH)

-----文献-----

Goryana, G.M. et al., *Khim. Prir. Soedin.*, 1976, 12, 400-401; 762-765; 810; 823-824; *Chem. Nat. Compd.* (Engl. Transl.), 1976, 12, 353-354; 684-686; 727; 743-744, (Asparagosides)

Liu, C. et al., *Huaxue Xuebao*, 1985, 20, 143-145, (分離)

Agrawal, P.K. et al., *Phytochemistry*, 1985, 24, 2479-2496, (C13-NMR, レビュー)

§ Spirostan-3-ol; (3 $\beta$ ,5 $\beta$ ,25 $S$ )-form, 3-O- $[\beta$ -D-Glucopyranosyl-(1 $\rightarrow$ 3)]- $[\alpha$ -D-xylopyranosyl-(1 $\rightarrow$ 4)]- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 4)]- $\beta$ -D-glucopyranoside

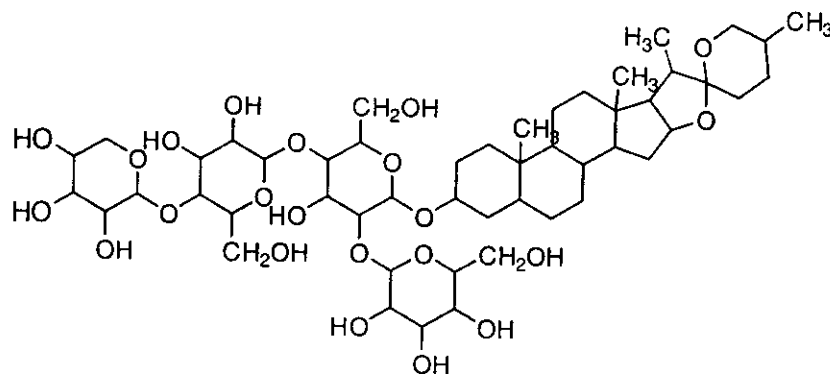
[化学名・別名] Asparagoside F

[CAS No.] 60267-26-7

[化合物分類] ステロイド

(Spirostane steroids). (C27).

[構造式]



[分子式]  $C_{50}H_{92}O_{22}$

[分子量] 1035.185

[天然基原] *Asparagus*

*officinalis*

[性状] 無定型

-----文献-----

Goryana, G.M. et al., *Khim. Prir. Soedin.*, 1976, 12, 400-401; 762-765; 810; 823-824; *Chem. Nat. Compd.* (Engl. Transl.), 1976, 12, 353-354; 684-686; 727; 743-744, (Asparagosides)

§ Zeaxanthin; Dihexadecanoyl

[化学名・別名] Physalien. Zeaxanthin dipalmitate

[CAS No.] 144-67-2

[化合物分類] テルペノイド (Tetraterpenoids)

[構造式]

[分子式]  $C_{77}H_{116}O_4$

[分子量] 1045.706

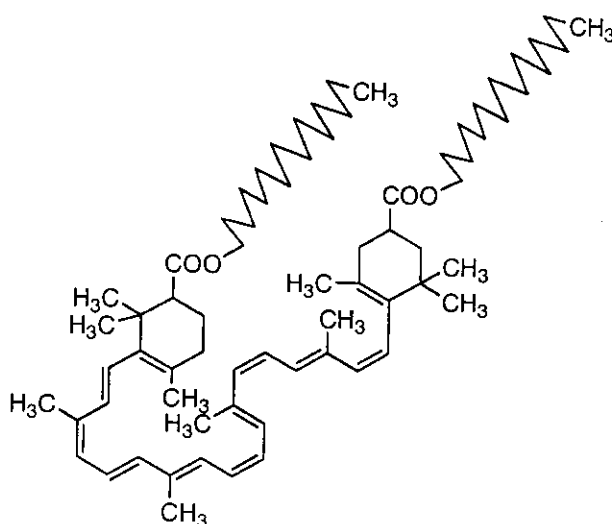
[天然基原] *Physalis* spp., *Lycium* spp., アスパラガス

(*Asparagus officinalis*), その他

[性状] 赤色の結晶 ( $C_6H_6/MeOH$ )

[融点] Mp 98.5-99.5 °C

[比旋光度]:  $[\alpha]_{D112} -45$  ( $CHCl_3$ )



-----文献-----

Curl, A.L. et al., *J. Food Sci.*, 1961, 26, 106-111, (分離)

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhuser Verlag, Basel, 1972, nos. 1839; 1840, (生育)

Parkes, K.E.B. et al., *Tet. Lett.*, 1986, 27, 2535, (分離)

Straub, O. et al., *Key to Carotenoids*, 2nd edn., Birkhuser Verlag, Basel and Boston, 1987, 119; 123, (成書)

Yokoyama, A. et al., *Tet. Lett.*, 1995, 36, 4901, (Thermozeaxanthins)

Kull, D.R. et al., *J. Nat. Prod.*, 1997, 60, 371-374, (配糖体)

§ § セリ科ミツバ (*Cryptotaenia japonica* Hasskari) の茎葉または幼茎

本調査研究では、成分に関する文献はなかった。

§ 2-(4-Hydroxyphenyl) ethanol; 1-O-4-Hydroxy-3-methoxycinnamoyl (E-)

[化学名・別名] *p*-Hydroxyphenethyl *trans*-ferulate

[CAS No.] 84873-15-4

[化合物分類] 単環芳香族 (Phenylacetic acid derivatives), 単環芳香族 (Simple phenylpropanoids)

[構造式]

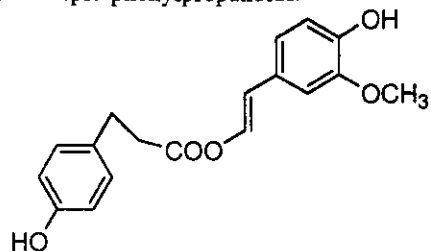
[分子式] C<sub>18</sub>H<sub>18</sub>O<sub>5</sub>

[分子量] 314.337

[天然基原] *Heracleum lanatum* var. *nipponicum*, *Oenanthe javanica*,  
*ania longa*

[性状] 粉末

[融点] Mp 165-166 °C



Steph

-----文献-----

Bridel, M. et al., C. R. Hebd. Seances Acad. Sci., 1926, 183, 231, (分離, Salidroside)

Veer, W.L.C. et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.), 1957, 76, 810-812, (分離)

Cross, B.E. et al., J.C.S., 1963, 2937-2943, (分離)

Thieme, H. et al., Naturwissenschaften, 1964, 51, 360, (分離, 構造決定, Salidroside)

Lou, H., Planta Med., 2001, 67, 345-349, (分離, H-NMR, C13-NMR)

§ 5-(2-Propenyl)-1,2,3-benzenetriol; 1,2-Methylene ether, 3-O-β-D-glucopyranoside

[化学名・別名] Oenanthoside A

[化合物分類] 単環芳香族 (Simple phenylpropanoids)

[構造式]

[分子式] C<sub>16</sub>H<sub>20</sub>O<sub>8</sub>

[分子量] 340.329

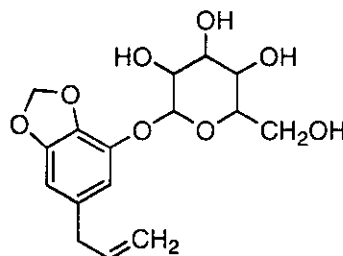
[天然基原] *Oenanthe javanica* (セリ科)

[性状] 粉末

[融点] Mp 155-156 °C

[比旋光度]: [α]<sub>D</sub><sup>24</sup> -55.2 (c, 0.03 in MeOH)

UV: [neutral] λ<sub>max</sub> 279 (ε 1820) (MeOH)



-----文献-----

Fujita, T. et al., Biosci., Biotechnol., Biochem., 1995, 59, 526, (Oenanthoside A)

§ § キク科シュンギク (*Chrysanthemum coronarium* L. var. *spatiosum* L. H. Bailey) の茎葉または幼茎  
本調査研究では、成分に関する文献はなかった。

§ § ウコギ科ウド (*Aralia cordata* Thunberg) の茎葉または幼茎  
本調査研究では、成分に関する文献はなかった。

\*\*\*\*\*ヨロイグサ (Yoroigusa) \*\*\*\*\*

§ § セリ科ヨロイグサ (*Angelica dahurica* Bentham et Hook) の根。

§ Alloisimperatorin

[化学名・別名] 4-Hydroxy-9-(3-methyl-2-butenyl)-7H-furo[3,2-g][1]benzopyran-7-one (CAS 名)

[CAS No.] 35214-83-6

[化合物分類] ベンゾピラノイド (Furanocoumarins), ベンゾピラノイド  
5,7-Dioxygenated coumarins)

[構造式]

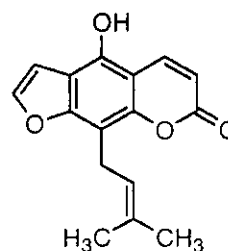
[分子式] C<sub>18</sub>H<sub>16</sub>O<sub>4</sub>

[分子量] 270.284

[天然基原] *Angelica dahurica*

[性状] 結晶

[融点] Mp 228-230 °C



[融点] Mp 228-230 °C

----- 文献 -----

- Saiki, Y. et al., *Yakugaku Zasshi*, 1971, 91, 1313; *CA*, 1972, 76, 56621  
Bhide, K.S. et al., *Indian J. Chem., Sect. B*, 1977, 15, 440, (Swietenocoumarins)  
Rao, A.V.R. et al., *Indian J. Chem., Sect. B*, 1980, 19, 1046, (Swietenocoumarin G)  
Murray, R.D.H. et al., *Phytochemistry*, 1989, 28, 227, (合成法, Swietenocoumarins)

§ **Byakangelicin; (R)-form, 2'-Ac**

[化合物分類] ベンゾピラノイド (Furanocoumarins), ベンゾピラノイド (5,7,8-Trioxxygenated coumarins)

[構造式]

[分子式]  $C_{19}H_{20}O_8$

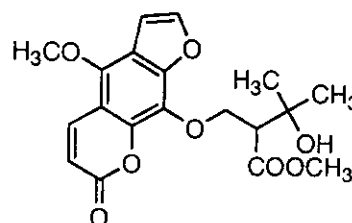
[分子量] 376.362

[天然基原] *Angelica pubescens*, *Angelica dahurica*

[性状] 結晶

[融点] Mp 140-141 °C

[比旋光度]:  $[\alpha]_D^{25} +11.1$  (EtOH),  $[\alpha]_D^{25} -15$  (Py)



----- 文献 -----

- Noguchi, T. et al., *Ber.*, 1938, 71, 344; 1428, (分離, 構造決定, 合成法)  
Perel'son, M.E. et al., *Khim. Prir. Soedin.*, 1971, 7, 576; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, 7, 557, (H-NMR)  
Saiki, Y. et al., *Yakugaku Zasshi*, 1971, 91, 1313, (Anhydrobyakangelicin)  
Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhuser Verlag, Basel, 1972, no. 580, (生育)  
Hata, K. et al., *Yakugaku Zasshi*, 1981, 101, 67, (acetate)  
Fujioka, T. et al., *Chem. Pharm. Bull.*, 1999, 47, 96-100, (Japoangelone)

§ **Byakangelicin; (R)-form, 3'-Me ether**

[化学名・別名] *tert-O-Methylbyakangelicin*

[化合物分類] ベンゾピラノイド (5,7,8-Trioxxygenated coumarins), ベンゾピラノイド (Furanocoumarins)

[構造式]

[分子式]  $C_{18}H_{20}O_7$

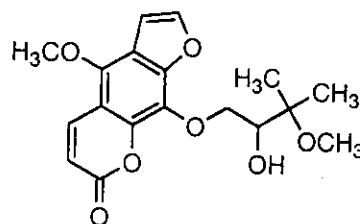
[分子量] 348.352

[天然基原] *Angelica dahurica*, *Angelica pachycarpa*

[性状] 結晶

[融点] Mp 95-96 °C

[比旋光度]:  $[\alpha]_D^{25} -17.8$  (EtOH)



----- 文献 -----

- Noguchi, T. et al., *Ber.*, 1938, 71, 344; 1428, (分離, 構造決定, 合成法)  
Reisch, J. et al., *Planta Med.*, 1969, 17, 116, ((-)-Byakangelicin)  
Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhuser Verlag, Basel, 1972, no. 580, (生育)

§ **Byakangelicin; (R)-form, 3'-Deoxy, 2'-ketone**

[化学名・別名] *Anhydrobyakangelicin*, *Isobyakangelicol*

[CAS No.] 35214-81-4

[化合物分類] ベンゾピラノイド (Furanocoumarins), ベンゾピラノイド (5,7,8-Trioxxygenated coumarins)

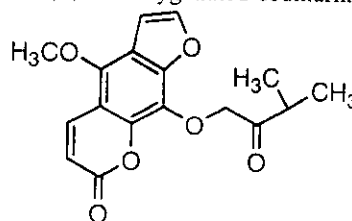
[構造式]

[分子式]  $C_{17}H_{16}O_6$

[分子量] 316.31

[天然基原] 次の植物から分離: *Angelica dahurica* の根

[融点] Mp 108-109 °C



----- 文献 -----

- Saiki, Y. et al., *Yakugaku Zasshi*, 1971, 91, 1313, (Anhydrobyakangelicin)

1972, no. 580, (生育)

§ 4,9-Dihydroxy-7H-furo [3,2-g] [1] benzopyran-7-one; Bis-O-(2,3-epoxy-3-methylbutyl)

[化学名・別名] Sen-byakangelicol

[CAS No.] 77063-74-2

[化合物分類] ベンゾピラノイド (Furanocoumarins), ベンゾピラノイド (5,7,8-Trioxxygenated coumarins)

[構造式]

[分子式]  $C_{21}H_{22}O_7$

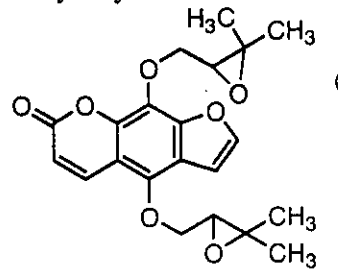
[分子量] 386.401

[天然基原] *Angelica dahurica*

[性状] 結晶

[融点] Mp 102-103 °C

[比旋光度]:  $[\alpha]_D^{25} +10$  (CHCl<sub>3</sub>)



-----文献-----

Briggs, L.H. et al., Tetrahedron, 1958, 2, 256, (分離, 誘導體)

Abu-Mustafa, G.A. et al., J. Het. Chem., 1973, 10, 443, (成書)

§ 4,9-Dihydroxy-7H-furo [3,2-g] [1] benzopyran-7-one; Bis-O-(2,3-dihydroxy-3-methylbutyl)

[CAS No.] 188818-25-9

[化合物分類] ベンゾピラノイド (5,7,8-Trioxxygenated coumarins), ベンゾピラノイド (Furanocoumarins)

[構造式]

[分子式]  $C_{21}H_{26}O_9$

[分子量] 422.431

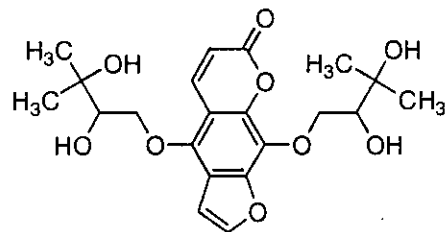
[天然基原] *Angelica dahurica*

[比旋光度]:  $[\alpha]_D^{20} +34$  (c, 0.1 in MeOH)

UV: [neutral]  $\lambda_{max}$  218 (log  $\epsilon$  2.03); 242 (log  $\epsilon$  2.68); 249

$\epsilon$  2.69); 267 (log  $\epsilon$  2.73); 312 (log  $\epsilon$  2.79) (MeOH)

neutral]  $\lambda_{max}$  218; 242; 249; 267; 312 (MeOH) (Berdy)



( log  
[

-----文献-----

Briggs, L.H. et al., Tetrahedron, 1958, 2, 256, (分離, 誘導體)

Abu-Mustafa, G.A. et al., J. Het. Chem., 1973, 10, 443, (成書)

Bohlmann, F. et al., Chem. Ber., 1975, 108, 2955, (誘導體)

§ Oxypeucedanin; (S)-form

[CAS No.] 26091-73-6

[化合物分類] ベンゾピラノイド (5,7-Dioxygenated coumarins), ベンゾピラノ  
(Furanocoumarins)

[構造式]

[分子式]  $C_{16}H_{14}O_5$

[分子量] 286.284

[天然基原] 次の植物から分離: *Prangos* spp., *Hippomarathrum caspicum*, *Ruta  
Peucedanum ostruthium*, *Ferulago turcomanica*, *Angelica dahurica*

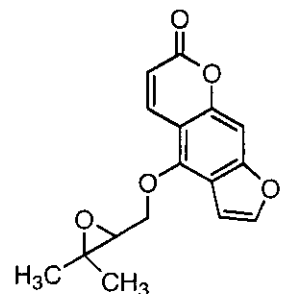
[用途] Weakly phototoxic

[性状] 結晶 (Et<sub>2</sub>O/CHCl<sub>3</sub>)

[融点] Mp 103-104 °C

[比旋光度]:  $[\alpha]_D^{20} -14$  (c, 0.9 in CHCl<sub>3</sub>)

[化学物質毒性データ総覧(RTECS)登録番号] LV1054000



イド

spp.,

-----文献-----

Ghosal, C.R. et al., Chem. Ind. (London), 1963, 1430, (分離, 構造決定)

Lemmich, J. et al., Phytochemistry, 1971, 10, 3333, (分離)

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1372, (生育)

González, A.G. et al., An. Quim., 1973, 69, 1141, (分離)

González, A.G. et al., An. Quim., 1973, 69, 1141, (分離)  
 Atkinson, E. et al., Phytochemistry, 1974, 13, 853, (分離)  
 Reisch, J. et al., Phytochemistry, 1975, 14, 1889, (分離)  
 Serkerov, S.V. et al., Khim. Prir. Soedin., 1976, 94, (分離)  
 Yost, G.S. et al., Phytochemistry, 1977, 16, 1097, (分離, 薬理)

\*\*\*RTECS (化学物質毒性データ) \*\*\*  
 \*\*\*健康障害に関するデータ\*\*\*  
 \*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 経口投与.  
 被験動物 : げっ歯類-マウス.  
 投与量・期間 : 1520 mg/kg  
 毒性影響 : [行動] 振戦.  
 [行動] 興奮.  
 [肺,胸郭,または呼吸] 呼吸困難.

参考文献

Zhongyao Tongbao. Bulletin of Chinese Materia Medica. (China International Book Trading Corp., POB 2820, Beijing, Peop. Rep. China) 10,564,1985

§ Phellopterin; Δ<sup>3</sup>-Isomer, 2'-hydroxy

[化学名・別名] Neobyakangelicol

[CAS No.] 35214-82-5

[化合物分類] ベンゾピラノイド(5,7,8-Trioxxygenated coumarins), ベンゾピラノイド(Furanocoumarins)  
 [構造式]

[分子式] C<sub>17</sub>H<sub>16</sub>O<sub>6</sub>

[分子量] 316.31

[天然基原] 次の植物から分離: *Angelica dahurica*

[性状] 結晶

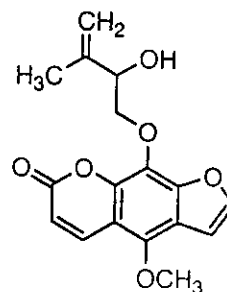
[融点] Mp 106-107 °C

[比旋光度]: [α]<sub>D</sub><sup>20</sup> -2 (EtOH)

[その他のデータ] Abs. config. of side chain not known

文献

Saiki, Y. et al., Yakugaku Zasshi, 1971, 91, 1313, (Neobyakangelicol)



§ § セリ科カラビヤクシ (*Angelica dahurica* Benth. et Hook. var. *pai-chi* Kimura, Hata et Yen) の根。  
 本調査研究では、成分に関する文献はなかった。

\*\*\*\*\*ライオンズフット (Lion's foot) \*\*\*\*\*

§ § バラ科ハゴロモグサ (*Alchemilla vulgaris* L.) の茎葉。  
 本調査研究では、成分に関する文献はなかった。

\*\*\*\*\*ライチ (Litchi) \*\*\*\*\*

§ § ムクロジ科レイシ (*Litchi chinensis* Sonnerat) の果実。

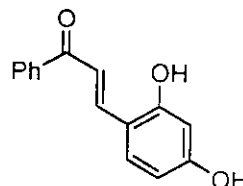
§ 2,4-Dihydroxychalcone

[化学名・別名] 3-(2,4-Dihydroxyphenyl)-1-phenyl-2-propen-1-one

[CAS No.] 92496-59-8

[化合物分類] フラボノイド (Chalcone flavonoids; 2 × O-置換基)

[構造式]



[分子量]240.258

[天然基原]*Litchi chinensis* の果実

-----文献-----

Jaiswal, B.P. et al., Indian J. Exp. Biol., 1987, 25, 66, (生育)

§ 4-Oxopentanoic acid (CAS 名)

[化学名・別名] Levulinic acid (旧 CAS 名). 3-Acetylpropionic acid. FEMA 2627

[CAS No.] 123-76-2

[関連 CAS No.] 591-64-0

[化合物分類] WE3500, 脂肪族化合物 (Saturated unbranched carboxylic acids and lactones)

[構造式]  $\text{H}_3\text{CCOCH}_2\text{CH}_2\text{COOH}$

[分子式]  $\text{C}_5\text{H}_8\text{O}_3$

[分子量] 116.116

[天然基原] sphagnum peat, 木くず, タバコ, bagasse, ビート, キャラメル等に見られる。また *Litchi chinensis*, *Basella rubra*, *Phyllophora* spp. によって生産される。Obt. by the action of dil. acids on carbohydrates, e.g. sucrose, glucose, starch

[用途] Used to make antacids, cathartics and shampoos, nylon, synthetic rubber, plastics and medicines. Flavour ingredient. Reagent for cleavage of oximes and 2,4-dinitrophenylhydrazones

[性状] 板状結晶あるいは酸っぱい, ウイスキー味の葉状結晶

[融点] Mp 33.5 °C

[沸点] Bp 245 °C. Bp<sub>10</sub> 143-147 °C

[溶解性] V. sol. H<sub>2</sub>O, EtOH, Et 2 O; insol. hydrocarbons

[PKa 値] pK<sub>a</sub> 4.62

[傷害・毒性] 皮膚を刺激する。50%致死量 (LD<sub>50</sub>) (ラット, 経口) 1850 mg/kg

[化学物質毒性データ総覧 (RTECS) 登録番号] OI1575000

[販売元] Aldrich:W26270-6; Fluka:61380; Sigma:L0626

-----文献-----

Cowley, M.A. et al., J.A.C.S., 1933, 55, 3463, (成書)

Leonard, R.H., Ind. Eng. Chem., 1956, 48, 1331, (レビュー)

EFS600; LFH000

\*\*\*RTECS (化学物質毒性データ)\*\*\*

生体影響物質 : 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 (Draize) 試験法.

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

反応の症度 : 軽度.

参照文献

Food and Cosmetics Toxicology. (London, UK) 17,847,1979

\*\*\*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 : 皮膚への塗布

被験動物 : げっ歯類-ウサギ.

投与量・期間 : >5 gm/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

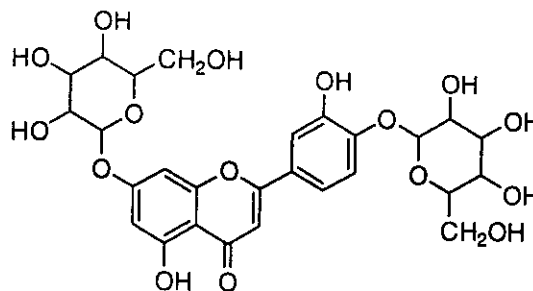
Food and Cosmetics Toxicology. (London, UK) 17,847,1979

\*\*\*\*\*ライフエバーラスティングフラワー (Life-everlasting flower) \*\*\*\*\*

§ § キク科エゾノチチコグサ (*Antennaria dioica* (L.) Gaertner) の花期の全草.

§ 3',4',5,7-Tetrahydroxyflavone; 4',7-Di-O-β-D-glucopyranoside

[化学名・別名] Luteolin 4',7-diglucoside  
 [CAS No.] 70404-47-6  
 [化合物分類] フラボノイド (Flavones; 4 × O-置換基)  
 [構造式]



[分子式]  $C_{27}H_{30}O_{16}$   
 [分子量] 610.524

[天然基原] 次の植物から分離: *Launaea* spp., *Antennaria dioica*, その他の植物属

----- 文献 -----

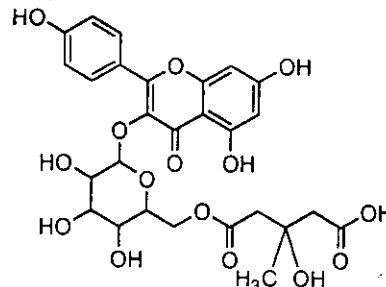
- Perkin, A.G., J.C.S., 1900, 77, 1315, (分離)  
 Diller, E., Ber., 1901, 34, 1452, (分離)  
 Spada, A. et al., Gazz. Chim. Ital., 1958, 88, 204, (4'-glucoside)  
 Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1470; 1473, (生育)  
 The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

\*\*\*\*\*ライム (Lime) \*\*\*\*\*

§ § ミカン科ライム (*Citrus aurantifolia* Swingle) の果実。

§ Astragalin; 6''-O-(4-Carboxy-3-hydroxy-3-methylbutanoyl)

[化学名・別名] Kaempferol 3-[6-O-(3-hydroxy-3-methylglutaroyl) glucoside]  
 [CAS No.] 157407-84-6  
 [化合物分類] フラボノイド (Flavonols; 4 × O-置換基)  
 [構造式]



[分子式]  $C_{27}H_{30}O_{15}$

[分子量] 592.509

[天然基原] *Polygala japonica* の葉, 10 year old callus cultures of *Citrus aurantifolia*

[性状] 黄色の粉末 (MeOH)

[融点] Mp 210-213 °C

----- 文献 -----

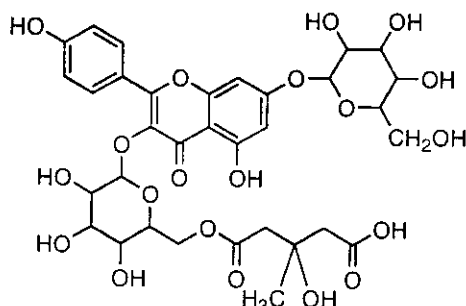
- The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988  
 Berkow, M.A. et al., Phytochemistry, 1994, 36, 1225-1227, (3-hydroxy-3-methylglutarates)

§ Astragalin; 6''-O-(4-Carboxy-3-hydroxy-3-methylbutanoyl), 7-O-β-D-glucopyranoside

[CAS No.] 157407-85-7

[化合物分類] フラボノイド (Flavonols; 4 × O-置換基)

[構造式]



[分子式]  $C_{33}H_{38}O_{20}$

[分子量] 754.651

[天然基原] 10 year old callus cultures of *Citrus aurantifolia*

----- 文献 -----

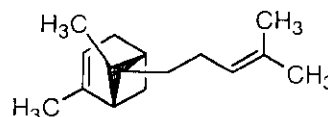
- The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988  
 Berkow, M.A. et al., Phytochemistry, 1994, 36, 1225-1227, (3-hydroxy-3-methylglutarates)

§ α-Bergamotene

[化学名・別名] Bergamotene

[CAS No.] 13474-59-4

[その他の CAS No.] 17699-05-7



[化合物分類]テルペノイド (Miscellaneous bicyclic sesquiterpenoids)

[構造式]

[分子式]  $C_{15}H_{24}$

[分子量] 204.355

[天然基原] ニンジン (*Daucus carota*) のオイル, ベルガモット (*Citrus bergamia*), またライム (*Citrus aurantifolia*), シトロネ (*Citrus medica*), 綿の実 (*Gossypium hirsutum*) のオイル

[性状] オイル

[比旋光度]:  $[\alpha]_D^{20} -44.1$  (CHCl<sub>3</sub>)

[濃度]  $d_{20} 0.855$

[屈折率]  $n_D^{20} 1.4904$

-----文献-----

Kováts, E., *Helv. Chim. Acta*, 1963, 46, 2705, (H-NMR, Mass, 構造決定)

Larsen, S.D. et al., *J.A.C.S.*, 1977, 99, 8015

Kulkarni, Y.S. et al., *J.O.C.*, 1985, 50, 2809, (合成法)

Snider, B.B. et al., *J.O.C.*, 1988, 53, 4508, (合成法)

§ 5,7-Dihydroxy-2H-1-benzopyran-2-one; 5-O-(3,7-Dimethyl-2,6-octadienyl), 7-O-Me

[化学名・別名] 5-Geranyloxy-7-methoxycoumarin

[CAS No.] 7380-39-4

[化合物分類] ベンゾピラノイド (5,7-Dioxygenated coumarins)

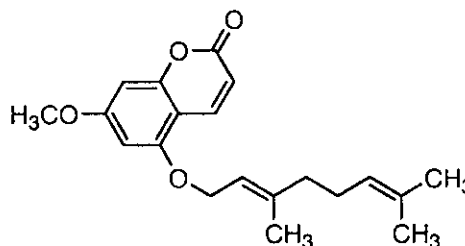
[構造式]

[分子式]  $C_{20}H_{30}O_3$

[分子量] 328.407

[天然基原] 次の植物から分離: *Citrus aurantifolia*

[融点] Mp 86-87 °C



-----文献-----

Ito, C. et al., *Chem. Pharm. Bull.*, 1996, 44, 2231, (5-Geranyloxy-7-hydroxycoumarin)

§ 5,7-Dihydroxy-2H-1-benzopyran-2-one; 5-O-(6-Hydroxy-3,7-dimethyl-2,7-octadienyl), 7-O-Me

[CAS No.] 40520-59-0

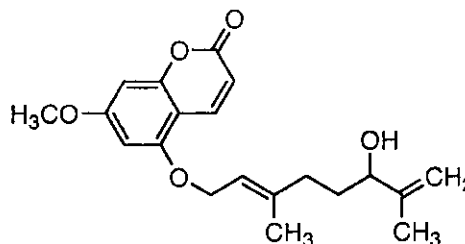
[化合物分類] ベンゾピラノイド (5,7-Dioxygenated coumarins)

[構造式]

[分子式]  $C_{20}H_{32}O_5$

[分子量] 344.407

[天然基原] 次の植物から分離: *Citrus aurantifolia*



-----文献-----

Talapatra, B. et al., *Indian J. Chem.*, 1975, 13, 835, (分離, 誘導体)

Günther, D.H. et al., *Org. Magn. Reson.*, 1975, 7, 339, (C13-NMR, 誘導体)

Gray, A.I. et al., *J.C.S. Perkin 2*, 1978, 391, (H-NMR)

Gashimov, N.F. et al., *Khim. Prir. Soedin.*, 1978, 14, 653; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, 14, 563, (誘導体)

Joseph-Nathan, P. et al., *J. Het. Chem.*, 1984, 21, 1141, (H-NMR, 誘導体)

Ito, C. et al., *Chem. Pharm. Bull.*, 1996, 44, 2231, (5-Geranyloxy-7-hydroxycoumarin)

§ *p*-Menth-3-en-1-ol

[化学名・別名] 1-Methyl-4-(1-methylethyl)-3-cyclohexen-1-ol. 4-[isopropyl-1-methyl-3-cyclohexen-1-ol. Terpinen-1-ol. FEMA 3563

[CAS No.] 586-82-3

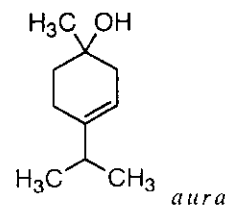
[化合物分類] WE9000, テルペノイド (*p*-Menthane monoterpenoids)

[構造式]

[分子式]  $C_{10}H_{18}O$

[分子量] 154.252

[天然基原] オレガノ *Origanum vulgare*, *Ferula peminervis*, ライムオイル (*Citrus*





*aurantifolia*), その他

[用途] 香料原料

[性状] オイル

[沸点] Bp 208-210 °C

[屈折率]  $n_D^{20}$  1.476

-----文献-----

Kováts, E., *Helv. Chim. Acta*, 1963, 46, 2705, (分離)

Brieskorn, C.H. et al., *Planta Med. (Suppl.)*, 1967, 96, (分離)

Goryaev, M.I. et al., *CA*, 1969, 70, 70998a, (分離)

Accrombessi, G. et al., *Tetrahedron*, 1981, 37, 3135, (合成法)

### § 2-(4-Methylphenyl)-2-propanol; Me ether

[化学名・別名] 1-(1-Methoxy-1-methylethyl)-4-methylbenzene. 8-Methoxy-*p*-cymene.

8-Methoxy-*p*-mentha-1,3,5-triene

[化合物分類] テルペノイド (p-Menthane monoterpenoids)

[構造式]

[分子式]  $C_{11}H_{16}O$

[分子量] 164.247

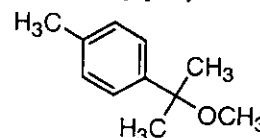
[天然基原] 次の植物から分離: *Citrus aurantifolia* のオイル

[性状] 液体

[沸点] Bp, 90-94 °C

[濃度]  $d_4^{20}$  0.934

[屈折率]  $n_D^{20}$  1.4958



-----文献-----

McBay, H.C. et al., *J.O.C.*, 1954, 19, 869, (合成法)

Marayama, K. et al., *Nippon Kagaku Kaishi*, 1960, 81, 1883; *CA*, 56, 3385, (合成法)

Oki, M. et al., *Bull. Chem. Soc. Jpn.*, 1963, 36, 1, (H-NMR)

Kugler, E. et al., *Helv. Chim. Acta*, 1963, 46, 1480, (分離)

### § Pinol

[化学名・別名] 4,7,7-Trimethyl-6-oxabicyclo[3.2.1]oct-3-ene (CAS 名). 6,8-Epoxy-*p*-menth-1-ene

[CAS No.] 2437-97-0

[関連 CAS No.] 497-31-4, 55822-06-5

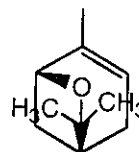
[化合物分類] テルペノイド (p-Menthane monoterpenoids)

[構造式]

[分子式]  $C_{10}H_{16}O$

[分子量] 152.236

[天然基原] 次の植物から分離: ライムオイル (*Citrus aurantifolia*)



-----文献-----

Kováts, E., *Helv. Chim. Acta*, 1963, 46, 2705, (分離, 合成法)

Garver, L. et al., *J.O.C.*, 1976, 41, 2773, (合成法)

Bondavalli, F. et al., *J.C.S. Perkin 1*, 1977, 430, (合成法)

### § Tetrahydro-2,2-dimethyl-5-(1-methyl-1-propenyl) furan

[CAS No.] 7416-35-5

[関連 CAS No.] 56058-69-6, 56058-70-9

[化合物分類] テルペノイド (Acyclic monoterpenoids)

[構造式]

[分子式]  $C_{11}H_{18}O$

[分子量] 154.252

[天然基原] 次の植物から分離: *Citrus aurantifolia* のオイル

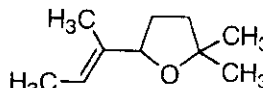
[性状] オイル

[比旋光度]:  $[\alpha]_D^{20}$  0

[濃度]  $d_4^{20}$  0.867

[屈折率]  $n_D^{20}$  1.4662

[販売元] Fluka: 74732



-----文献-----

Kováts, E. et al., *Helv. Chim. Acta*, 1963, 46, 2705; 1966, 49, 2055, (分離)  
Corbier, B. et al., *Recherches*, 1974, 19, 235, (合成法)

### § Toluene (旧 CAS 名)

[化学名・別名] Methylbenzene (CAS 名)

[CAS No.] 108-88-3

[関連 CAS No.] 1124-18-1, 2037-26-5, 6711-19-9, 18860-15-6, 34504-47-7

[化合物分類] 単環芳香族 (Simple benzene derivatives)

[構造式] PhCH<sub>3</sub>

[分子式] C<sub>7</sub>H<sub>8</sub>

[分子量] 92.14

[天然基原] 多くのミネラルオイルやコールタールオイルの主成分。トルーバルサム (*Myroxylon balsamum*) から蒸留して分離; またライムオイル (*Citrus aurantifolia*) の微量成分。Manuf. by reforming and fractionation of petroleum fractions

[用途] Important industrial intermed., used for prodn. of Benzene, Benzoic acid, 2,4-Diisocyanato-1-methylbenzene, Hexahydro-2H-azepin-2-one and Phenol. Solvent, high-octane blending component for gasoline. Important industrial chemical, 27th in order of volume for USA in 1994 (production 3.37 million tons/year)

[性状] 液体

[融点] Fp -95 °C

[沸点] Bp 110.6 °C. Bp<sub>1+56</sub> 14.5 °C

[濃度] d<sub>20</sub><sup>4</sup> 0.866

[PKa 値] pK<sub>a</sub> 54 (MeCN)

[屈折率] n<sub>D</sub><sup>20</sup> 1.4967

[傷害・毒性] 発火しやすい, 引火点: 4 °C, 自然発火点: 480 °C. 多くのオキシダントと激しく反応する。中枢神経抑制薬。低濃度で (100 ppm) 眼, 呼吸器刺激, 頭痛, めまいを引き起こす。高濃度で精神混乱, 整合性の喪失, 数分以内に意識を失う。Not associated with the haemopoietic effects of benzene. Chronic exposure or abuse can injure kidneys and liver, and cause teratogenic effects. OES: long-term 50 ppm; short-term 150 ppm (Sk)

[化学物質毒性データ総覧 (RTECS) 登録番号] XS5250000

[販売元] Aldrich: 17941-8; Fluka: 89676; Sigma: T2790; Supelco: 4-8572

-----文献-----

Kirk-Othmer *Encycl. Chem. Technol.*, 3rd edn., Wiley, 1978, 23, 246, (レビュー)

Antti-Poika, M. et al., *Ethel Browning's Toxicity and Metabolism of Industrial Solvents*, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1, 1987, 38, (レビュー, 毒性)

\*\*\*\*\*ライラック (Lilac) \*\*\*\*\*

§ § モクセイ科ライラック (*Syringa vulgaris* L.) の花。

### § 2-(3,4-Dihydroxyphenyl) ethanol; 1-O-β-D-Glucopyranoside

[化学名・別名] 3,4-Dihydroxyphenethyl glucoside

[CAS No.] 76873-99-9

[その他の CAS No.] 123078-38-6, 147731-98-4

[化合物分類] 単環芳香族 (Simple phenols)

[構造式]

[分子式] C<sub>11</sub>H<sub>12</sub>O<sub>8</sub>

[分子量] 316.307

[基原] *Ligustrum* spp., *Osmanthus* spp., *Prunus* sp., *Syringa vulgaris*

[用途] 細胞毒剤

[性状] 青白い黄色の粉末

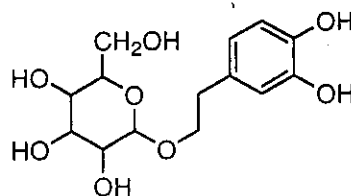
[融点] Mp 40.5-42 °C (as hexa-Ac)

[比旋光度]: [α]<sub>D</sub><sup>20</sup> -23.8 (c, 1 in MeOH). [α]<sub>D</sub><sup>20</sup> -12.3 (c, 7.1 in CHCl<sub>3</sub>) (hexa-Ac)

-----文献-----

Kudo, K. et al., *Planta Med.*, 1980, 40, 250, (1-glucoside)

Jimenez, C. et al., *Nat. Prod. Rep.*, 1994, 591, (レビュー, 配糖体)



§ 2-(3,4-Dihydroxyphenyl) ethanol; 1-O-[4-Hydroxy-3-methoxycinnamoyl-(→4)-β-D-glucopyranoside]

[化学名・別名] Syringalide C

[CAS No.] 124761-15-5

[化合物分類] 単環芳香族 (Simple phenols), 単環芳香族 (Simple phenylpropanoids)

[構造式]

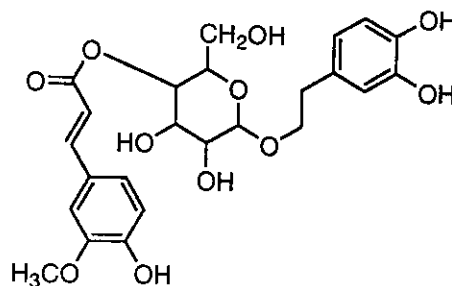
[分子式] C<sub>14</sub>H<sub>12</sub>O<sub>11</sub>

[分子量] 492.479

[基原] *Syringa vulgaris*

[融点] Mp 74 °C (as hexa-Ac)

[比旋光度]: [α]<sub>D</sub><sup>25</sup> -36.5 (c, 1.3 in CHCl<sub>3</sub>)



----- 文献 -----

Baraldi, P.G. et al., *Annalen*, 1983, 684, (合成法, IR, H-NMR, 成書)

Kikuchi, M. et al., *Yakugaku Zasshi*, 1987, 107, 350; 647, (Isosyringalide, Neosyringalide)

Jimenez, C. et al., *Nat. Prod. Rep.*, 1994, 591, (レビュー, 配糖体)

§ 2-(3,4-Dihydroxyphenyl) ethanol; 4'-O-β-D-Glucopyranoside

[化学名・別名] Decoumaroylibotanolide

[CAS No.] 54695-80-6

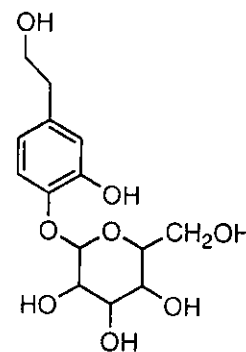
[化合物分類] 単環芳香族 (Simple phenols)

[構造式]

[分子式] C<sub>14</sub>H<sub>20</sub>O<sub>8</sub>

[分子量] 316.307

[基原] *Clematis koreana*, *Ligustrum obtusifolium*, *Osmanthus asiaticus*, *Olea* sp., *Syringa vulgaris*



----- 文献 -----

Baraldi, P.G. et al., *Annalen*, 1983, 684, (合成法, IR, H-NMR, 成書)

Kikuchi, M. et al., *Yakugaku Zasshi*, 1987, 107, 350; 647, (Isosyringalide, Neosyringalide)

Jimenez, C. et al., *Nat. Prod. Rep.*, 1994, 591, (レビュー, 配糖体)

§ 3,3',4,4',9,9'-Hexahydroxylignan; (8ξ,8'ξ)-form, 3,4;3',4'-Bis(methylene) ether, 9-O-β-D-glucopyranoside

[化学名・別名] Syringanide

[CAS No.] 124846-49-7

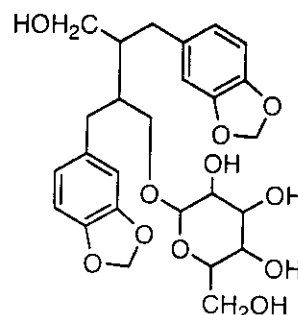
[化合物分類] リグナン化合物 (Side-chain oxygenated dibenzylbutane lignans)

[構造式]

[分子式] C<sub>26</sub>H<sub>32</sub>O<sub>11</sub>

[分子量] 520.532

[基原] *Syringa vulgaris* の葉



----- 文献 -----

Kikuchi, M. et al., *Annu. Rep. Tohoku Coll. Pharm.*, 1988, 105; *CA*, 113, 187988, (Syringanide)

§ Isoligustrosidic acid; Me ester

[化学名・別名] Isoligustroside

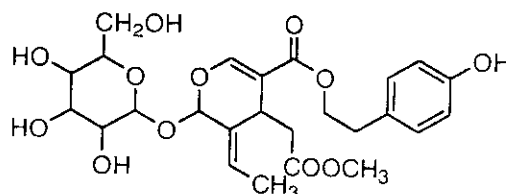
[CAS No.] 108789-18-0

[化合物分類] テルペノイド (Secoiridoid monoterpeneoids)

[構造式]

[分子式] C<sub>33</sub>H<sub>40</sub>O<sub>12</sub>

[分子量] 524.521



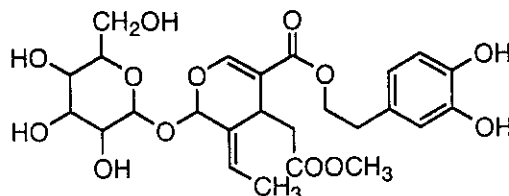
[性状] 結晶 (as penta-Ac)  
[融点] Mp 45-50 °C (penta-Ac)  
[比旋光度]:  $[\alpha]_D^{20} -122.7$  (c, 1.1 in CHCl<sub>3</sub>) (penta-Ac)

-----文献-----

Kikuchi, M. et al., Yakugaku Zasshi, 1987, 107, 245, (Isoligustroside)

§ **Isoligustrosidic acid; 3''-Hydroxy, Me ester**

[化学名・別名] Isooleuropein  
[CAS No.] 108789-17-9  
[化合物分類] テルペノイド (Secoiridoid monoterpeneoids)  
[構造式]  
[分子式] C<sub>25</sub>H<sub>32</sub>O<sub>13</sub>  
[分子量] 540.52



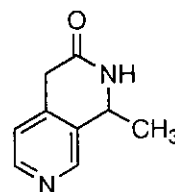
[基原] *Syringa vulgaris*  
[性状] 無定型の塊  
[比旋光度]:  $[\alpha]_D -105.4$  (CHCl<sub>3</sub>) (hexa-Ac)

-----文献-----

Kikuchi, M. et al., CA, 1987, 107, 28255, (Isooleuropein)

§ **Jasminidine**

[CAS No.] 68711-43-3  
[化合物分類] アルカロイド化合物 (Secologanin-derived monoterpeneoid alkaloids)  
[構造式]  
[分子式] C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>O  
[分子量] 162.191  
[基原] 次の植物から得られるアルカロイド: *Syringa vulgaris* の葉 (モクセイ科)  
[性状] 結晶 (CHCl<sub>3</sub>/Et<sub>2</sub>O)  
[融点] Mp 190-194 °C で分解  
[比旋光度]:  $[\alpha]_D^{27} -3.2$  (c, 0.35 in CHCl<sub>3</sub>)

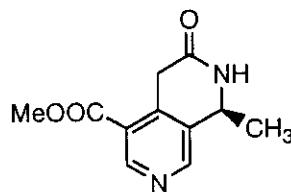


-----文献-----

Ripperger, H., Phytochemistry, 1978, 17, 1069, (分離, IR, H-NMR, Mass, 構造決定)

§ **Jasminine**

[CAS No.] 19634-30-1  
[化合物分類] アルカロイド化合物 (Secologanin-derived monoterpeneoid alkaloids)  
[構造式]  
[分子式] C<sub>11</sub>H<sub>13</sub>N<sub>2</sub>O<sub>3</sub>  
[分子量] 220.227  
[基原] 次の植物から得られるアルカロイド: *Jasminum gracile*, その他数種の *Jasminum* spp., *Ligustrum novoguineense*, *Olea paniculata*, *Syringa vulgaris* (モクセイ科)  
[融点] Mp 175-176 °C  
[比旋光度]:  $[\alpha]_D^{24} -29.8$  (c, 1 in CHCl<sub>3</sub>)



Absolute configuration  
mon

-----文献-----

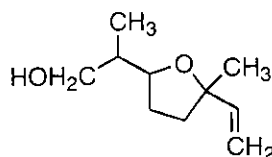
Hart, N.K. et al., Aust. J. Chem., 1968, 21, 1321, (UV, IR, H-NMR, Mass, 分離, 構造決定)

Ripperger, H., Phytochemistry, 1978, 17, 1069, (IR, H-NMR, Mass, 構造)

Benkrief, R. et al., Phytochemistry, 1998, 47, 825-832, (分離, H-NMR)

§ **Lilac alcohol; (β S,2S,5S)-form**

[化学名・別名] Lilac alcohol a  
[CAS No.] 33081-34-4  
[化合物分類] テルペノイド (Acyclic monoterpeneoids)  
[構造式]  
[分子式] C<sub>10</sub>H<sub>18</sub>O<sub>2</sub>  
[分子量] 170.251  
[基原] *Syringa vulgaris*  
[比旋光度]:  $[\alpha]_D^{23} +12.2$  (c, 4.1 in CHCl<sub>3</sub>)



[比旋光度]:  $[\alpha]_D^{25} +12.2$  (c, 4.1 in  $\text{CHCl}_3$ )

-----文献-----

Wakayama, S. et al., Bull. Chem. Soc. Jpn., 1973, 46, 3183

§ Lilac alcohol; ( $\beta$  R,2S,5S)-form

[化学名・別名] Lilac alcohol b

[CAS No.] 33081-35-5

[化合物分類] テルペノイド (Acyclic monoterpenoids)

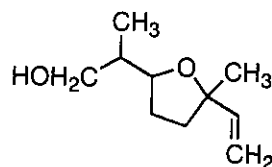
[構造式]

[分子式]  $\text{C}_{10}\text{H}_{18}\text{O}_2$

[分子量] 170.251

[基原] *Syringa vulgaris*

[比旋光度]:  $[\alpha]_D^{25} -6.6$  (c, 3.6 in  $\text{CHCl}_3$ )



-----文献-----

Wakayama, S. et al., Bull. Chem. Soc. Jpn., 1973, 46, 3183

§ Lilac alcohol; ( $\beta$  R,2R,5S)-form

[化学名・別名] Lilac alcohol c

[CAS No.] 33081-36-6

[化合物分類] テルペノイド (Acyclic monoterpenoids)

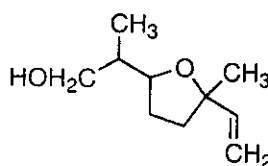
[構造式]

[分子式]  $\text{C}_{10}\text{H}_{18}\text{O}_2$

[分子量] 170.251

[基原] *Syringa vulgaris*

[比旋光度]:  $[\alpha]_D^{25} -1.4$  (c, 1.8 in  $\text{CHCl}_3$ )



-----文献-----

Wakayama, S. et al., Bull. Chem. Soc. Jpn., 1973, 46, 3183

§ Lilac alcohol; ( $\beta$  S,2R,5S)-form

[化学名・別名] Lilac alcohol d

[CAS No.] 33081-37-7

[化合物分類] テルペノイド (Acyclic monoterpenoids)

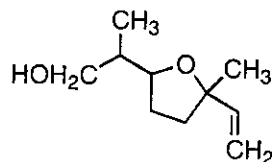
[構造式]

[分子式]  $\text{C}_{10}\text{H}_{18}\text{O}_2$

[分子量] 170.251

[基原] *Syringa vulgaris*

[比旋光度]:  $[\alpha]_D^{25} +4.3$  (c, 1.7 in  $\text{CHCl}_3$ )



-----文献-----

Wakayama, S. et al., Bull. Chem. Soc. Jpn., 1973, 46, 3183

§ Loganic acid; 7-Ketone, 3-(4-hydroxyphenyl) propanoyl ester

[化学名・別名] Syringopicroside

[CAS No.] 29118-80-7

[化合物分類] テルペノイド (Iridoid monoterpenoids)

[構造式]

[基原] *Syringa vulgaris* の葉

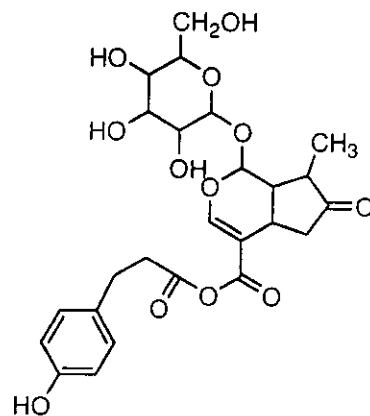
[性状] 無定型; 板状結晶 (EtOH) (as penta-Ac)

[融点] Mp 156-156.5 °C (penta-Ac)

[比旋光度]:  $[\alpha]_D^{20.5} -116.5$  (c, 1 in  $\text{CHCl}_3$ ) (penta-Ac)

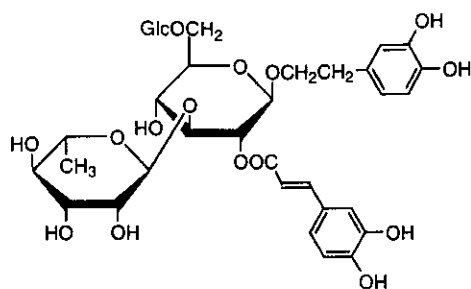
-----文献-----

Asaka, Y. et al., Tetrahedron, 1970, 26, 2365. (Syringopicroside)



§ Neoacteoside

[CAS No.] 27625-93-0  
[化合物分類] 炭水化物 (Oligosaccharides)  
[構造式]



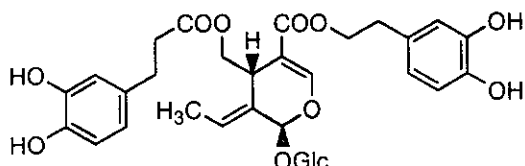
[分子式]  $C_{35}H_{46}O_{20}$   
[分子量] 786.736  
[基原] *Syringa vulgaris* の葉  
[融点] Mp 160 °C

-----文献-----

Birkhofer, L. et al., Z. Naturforsch., B, 1968, 23, 1051-1058, (分離, 構造決定)

#### § Neoleuropein

[化学名・別名] Jasmultiside  
[CAS No.] 108789-16-8  
[化合物分類] テルペノイド (Secoiridoid monoterpenoids)  
[構造式]



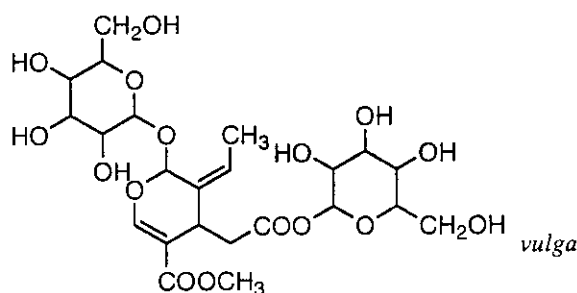
[分子式]  $C_{32}H_{38}O_{15}$   
[分子量] 662.643  
[一般的性質] Jasmultiside appears to be identical to the prev. known Neoleuropein  
[基原] *Syringa vulgaris*, *Jasminum multiflorum*  
[性状] 無定型の粉末  
[比旋光度]:  $[\alpha]_D^{20}$  -42.6 (c, 1 in MeOH)

-----文献-----

Chen, H.-Y. et al., J. Nat. Prod., 1991, 54, 1087, (Jasmultiside)

#### § 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 monoterpenoids)  
[構造式]  
[分子式]  $C_{32}H_{34}O_{16}$   
[分子量] 566.512  
[基原] *Ligustrum japonicum*, *Jasminum polyanthum*, *Syringa ris*, *Fraxinus excelsior*  
[性状] 粉末  
[比旋光度]:  $[\alpha]_D^{20}$  -164.7 (c, 0.51 in MeOH)



-----文献-----

Inouye, H. et al., Tetrahedron, 1974, 30, 201, (Oleoside, 構造決定)

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; Parent acid

[化学名・別名] Demethyloleuropein  
[CAS No.] 52077-55-1  
[化合物分類] テルペノイド (Secoiridoid monoterpenoids)  
[構造式] 有効な構造式はない  
[分子式]  $C_{32}H_{38}O_{15}$   
[分子量] 526.493  
[基原] *Syringa vulgaris* のオリーブ果実と樹皮に存在する  
[用途] Indicator of maturity in olives which increases as the fruit ripens  
[性状] 結晶 (EtOH)  
[融点] Mp 145-147 °C  
[比旋光度]:  $[\alpha]_D^{20}$  -157 (c, 0.4 in EtOH)

-----文献-----

Shasha, B. et al., J.O.C., 1961, 26, 1948. (分離)

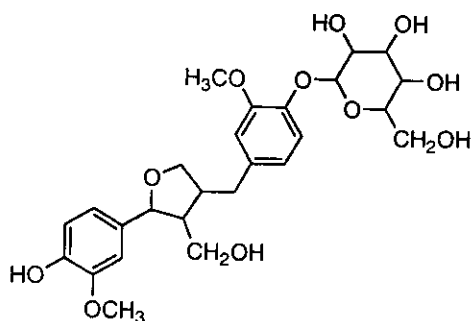
Panizzi, L. et al., Gazz. Chim. Ital., 1965, 95, 1279, (分離)  
 Asaka, Y. et al., Chem. Lett., 1972, 141, (分離, 構造決定)  
 Kurkin, V.A. et al., Khim. Prir. Soedin., 1990, 695-697; Chem. Nat. Compd. (Engl. Transl.), 1990, 26, 592-593, (demethyl, 分離, UV)  
 Damtoft, S. et al., Phytochemistry, 1992, 31, 4197; 1993, 34, 1291; 1995, 40, 785, (合成, Oleuropein, Ligustroside)

§ **3,3',4,4',9-Pentahydroxy-7,9'-epoxylignan; (7S,8R,8'R)-form, 3,3'-Di-Me ether, 4'-O-β-D-glucopyranoside**

[CAS No.] 143663-00-7

[化合物分類] リグナン化合物 (7,9'-Epoxytetrahydrofuranoid lignans)

[構造式]



[分子式]  $C_{26}H_{32}O_{11}$

[分子量] 522.548

[基原] *Arum italicum*, *Osmanthus asiaticus*, *Rhodiola rosea*,

*Syringa vulgaris*

[性状] 淡黄色の無定型粉末

[比旋光度]:  $[\alpha]_D^{20} -25.9$  (c, 1.1 in EtOH).  $[\alpha]_D^{20} -19.3$  (c, 0.4 in MeOH)

-----文献-----

Kurkin, V.A. et al., Khim. Prir. Soedin., 1991, 27, 481; 768; Chem. Nat. Compd. (Engl. Transl.), 1991, 27, 419; 678, (配糖体)

Sugiyama, M. et al., Heterocycles, 1993, 36, 117, (分離, 配糖体)

§ **Secologanol; 7-O-(2,5-Dihydroxybenzoyl)**

[化学名・別名] Syringalactone B. Lilacoside

[CAS No.] 111116-40-6

[化合物分類] テルペノイド (Secoiridoid monoterpenoids)

[構造式]

[分子式]  $C_{26}H_{30}O_{13}$

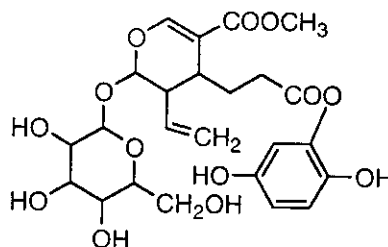
[分子量] 526.493

[基原] *Syringa vulgaris*, *Gentiana verna*

[性状] 結晶 (as hexa-Ac)

[融点] Mp 58 °C (hexa-Ac)

[比旋光度]:  $[\alpha]_D -35.6$  (CHCl<sub>3</sub>) (hexa-Ac)



-----文献-----

Kikuchi, M. et al., CA, 1988, 109, 89748, (Syringalactone B)

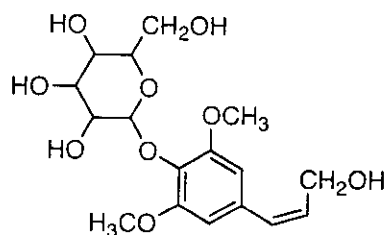
§ **Sinapyl alcohol; (E)-form, 4'-O-β-D-Glucopyranoside**

[化学名・別名] Syringin. Lilacin. Methoxyconiferin. Eleutheroside B. Magnolenin. Alyposide. Syringoside. Ligustrin. Hexanthin A

[CAS No.] 118-34-3

[化合物分類] 単環芳香族 (Simple phenylpropanoids)

[構造式]



[分子式]  $C_{17}H_{18}O_6$

[分子量] 372.371

[基原] 次の植物から分離: *Syringa vulgaris*, *Ligustrum* spp., *Jasminum* spp., *Phyllyrea latifolia*, *Phyllyrea decora*, *Paulownia tomentosa*, *Forsythia suspensa*, *Fraxinus* spp., その他

[性状] 板状結晶もしくはプリズム結晶 (H<sub>2</sub>O)

[融点] Mp 191-192 °C

[比旋光度]:  $[\alpha]_D -18$  (H<sub>2</sub>O)

-----文献-----

Sutarjadi, T.M.M. et al., Phytochemistry, 1978, 17, 564, (分離, UV, IR, H-NMR, Syringin)

Daubresse, N. et al., Synthesis, 1998, 157-161, (合成法, Syringin)

### § Syringalactone A

[化学名・別名] Fliederoside

[CAS No.] 115623-13-7

[化合物分類] テルペノイド (Secoiridoid monoterpenoids)

[構造式]

[分子式]  $C_{24}H_{30}O_{12}$

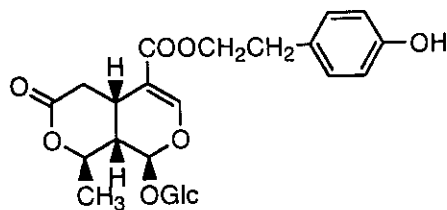
[分子量] 510.494

[基原] *Syringa vulgaris*

[性状] 結晶 (as penta-Ac)

[融点] Mp 64-66 °C (penta-Ac)

[比旋光度]:  $[\alpha]_D -38.2$  (CHCl<sub>3</sub>) (penta-Ac)



-----文献-----

Kikuchi, M. et al., CA, 1988, 109, 89748, (分離, H-NMR, C13-NMR)

Damtoft, S. et al., Phytochemistry, 1995, 40, 785, (分離, H-NMR, C13-NMR)

### § Syringenone

[CAS No.] 58546-53-5

[化合物分類] テルペノイド (Iridoid monoterpenoids)

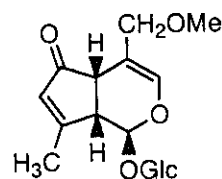
[構造式]

[分子式]  $C_{17}H_{24}O_9$

[分子量] 372.371

[基原] 次の植物から分離: *Syringa vulgaris*

[性状] 無定型



-----文献-----

Popov, S.S. et al., Dokl. Bolg. Akad. Nauk, 1975, 28, 1509

### § Syringenone; 7 β,8 β-Epoxyde

[化学名・別名] Syringoxide

[CAS No.] 56222-02-7

[化合物分類] テルペノイド (Iridoid monoterpenoids)

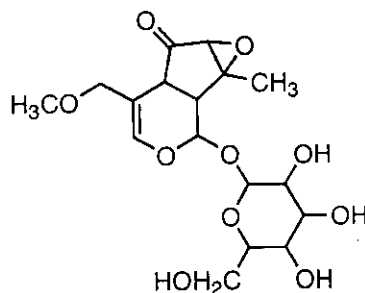
[構造式]

[分子式]  $C_{17}H_{24}O_{10}$

[分子量] 388.371

[基原] *Syringa vulgaris*

[性状] 無定型



-----文献-----

Popov, S.S. et al., Dokl. Bolg. Akad. Nauk, 1975, 28, 1509

\*\*\*\*\* ラカンカ (Rakanka, Lo han kuo) \*\*\*\*\*

§ § ウリ科ラカンカ (*Momordica grosvenori* Swingle) の果実。

### § Cycloarta-7,24-diene-3,21-diol; 3 α-form, Dibenzoyl

[化学名・別名] Mogroester

[CAS No.] 143086-36-6

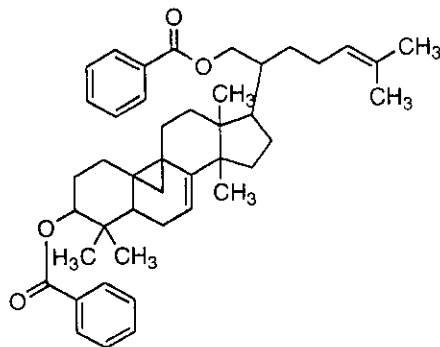
[化合物分類] テルペノイド (Cycloartane triterpenoids)

[構造式]

[分子式]  $C_{44}H_{76}O_4$

[分子量] 648.924

[基原] *Momordica grosvenori*



-----文献-----

Wang, Y. et al., Zhongcaoyao. 1992, 23, 61; CA, 117, 108097k, (分離, H-NMR, C13-NMR)



Wang, Y. et al., Zhongcaoyao, 1992, 23, 61; CA, 117, 108097k, (分離, H-NMR, C13-NMR)

\*\*\*\*\*ラカンシヨウ (Long-leaved podocarp) \*\*\*\*\*

§ § マキ科マキ (*Podocarpus macrophylla* D. Don) の果実。

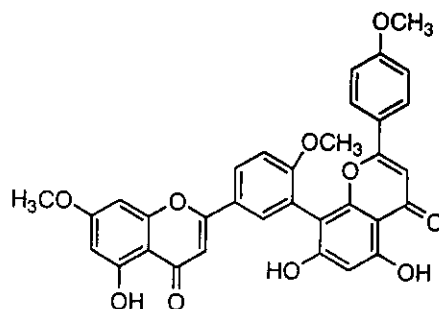
§ Amentoflavone; 4',4'',7''-Tri-Me ether

[化学名・別名] Sciadopitysin

[CAS No.] 521-34-6

[化合物分類] フラボノイド (Biflavonoids and polyflavonoids)

[構造式]



[分子式]  $C_{33}H_{24}O_{10}$

[分子量] 580.547

[基原] *Sciadopitys verticillata*, *Torreya nucifera*, *Metasequoia glyptostroboides*, *Juniperus horizontalis*, *Podocarpus macrophylla*

[性状] 結晶 ( $Me_2CO$ )

[融点] Mp 287-289 °C. Mp 295-297 °C で分解

UV: [neutral]  $\lambda_{max}$  271 ( $\epsilon$  37600); 330 ( $\epsilon$  35000) (EtOH) (Berdy) [base]  $\lambda_{max}$  287 ( $\epsilon$  50800); 378 ( $\epsilon$  16000) (EtOH-NaOH) (Berdy)

-----文献-----

Konda, Y. et al., J. Het. Chem., 1995, 32, 1531, (Ginkgetin, Sciadopitysin, 結晶構造, H-NMR, C13-NMR)  
Krauze-Baranowska, M., Planta Med., 1999, 65, 482-484, (2,3-Dihydrosciadopitysin)

§ Ergost-5-ene-3,26-diol; (3  $\beta$ , 24  $\xi$ , 25  $\xi$ )-form

[CAS No.] 74730-03-3

[化合物分類] ステロイド (Ergostane steroids; excluding withanolides and brassinolides). (C28).

[構造式]

[分子式]  $C_{28}H_{48}O_2$

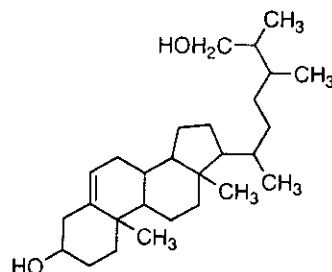
[分子量] 416.686

[基原] *Podocarpus macrophylla*

[性状] 板状結晶 ( $Me_2CO$ )

[融点] Mp 162-164 °C

[比旋光度]:  $[\alpha]_D^{25}$  -36.5 (c, 0.85 in  $CHCl_3/MeOH$ )



-----文献-----

Ohmoto, T. et al., Chem. Pharm. Bull., 1980, 28, 1894

§ Hinokiflavone; 7-Me ether

[化学名・別名] Neocryptomerin

[CAS No.] 20931-36-6

[化合物分類] フラボノイド

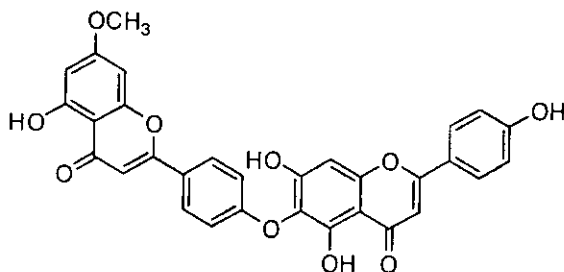
(Biflavonoids and polyflavonoids)

[構造式]

[分子式]  $C_{33}H_{20}O_{10}$

[分子量] 552.493

[基原] *Podocarpus macrophylla* の葉



-----文献-----

Voirin, B. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1966, 262, 707, (分離)

Jayaprakasam, B. et al., Phytochemistry, 2000, 53, 515-517, (Tetrahydrodimethylhinokiflavone)

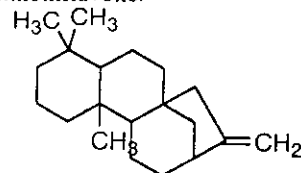
§ 16-Kaurene; (-)-form

[化学名・別名] *ent*-form.  $\alpha$ -Podocarpene.  $\alpha$ -Podocarpene

[CAS No.] 562-28-7

[化合物分類] テルペノイド (Kaurane diterpenoids)

[構造式]



[分子量] 272.473

[基原] *Agathis australis*; produced by *Gibberella fujikuroi*. また *Cryptomeria japonica*, *Hordeum vulgare*, *Podocarpus macrophylla*, *Sciadopitys verticillata*, その他からも得られる

[用途] 結晶 (MeOH)

[融点] Mp 50 °C

[比旋光度]:  $[\alpha]_D^{20}$  -80 (c, 1.0 in CHCl<sub>3</sub>)

-----文献-----

Briggs, L.H. et al., J.C.S., 1963, 1345, (分離, 構造決定)

Cross, B.E. et al., J.C.S., 1963, 2937, (分離, 構造決定)

Overton, K.H. et al., Prog. Chem. Org. Nat. Prod., 1977, 34, 249, (合成, レビュー)

### § Macrophylllic acid

[CAS No.] 2785-58-2

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

[構造式]

[分子式] C<sub>30</sub>H<sub>54</sub>O<sub>6</sub>

[分子量] 630.863

[基原] *Podocarpus macrophylla* の心材, *Podocarpus lambertius* 皮

[性状] 絹のような針状結晶 (Et<sub>2</sub>O/hexane あるいは C<sub>6</sub>H<sub>6</sub>/petrol)

[融点] Mp 237-238 °C で分解

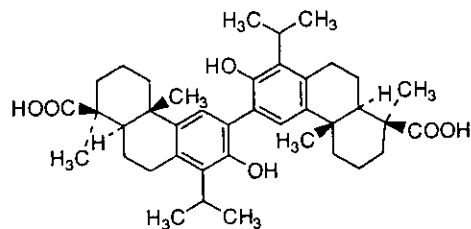
[比旋光度]:  $[\alpha]_D^{20}$  +79 (c, 1.05 in EtOH)

-----文献-----

Bocks, S.M. et al., Tetrahedron, 1963, 19, 1109, (分離, UV, IR, H-NMR)

Campello, J., Tetrahedron, de P. et al., Phytochemistry, 1975, 14, 243, (分離)

Bendall, J.G. et al., Aust. J. Chem., 1995, 48, 883, (レビュー)



の樹

### § Podototarin

[CAS No.] 2539-02-8

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

[構造式]

[分子式] C<sub>40</sub>H<sub>58</sub>O<sub>2</sub>

[分子量] 570.897

[基原] 次の植物から分離: *Podocarpus totara* の心材, *Podocarpus hallii*, *Podocarpus macrophylla*, *Podocarpus mannii*, *Podocarpus nagi*

[融点] Mp 225-226 °C

[比旋光度]:  $[\alpha]_D^{24}$  +76

[その他のデータ] Nmr shows hindered rotation

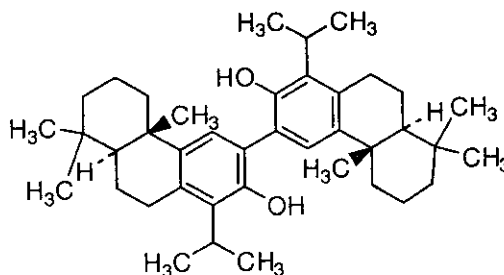
-----文献-----

Falshaw, C.P. et al., J.C.S., 1963, 2422, (分離)

Cambie, R.C. et al., Tetrahedron, 1963, 19, 209, (分離)

Bennett, C.R. et al., Phytochemistry, 1967, 6, 883, (分離)

Bendall, J.G. et al., Aust. J. Chem., 1995, 48, 883, (レビュー)



### § Stigmast-5-ene-3,26-diol; (3β,24ξ,25ξ)-form

[CAS No.] 66760-37-0

[化合物分類] ステロイド (Stigmastane steroids). (C<sub>29</sub>).

[構造式]

[分子式] C<sub>29</sub>H<sub>50</sub>O<sub>2</sub>

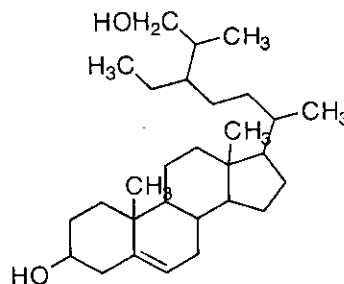
[分子量] 430.713

[基原] *Podocarpus macrophylla*

[性状] 板状結晶 (Me<sub>2</sub>CO)

[融点] Mp 148-150 °C

[比旋光度]:  $[\alpha]_D^{18}$  -23.5 (c, 2 in CHCl<sub>3</sub>/MeOH)



[比旋光度]:  $[\alpha]_D^{25} -23.5$  (c, 2 in  $\text{CHCl}_3/\text{MeOH}$ )

-----文献-----

Ohmoto, T. et al., Chem. Pharm. Bull., 1980, 28, 1894

Saba et al., Phytochemistry, 1999, 50, 1375-1377, (26-benzoyl)

\*\*\*\*\*ラズベリー (Raspberry) \*\*\*\*\*

§ §バラ科セイヨウキイチゴ (*Rubus idaeus* L.)

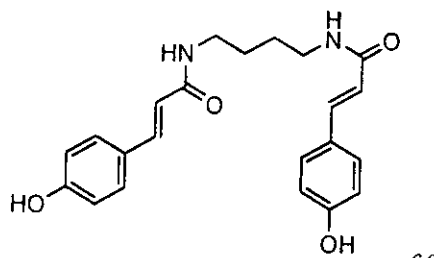
§ Di-4-coumaroylputrescine

[化学名・別名] *N,N*-1,4-Butanediybis[3-(4-hydroxyphenyl)-2-propenamido] (CAS名). *N,N*-Bis(4-hydroxycinnamoyl)-1,4-butanediamine

[CAS No.] 37946-59-1

[化合物分類] アルカロイド化合物 (Putrescine alkaloids)

[構造式]



[分子式]  $\text{C}_{22}\text{H}_{22}\text{N}_2\text{O}_4$

[分子量] 380.443

[基原] 次の植物から得られるアルカロイド: *Dianthus*

*ryophyllus*, *Helianthus annuus*, *Nicotiana tabacum*, *Pyrus communis*, *Rubus idaeus*, *Vicia faba* (ナデシコ科, キク科, ナス科, バラ科, マメ科)

-----文献-----

Martin-Tanguy, J. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1973, 276, 1433, (UV, 構造決定, 合成法, Diferuloylputrescine)

Cabanne, F. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1976, 282, 1959, (UV, 構造決定, Dicafeoylputrescine)

Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927, (生育, 誘導体)

§ 3-Hexenoic acid (CAS名)

[化学名・別名] 2-Pentene-1-carboxylic acid. Hydrosorbic acid. FEMA 3170

[CAS No.] 4219-24-3

[関連 CAS No.] 1775-43-5

[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones), WE9000

[構造式]  $\text{H}_3\text{CCH}_2\text{CH}=\text{CHCOOH}$

[分子式]  $\text{C}_6\text{H}_{10}\text{O}_2$

[分子量] 114.144

[基原] 次の植物から分離: キイチゴ (*Rubus idaeus*), チャ (*Thea sinensis*)

[用途] お茶の香り付けに用いられる

[融点] Mp 12 °C

[沸点] Bp 208 °C. Bp<sub>25</sub> 118-119 °C

[化学物質毒性データ総覧 (RTECS) 登録番号] MP7730000

[販売元] Aldrich: W31700-4

-----文献-----

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, 1, 985A, (NMR)

Boxer, J.E. et al., J.C.S., 1931, 748, (合成法)

Takei, S. et al., Ber., 1935, 68, 95, (合成法)

Isaacs, E. et al., J.C.S., 1936, 202, (合成法)

Birch, A.J. et al., Aust. J. Chem., 1976, 29, 2737, (合成法)

Kawashima, M. et al., Bull. Chem. Soc. Jpn., 1988, 61, 3255, (合成法)

Wolber, E.K.A. et al., Chem. Ber., 1992, 125, 525, (nitrile)

Marson, C.M. et al., J.O.C., 1994, 59, 284, (amide)

Shi, L. et al., CA, 1995, 123, 179192x, (2-propenyl ester)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 992; 1306; 1777, (生育, 性質, esters)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, HFD000

<<試験方法>> LD50 試験 (50%致死量試験).  
 曝露経路 : 腹腔内投与.  
 被験動物 : げっ歯類-マウス.  
 投与量・期間 : 1840 mg/kg  
 毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

Journal of Pharmacy and Pharmacology. (Pharmaceutical Soc. of Great Britain, 1 Lambeth High St., London SE1 7JN, UK) 21,85,1969

§ 4-(4-Hydroxyphenyl)-2-butanone (CAS 名)

[化学名・別名] Raspberry ketone. Rheosmine. Frambinone

[CAS No.] 5471-51-2

[化合物分類] 単環芳香族 (Simple aryl ketones)

[構造式]

[分子式] C<sub>10</sub>H<sub>12</sub>O<sub>2</sub>

[分子量] 164.204

[基原] 次の植物から分離: キイチゴ (*Rubus idaeus*), ルバーブ (*Rheum* spp.)

[用途] 香料原料として重要

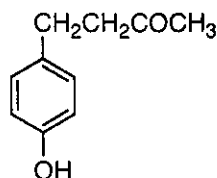
[性状] 針状結晶 (H<sub>2</sub>O)

[融点] Mp 82.5 °C

[傷害・毒性] 50%致死量 (LD<sub>50</sub>) (ラット, 経口) 1320 mg/kg

[化学物質毒性データ総覧 (RTECS) 登録番号] EL8925000

[販売元] Aldrich:17851-9; Fluka:56110



-----文献-----

Schinz, H. et al., Helv. Chim. Acta, 1957, 40, 1839; 1961, 44, 278, (分離, 構造決定)

Murakami, T. et al., Tet. Lett., 1972, 2965-2968, (分離, 配糖体)

Opdyke, D.L.J., Food Cosmet. Toxicol., 1978, 16, 781, (レビュー, 毒性)

Pabst, A. et al., Phytochemistry, 1990, 29, 3853-3858, (分離, 配糖体)

Fan, W. et al., Chem. Pharm. Bull., 2000, 48, 1055-1061, (分離, H-NMR, C13-NMR, 配糖体)

\*\*\*RTECS (化学物質毒性データ)\*\*\*

\*\*\*健康障害に関するデータ\*\*\*

\*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> 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 : 1320 mg/kg

毒性影響 : [行動] 睡眠時間の変化 (立ち直り反射の変化を含む).

[行動] 鎮痛.

参照文献

Food and Cosmetics Toxicology. (London. UK) 8,349,1970

§ 4,7-Megastigmadiene-3,9-diol; (3S,7E,9R)-form, 3-Ketone, 9-O-β-D-glucopyranoside

[化合物分類] テルペノイド (Megastigmane nortriterpenoids)

[構造式]

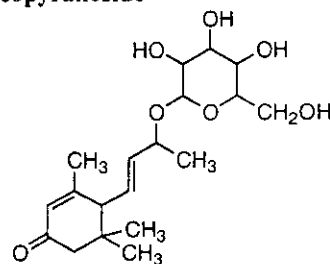
[分子式] C<sub>19</sub>H<sub>30</sub>O<sub>7</sub>

[分子量] 370.442

[基原] 次の植物から分離: *Polystichum tripterum*, *Dennstaedtia wilfordii*, ブクベリイ (*Rubus idaeus*), ダルメシアンセージ (*Salvia officinalis*) の葉

[性状] オイル

[比旋光度]: [α]<sub>D</sub><sup>20</sup> +58.6 (c, 1.5 in MeOH)



-----文献-----

Murakami, T. et al., Chem. Pharm. Bull., 1981, 29, 866-868. (3-ketone 9-glucoside)

Wang, M. et al., J. Agric. Food Chem., 1998, 46, 2509-2511, (3-ketone glucoside, 分離, NMR)

§ 4,7-Megastigmadiene-3,9-diol; (3S,7E,9S)-form, 3-Ketone, 9-O-β-D-glucopyranoside