

§ 6,7-Dihydroxy-1-methylisoquinoline; Di-Me ether, N-oxide

[化学名・別名] Nigellimine N-oxide

[CAS No.] 96562-85-5

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

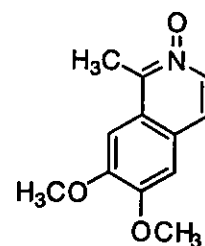
[構造式]

[分子式]  $C_{12}H_{13}NO_3$

[分子量] 219.24

[基原] 次の植物の種子に含まれるアルカロイド微量成分: *Nigella sativa* (キンボウゲ科)

[性状] 無定型



----- 文献 -----

Atta-ur-Rahman et al., *Heterocycles*, 1985, 23, 953, (Nigellimine oxide)

§ Diisopropyl disulfide

[化学名・別名] Bis(1-methylethyl) disulfide (CAS 名). Isopropyl disulfide

[CAS No.] 4253-89-8

[化合物分類] 脂肪族化合物 (Disulfides, trisulfides)

[構造式]  $(H_3C)_2CHSSCH(CH_3)_2$

[分子式]  $C_6H_{14}S_2$

[分子量] 150.309

[基原] *Durio zibethinus* の果実, *Nigella sativa* の種子

[沸点] Bp 177 °C. Bp<sub>56</sub> 95 °C

[販売元] Aldrich:I-2200-5

----- 文献 -----

Cumper, C.W.N. et al., *J.C.S.*, 1965, 5323; *J.C.S. (A)*, 1966, 239, (性質)

Cohen, V.I., *Helv. Chim. Acta*, 1976, 59, 840, (合成法, 成書)

Naef, R. et al., *Fragrance J.*, 1996, 11, 295-303, (生育)

§ 3,7-Dimethyl-6-octen-1-ol; (R)-form

[CAS No.] 1117-61-9

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

[構造式]

[分子式]  $C_{10}H_{20}O$

[分子量] 156.267

[基原] *Nigella sativa* の種子, *Cymbopogon distans*. 通常の植物オイル, 特にミカン科. Also isol. from alligator secretions. Richest source is *Boronia citriodora* オイル (80%). Mostly prod. by partial or total synth.

[性状] 甘いバラ様の香りを持つオイル

[沸点] Bp 108 °C. Bp<sub>0.5</sub> 68 °C

[比旋光度]:  $[\alpha]_D +5.45$  (neat)

[濃度]  $d^{20}_D$  0.86

[屈折率]  $n^{20}_D$  1.4558

[販売元] Aldrich:30346-1; Fluka:27478; Sigma:C5161

----- 文献 -----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 111, (生育)

Wollmann, H. et al., *Pharmazie*, 1973, 28, 56, (分離)

Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1975, 13, 757-758, (レビュー, 毒性)

Ackermann, I.E. et al., *Annalen*, 1989, 79-81, (合成法, 配糖体)

Bauer, K. et al., *Common Fragrance and Flavor Materials, Preparation, Properties and Uses*, VCH, Weinheim, 2nd. edn., 1990, 25, (レビュー)

Ford, R.A. et al., *Food Chem. Toxicol.*, 1992, 30, 113S-114S, (レビュー, 毒性)

§ Ethyl propyl disulfide

[化学名・別名] 3,4-Dithiaheptane

[CAS No.] 30453-31-7

[化合物分類] 脂肪族化合物 (Disulfides, trisulfides)

[構造式] EtS-S-CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>

[分子式] C<sub>5</sub>H<sub>12</sub>S<sub>2</sub>

[分子量] 136.282

[基原] *Allium* spp., *Durio zibethinus*, *Nigella sativa*

[沸点] Bp<sub>90</sub> 104-106 °C. Bp<sub>7</sub> 47-48 °C

----- 文献 -----

Gupta, D. et al., Can. J. Chem., 1981, 59, 543-548, (Mass)

Naef, R. et al., Fragrance J., 1996, 11, 295-303, (分離)

§ 4-Hydroxy-4-methyl-2-cyclohexen-1-one; (ξ)-form

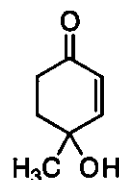
[化合物分類] 脂肪族化合物 (Monocarbocyclic aldehydes and ketones)

[構造式]

[分子式] C<sub>7</sub>H<sub>10</sub>O<sub>2</sub>

[分子量] 126.155

[基原] *Jungermannia obovata*, *Nigella sativa*, ペパーミントオイル (*Mentha piperita*)



----- 文献 -----

Takahashi, K. et al., Agric. Biol. Chem., 1980, 44, 1535-1543, (分離, 合成法)

Bueno, A.B. et al., Tet. Lett., 1995, 36, 3737-3740, (合成法)

Buchanan, M.S. et al., J. Indian Chem. Soc., 1998, 75, 613-615

§ Isoquercitrin; 2''-O-[β-D-Glucopyranosyl-(1 → 2)-β-D-galactopyranosyl]

[CAS No.] 197250-97-8

[化合物分類] フラボノイド (Flavonols; 5 × O-置換基)

[構造式]

[分子式] C<sub>33</sub>H<sub>40</sub>O<sub>22</sub>

[分子量] 788.666

[基原] *Nigella sativa* の種子

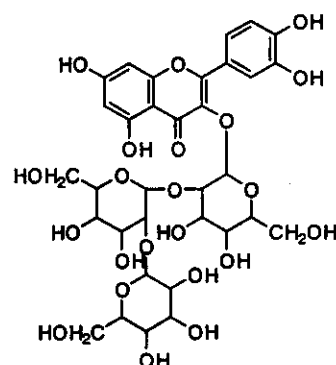
[性状] 無定型の黄色の粉末

[溶解性] BERDY SOL: 水に可溶; メタノールに易溶; ブタノール, ヘキサンに難溶

UV: [neutral] λ<sub>max</sub> 255 ; 265 (sh); 355 (MeOH) [neutral] λ<sub>max</sub> (H<sub>2</sub>O)

(Berdy)

[傷害・毒性] BERDY HAZD : 50 %致死量 (LD<sub>50</sub>) (マウス, 静脈内) 62 mg/kg



----- 文献 -----

Merfort, I. et al., Phytochemistry, 1997, 46, 359-363, (2''-glucosylgalactosyl)

§ Isoquercitrin; 2''-O-[4-Hydroxy-3-methoxycinnamoyl-(→ 6)-β-D-glucopyranosyl-(1 → 2)-β-D-galactopyranosyl]

[CAS No.] 197294-29-4

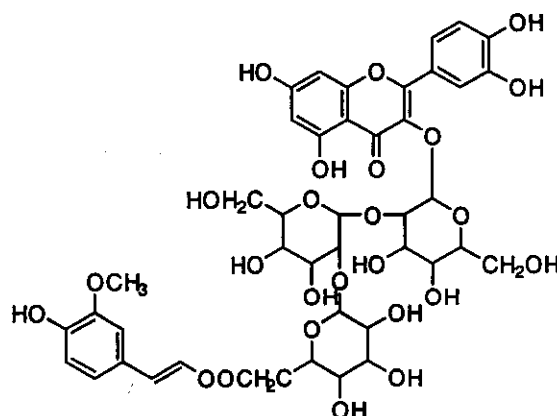
[化合物分類] フラボノイド (Flavonols; 5 × O-置換基)

[構造式]

[分子式] C<sub>43</sub>H<sub>48</sub>O<sub>25</sub>

[分子量] 964.837

[基原] *Nigella sativa* の種子



----- 文献 -----

§ p-Mentha-3,6-diene-2,5-dione

[化学名・別名] 2-Methyl-5-(1-methylethyl)-2,5-cyclohexadiene-1,4-dione (CAS名)

2-Isopropyl-5-methyl-1,4-benzoquinone. p-Cymene-2,5-dione. Thymoquinone. Thymoil

[CAS No.] 490-91-5

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

[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] *Callitris quadrivalvis* と *Monarda fistulosa* の木部にみられる。また *Juniperus cedrus*, *Tetraclinis articulata*, *Nepeta leucophylla* から得られる。次の植物の種子オイルの主成分: *Nigella sativa* (24%)

[性状] 浸透性の臭気を持つ淡黄色の結晶 (pentane)

[融点] Mp 44-45 °C

[溶解性] BERDY SOL: メタノール, エーテルに可溶; クロロホルムに易溶; 水に難溶

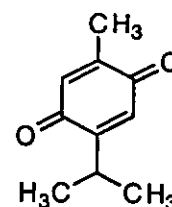
UV: [neutral] λ<sub>max</sub> 276 (ε 2610); 282 (ε 2450) (EtOH) (Berdy)

[その他のデータ] 水蒸気蒸留で得られる

[傷害・毒性] 50%致死量(LD<sub>50</sub>) (ラット, 腹膜内) 10 mg/kg

[化学物質毒性データ総覧(RTECS)登録番号] GU5330000

[販売元] Aldrich:27466-6; Sigma:T8146



-----文献-----

El-Dakhkhny, M., *Planta Med.*, 1963, 11, 465, (分離)

Jacobsen, N., *J.C.S. Perkin 2*, 1979, 569, (合成法, H-NMR, Mass)

Liebeskind, L.S. et al., *J.O.C.*, 1992, 57, 4345, (合成法, H-NMR, IR)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, IQF000

\*\*\*RTECS (化学物質毒性データ)\*\*\*

生体影響物質 : 変異原性物質.

\*\*\*健康障害に関するデータ\*\*\*

\*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 腹腔内投与.

被験動物 : げっ歯類-ラット.

投与量・期間 : 10 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

*Arzneimittel-Forschung. Drug Research.* (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) 15,1227,1965

\*\*\*変異原性に関するデータ\*\*\*

<<試験方法>> 微生物を用いた突然変異試験.

試験系 : 大腸菌 *Salmonella typhimurium*

投与量・期間 : 20 nmol/plate

参照文献

*Mutation Research.* (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherlands) 347,37,1995

\*\*\*米国に於ける状況\*\*\*

EPA TSCA Section 8(b) CHEMICAL INVENTORY

### § Nigellicine

[CAS No.] 98063-20-8

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

[構造式]

[分子式] C<sub>13</sub>H<sub>14</sub>N<sub>2</sub>O<sub>3</sub>

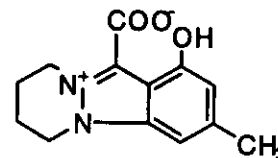
[分子量] 246.265

[基原] 次の植物の種子から得られるアルカロイド: *Nigella sativa* (キンポウゲ科)

[性状] 黄色の結晶 (EtOH)

UV: [neutral] λ<sub>max</sub> 240 (ε 20000); 288 (ε 3310); 296 (ε 3240); 353 (ε 3390) (EtOH) (Derep)

[その他のデータ] Dec. over a wide temp. range



-----文献-----

Atta-ur-Rahman et al., *Tet. Lett.*, 1985, 26, 2759, (分離, UV, IR, H-NMR, C13-NMR, Mass, 結晶構造)

### § Nigellidine

[化学名・別名] 6,7,8,9-Tetrahydro-1-hydroxy-11-(4-hydroxyphenyl)-3-methylpyridazino[1,2-a]

indazol-5-ium inner salt (CAS 名)

[CAS No.] 120993-86-4

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

[構造式]

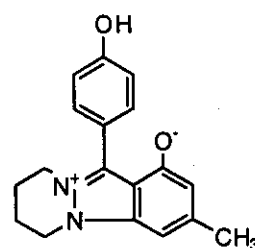
[分子式]  $C_{18}H_{18}N_2O_2$

[分子量] 294.352

[基原] 次の植物の種子から得られるアルカロイド: *Nigella sativa* (キンポウゲ科)

UV: [neutral]  $\lambda_{max}$  230 ( $\epsilon$ ); 280 ( $\epsilon$ ); 328 ( $\epsilon$ ) (MeOH) (Derep)

[その他のデータ] 化学構造は次の化合物と似ている: Nigellicine



-----文献-----

Atta-ur-Rahman et al., Tet. Lett., 1995, 36, 1993, (分離, UV, IR, H-NMR, C13-NMR, Mass, 結晶構造)

### § § キンポウゲ科クロタネソウ (*Nigella damascena* L.) の種子。

#### § Abscisic acid; (S)-form, 14-Hydroxy

[化学名・別名] Nigellinic acid

[CAS No.] 91897-25-5

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

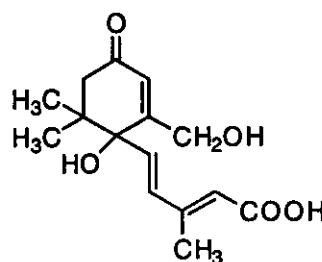
[構造式]

[分子式]  $C_{15}H_{20}O_5$

[分子量] 280.32

[基原] 次の植物から分離: *Xanthium strumarium*, *Nigella damascena*, *Vicia faba* の葉

[性状] ガム



-----文献-----

Lehmann, H. et al., Phytochemistry, 1983, 22, 1277; 1988, 27, 677, (Nigellinic acid)

Boyer, G.L. et al., Phytochemistry, 1986, 25, 1103, (Nigellinic acid)

#### § 2-Amino-3-hydroxybenzoic acid; O,N-Di-Me, Me ester

[化学名・別名] Damascenine

[CAS No.] 483-64-7

[化合物分類] アルカロイド化合物 (Simple anthranilic acid alkaloids), 単環芳香族 (Simple benzoic acids and esters)

[構造式]

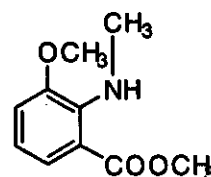
[分子式]  $C_{10}H_{13}NO_3$

[分子量] 195.218

[基原] 次の植物の種子から得られるアルカロイド: *Nigella damascena* (キンポウゲ科)

[融点] Mp 24-26 °C

[沸点] Bp 270 °C で分解. Bp<sub>10</sub> 147-148 °C



-----文献-----

Ewins, A.J., J.C.S., 1912, 101, 544, (Damascenine)

Thoinet, M. et al., Ann. Pharm. Fr., 1978, 36, 337, (合成法, Damascenine)

#### § 2,4-Diamino-3-hydroxybenzoic acid; N<sup>2</sup>,N<sup>4</sup>-Di-Me, Me ester

[化学名・別名] Damascinine. Methyl 3-hydroxy-2,4-bis(methylamino) benzoate (CAS 名)

[CAS No.] 28917-01-3

[化合物分類] アルカロイド化合物 (Simple anthranilic acid alkaloids)

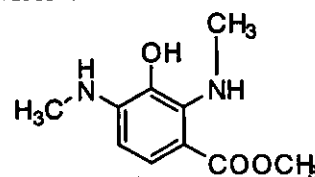
[構造式]

[分子式]  $C_{10}H_{14}N_2O_3$

[分子量] 210.232

[基原] 次の植物の種子から得られるアルカロイド: *Nigella damascena* (キンポウゲ科)

[融点] Mp 75-79 °C



-----文献-----

Doepke, W. et al., Pharmazie, 1970, 25, 69, (IR, H-NMR, Mass)

\*\*\*\*\*ブラックベリー (Blackberry) \*\*\*\*\*

§ §バラ科セイヨウヤブイチゴ (*Rubus fruticosus* L.) の果実, 葉または樹皮.

§ 3,7-Dihydroxy-12-ursen-28-oic acid; (3  $\beta$ , 7  $\alpha$ )-form

[化学名・別名] Rubitic acid

[CAS No.] 28348-90-5

[化合物分類] テルペノイド (Ursane triterpenoids)

[構造式]

[分子式]  $C_{30}H_{48}O_4$

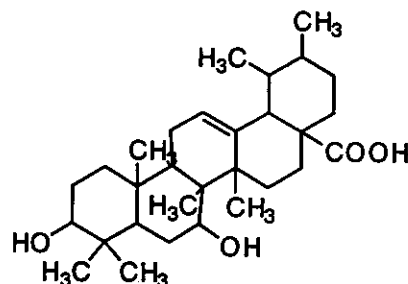
[分子量] 472.707

[基原] *Rubus fruticosus*

[性状] 無定型の塊

[融点] Mp 252-254 °C

[比旋光度]:  $[\alpha]_D^{25} +65$  (MeOH)



----- 文献 -----

Sarkar, A. et al., Phytochemistry, 1978, 17, 1983

ukherjee, M. et al., Phytochemistry, 1984, 23, 2581

§ 3,7-Dihydroxy-12-ursen-28-oic acid; (3  $\beta$ , 7  $\alpha$ )-form, 3-Ketone

[化学名・別名] 7  $\alpha$ -Hydroxy-3-oxo-12-ursen-28-oic acid. Rubinic acid

[CAS No.] 94662-96-1

[化合物分類] テルペノイド (Ursane triterpenoids)

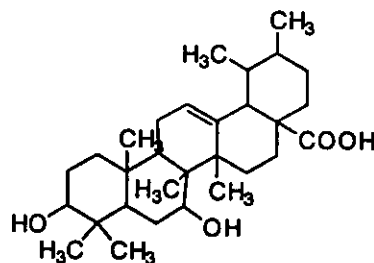
[構造式]

[基原] *Rubus fruticosus*

[性状] 結晶 (MeOH/CHCl<sub>3</sub>)

[融点] Mp 259-261 °C

[比旋光度]:  $[\alpha]_D^{25} +72$  (MeOH)



----- 文献 -----

Sarkar, A. et al., Phytochemistry, 1978, 17, 1983

ukherjee, M. et al., Phytochemistry, 1984, 23, 2581

§ 3-Hydroxy-12-ursen-28-oic acid; 3  $\beta$ -form, 3-Ketone

[化学名・別名] 3-Oxo-12-ursen-28-oic acid. Ursonic acid

[CAS No.] 6246-46-4

[化合物分類] テルペノイド (Ursane triterpenoids)

[構造式]

[分子式]  $C_{30}H_{46}O_3$

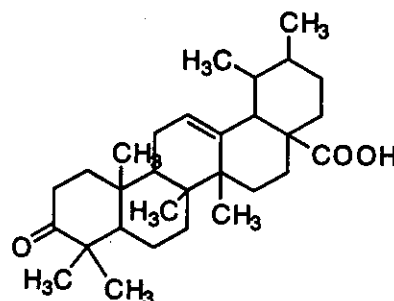
[分子量] 454.692

[基原] dammar resin, *Rubus fruticosus*, その他の植物

[性状] 結晶 (MeOH)

[融点] Mp 270-275 °C で分解

[比旋光度]:  $[\alpha]_D^{25} +80$  (c, 0.9 in CHCl<sub>3</sub>)



----- 文献 -----

Mills, J.S. et al., J.C.S., 1955, 3132, (Ursonic acid)

Poehland, B.L. et al., J. Nat. Prod., 1987, 50, 706, (Ursonic acid, H-NMR, C13-NMR)

§ Pedunculagin; 1-O-(3,4,5-Trihydroxybenzoyl) (1  $\beta$ -)

[化学名・別名] 1-O-Galloylpedunculagin

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

[構造式]

[分子式]  $C_{41}H_{28}O_{26}$

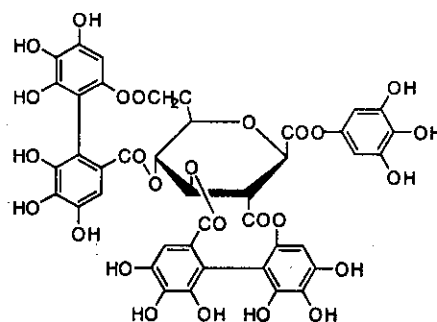
[分子量] 936.657

[基原] 次の植物から得られるタンニン: *Rosa canina*, *Quercus*

*infectoria*, *Rubus fruticosus*, *Rubus idaeus*

[性状] 淡褐色の無定型の粉末・一水和物

[比旋光度]:  $[\alpha]_D^{20} +34.9$  (c, 0.6 in MeOH)



-----文献-----

Schmidt, O.T. et al., *Annalen*, 1965, 690, 150

Gupta, R.K. et al., *J.C.S. Perkin 1*, 1982, 2525, (1-O-Galloylpedunculagin)

Okuda, T. et al., *J.C.S. Perkin 1*, 1983, 1765, (IR, UV, CD, H-NMR, C13-NMR)

Ishimatea, M. et al., *Phytochemistry*, 1989, 28, 3179, (分離, H-NMR)

Feldman, K.S. et al., *J.O.C.*, 1996, 61, 2606, (合成法, H-NMR, C13-NMR)

### § 3,3',4',5,7-Pentahydroxyflavan (4 → 8)-3,3',4',5,7-pentahydroxyflavan; (2R,2'R,3S,3'R,4S)-form

[化学名・別名] Procyanidin B. Catechin (4 α → 8) epicatechin

[CAS No.] 29106-51-2

[化合物分類] フラボノイド (Proanthocyanidin flavonoids),

フラボノイド (Neoflavonoids)

[構造式]

[分子式]  $C_{30}H_{26}O_{12}$

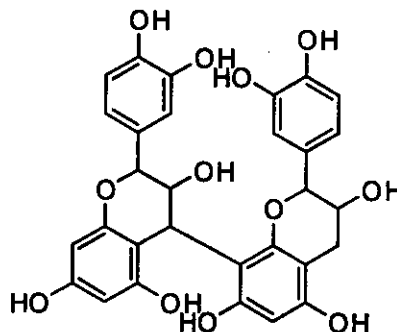
[分子量] 578.528

[基原] *Rubus fruticosus* (ブラックベリー), *Rubus idaeus*

[性状] 結晶 (EtOH) (as deca-Ac)

[融点] Mp 172-173 °C (deca-Ac)

[比旋光度]:  $[\alpha]_D -194$  (EtOH)



-----文献-----

Bae, Y.-S. et al., *Phytochemistry*, 1994, 35, 473, (Procyanidin B 3 3-glucoside)

Weinges, K. et al., *Tetrahedron*, 2001, 57, 2327-2330, (Procyanidin B 1,cryst struct)

### § Sanguin H6

[CAS No.] 82978-00-5

[化合物分類] タンニン化合物

(Sanguisorbyl ester tannins)

[構造式]

[分子式]  $C_{52}H_{34}O_{32}$

[分子量] 1871.297

[一般的性質構造式は 1985 年に改正された]

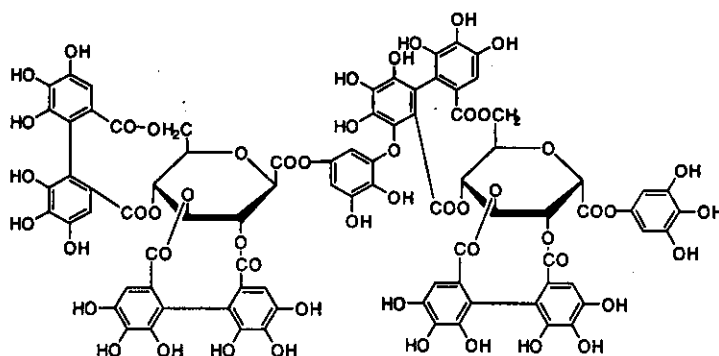
[基原] 次の植物から得られるタンニン:

*Sanguisorba officinalis*, *Rubus chingii*,

*Rubus fruticosus*, *Rubus idaeus*

[性状] 茶色の無定型の粉末

[比旋光度]:  $[\alpha]_D +72$  (Me<sub>2</sub>CO)



-----文献-----

Nonaka, G. et al., *Chem. Pharm. Bull.*, 1982, 30, 2255, (分離)

Tanaka, T. et al., *J. Chem. Res., Synop.*, 1985, 176, (構造決定)

Tanaka, T. et al., *Chem. Pharm. Bull.*, 1993, 41, 1214, (Lambertianin A, Lambertianin B)

### § 1,2,6-Trigalloylglucose; β-D-Pyranose-form

[CAS No.] 79886-49-0

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

[構造式]

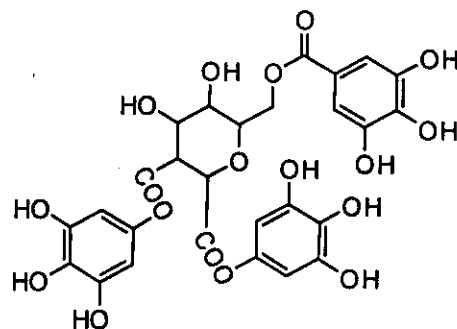
[分子式]  $C_{27}H_{34}O_{18}$

[分子量] 636.476

[基原] 次の植物から分離: *Rubus fruticosus*, *Rubus idaeus*, *Rosa canina*

[性状] 淡黄褐色の無定型の粉末・一水和物

[比旋光度]:  $[\alpha]_D^{20} +10.3$  (c, 0.5 in Me<sub>2</sub>CO)



----- 文献 -----

Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515, (分離, 構造決定, H-NMR, C13-NMR)

Ishimatsu, M. et al., Chem. Pharm. Bull., 1989, 37, 129, (構造決定)

Nawwar, M.A.M. et al., Phytochemistry, 1994, 36, 793, (分離, H-NMR, C13-NMR)

Amakura, Y. et al., Can. J. Chem., 1997, 75, 727-733, (分離,  $\alpha$ -D-glucose)

\*\*\*\*\*プラム (Plum) \*\*\*\*\*

§ §バラ科セイヨウスモモ (*Prunus domestica* L.) の果実。

§ Acaciabiuronic acid

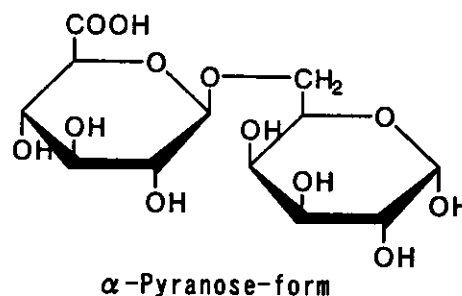
[化学名・別名] 6-O- $\beta$ -D-Glucopyranuronosyl-D-galactose (CAS名) (旧CAS名)

[CAS No.] 7264-19-9

[関連CAS No.] 1693-80-7, 5566-99-4

[化合物分類] 炭水化物 (Glycuronic acids),  
炭水化物 (Disaccharides)

[構造式]



[分子式]  $C_{17}H_{26}O_{12}$

[分子量] 356.283

[基原] Probably the commonest aldobiouronic acid present as a structural unit in plant gums. Isol. from partial acid hydrolysates from the following plants; black wattle (*Acacia mollissima*), *Acacia senegal*, *Acacia pycnantha*, *Acacia karroo*, *Acacia cyanophylla*, egg plum (*Prunus domestica*), アーモンド (*Prunus amygdalus*), モモ (*Prunus persica*), *Anogeissus latifolia* (gum ghatti), *Vigilia oroboides*, *Afraegle paniculata*, *Ferula* と *Chorisia* spp. また次の植物の加水分解でも得られる: カイガンシヨウ (*Pinus pinaster*) hemicellulose, 麦藁

[融点] Mp 118-119 °C (hydrate)

[比旋光度]:  $[\alpha]_D +11.6 \rightarrow -8.6$  (H<sub>2</sub>O)

----- 文献 -----

Goebel, W.F. et al., J. Biol. Chem., 1938, 124, 207, (分離)

Aspinall, G.O. et al., J.C.S., 1955, 1160; 1961, 3461, (分離)

Mukherjee, S. et al., J.A.C.S., 1958, 80, 2536, (分離)

Jones, J.K.N. et al., Can. J. Chem., 1961, 39, 162, (分離)

Di Fabio, J.L. et al., Carbohydr. Res., 1982, 99, 41, (分離)

§ 12'-Apo- $\beta$ -carotene-3,12'-diol; 5 $\alpha$ ,6 $\alpha$ -Epoxide

[化学名・別名] 5,6-Epoxy-5,6-dihydro-12'-apo- $\beta$ -carotene-3,12'-diol.

Persicaxanthin

[CAS No.] 80952-82-5

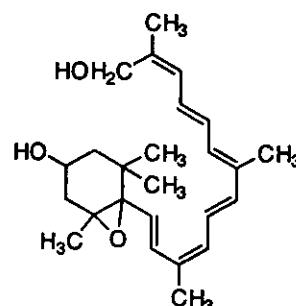
[化合物分類] テルペノイド (Apocarotenoids)

[構造式]

[分子式]  $C_{25}H_{36}O_3$

[分子量] 384.558

[基原] 次の植物から分離: プラム *Prunus domestica*



[性状]黄色の板状結晶 (C<sub>6</sub>H<sub>6</sub>/petrol)

[融点]Mp 92 °C

-----文献-----

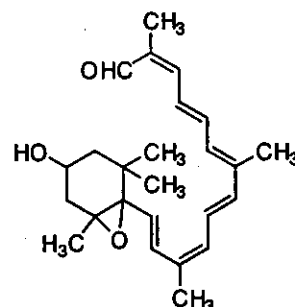
Gross, J. et al., *Phytochemistry*, 1981, 20, 2267, (Persicaxanthin)

§ 12'-Apo-β-carotene-3,12'-diol; 12'-Aldehyde, 5 α,6 α-epoxide

[化学名・別名]5,6-Epoxy-5,6-dihydro-3 β-hydroxy-12'-apo-β-caroten-12'-al. Apo-12'-violaxanthal

[化合物分類]テルペノイド (Apocarotenoids)

[構造式]



[分子式]C<sub>25</sub>H<sub>34</sub>O<sub>3</sub>

[分子量]382.542

[基原]次の植物から分離: プラム *Prunus domestica*

[性状]黄色色素

-----文献-----

Gross, J. et al., *Phytochemistry*, 1981, 20, 2267, (Persicaxanthin)

Molnaacuter, P. et al., *Phytochemistry*, 1987, 26, 1493, (絶対構造)

Märki-Fischer, E. et al., *Helv. Chim. Acta*, 1988, 71, 1689, (分離, H-NMR, UV)

§ Fucose; L-form, 2-Me

[化学名・別名]2-O-Methyl-L-fucose

[CAS No.]34299-00-8

[化合物分類]AF6100, 炭水化物 (6-Deoxygalactoses)

[構造式]

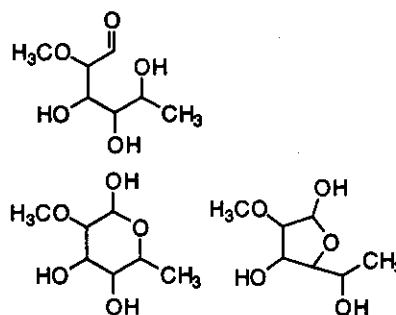
[分子式]C<sub>7</sub>H<sub>14</sub>O<sub>5</sub>

[分子量]178.185

[基原]次の植物の多糖類に存在する。例えば, *Prunus domestica*

[融点]Mp 150-152 °C

[比旋光度]:[α]<sub>D</sub><sup>25</sup> -88 (c, 1.02 in H<sub>2</sub>O)



-----文献-----

Andrews, P. et al., *Chem. Ind. (London)*, 1956, 658; 1453, (分離, 2-O-Me)

Morgenlie, S., *Carbohydr. Res.*, 1975, 41, 77, (α-D-pyr isopropylidene, α-D-pyr 2-Me)

Flowers, H.M., *Adv. Carbohydr. Chem. Biochem.*, 1981, 39, 280, (レビュー)

Kinoshita, T. et al., *Carbohydr. Res.*, 1985, 143, 249, (α-D-fur derivs, β-D-fur derivs)

§ 2-O-Methylxylose; D-form

[CAS No.]7434-28-8

[化合物分類]AF0500, 炭水化物 (xylo-Pentoses)

[構造式]

[分子式]C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>

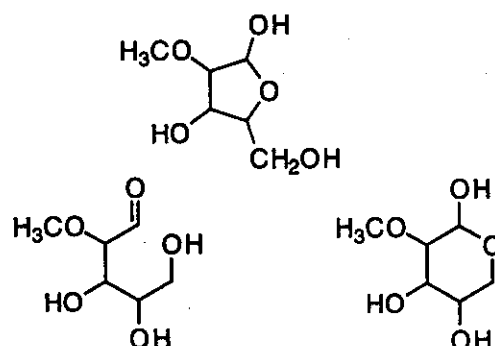
[分子量]164.158

[基原]次の植物の加水分解で分離: *Prunus domestica* の多糖類

[融点]Mp 137-138 °C

[比旋光度]:[α]<sub>D</sub> -21 → +34 (2 hr.) (H<sub>2</sub>O)

[販売元]Sigma:M9013



-----文献-----

Ehrenthal, I. et al., *J.A.C.S.*, 1954, 76, 5509, (D-form, β-D-Me pyr)

Maher, G.G., *Adv. Carbohydr. Chem.*, 1955, 10, 257, (レビュー, 誘導体)

Andrews, P. et al., *Chem. Ind. (London)*, 1956, 1278, (D-form, 分離)

§ Norepinephrine

[化学名・別名]4-(2-Amino-1-hydroxyethyl)-1,2-benzenediol (CAS名). α-(Aminomethyl)-3,4-dihydroxybenzyl alcohol (旧CAS名). 2-Amino-1-(3,4-dihydroxyphenyl)ethanol. 4-(β-Amino-α



-hydroxyethyl) catechol. Noradrenaline, BAN. Arterenol

[関連 CAS No.] 5794-08-1, 69815-49-2

[化合物分類] 薬物:  $\alpha$ -アドレナリン受容体作用薬 ( $\alpha$ -Adrenoceptor agonists), 薬物:  $\beta$ -アドレナリン受容体作用薬 ( $\beta$ -Adrenoceptor agonists), 薬物: 交感神経作用薬 (Sympathomimetic agents), アルカロイド化合物 (Simple tyramine alkaloids), 薬物: 血管収縮 (Vasoconstrictors)

[構造式]

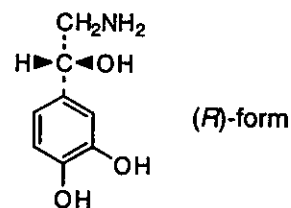
[分子式]  $C_8H_{11}NO_2$

[分子量] 169.18

[基原] 次の植物のアルカロイド: *Albizia julibrissin*, *Mimosa pudica*, *Phaseolus multiflorus*, *Samanea saman*, *Musa paradisiaca*, *Musa sapientium*, *Passiflora quadrangularis*, *Portulaca oleracea*, *Prunus domestica*, *Citrus sinensis*, *Aconitum napellus*, *Aconitum paniculatum*, *Solanum tuberosum* (マメ科, バショウ科, トケイソウ科, スペリヒユ科, パラ科, ミカン科, キンボウゲ科, ナス科)

[用途]  $\alpha$ ,  $\beta$ -アドレナリン受容体作用薬, 気管拡張薬, 交感神経遮断薬, 昇圧薬

[Log P 計算値] Log P -0.99 (計算値)



-----文献-----

Biel, J.H. et al., J.A.C.S., 1954, 76, 3149-3153, (合成法, 薬理)

Waalkes, T.P. et al., Science (Washington, D.C.), 1958, 127, 648-650, (分離)

Pratesi, P. et al., J.C.S., 1959, 4062-4065, (絶対構造)

Levy, B. et al., Drill's Pharmacol. Med., 4th edn., McGraw-Hill, New York, 1971, 627, (レビュー, 薬理)

Karlson, P. et al., Hoppe Seyler's Z. Physiol. Chem., 1972, 327, 86-94, (分離, 合成法, N-Ac)

Smith, T.A., Phytochemistry, 1977, 16, 9-18, (生育, 成書)

Wilson, T.D. et al., Anal. Profiles Drug Subst., 1982, 11, 555, (レビュー)

### § 3,4',5,6,7-Pentahydroxyflavanone; 4',6-Di-Me ether

[化学名・別名] 3,5,7-Trihydroxy-4',6-dimethoxyflavanone

[CAS No.] 143114-81-2

[化合物分類] フラボノイド (Dihydroflavonols; 5 × O-置換基)

[構造式]

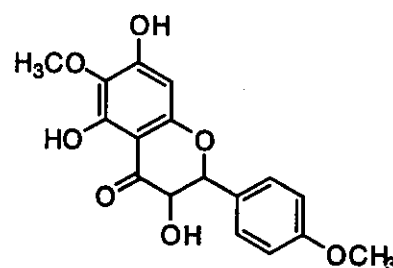
[分子式]  $C_{17}H_{16}O_7$

[分子量] 332.309

[基原] *Prunus domestica* の心材

[性状] 黄色の塊

[融点] Mp 164 °C



-----文献-----

Parmar, V.S. et al., Phytochemistry, 1992, 31, 2185

### § Persicachrome

[化学名・別名] 5,8-Epoxy-5,8-dihydro-12'-apo- $\beta$ -carotene-3,12'-diol

[CAS No.] 80931-31-3

[化合物分類] テルペノイド (Apocarotenoids)

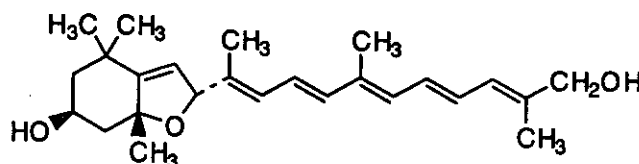
[構造式]

[分子式]  $C_{25}H_{36}O_3$

[分子量] 384.558

[基原] *Prunus domestica* (no stereochem. indicated)

[性状] 黄色色素



-----文献-----

Gross, J. et al., Phytochemistry, 1981, 20, 2267

Märki-Fischer, E. et al., Helv. Chim. Acta, 1988, 71, 1689, (分離, H-NMR, UV, CD, 絶対構造)

### § 3,4',5,7-Tetrahydroxyflavanone; (2R,3R)-form, 3-Me ether

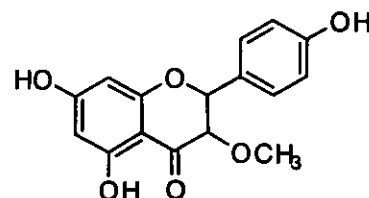
[化学名・別名] 4',5,7-Trihydroxy-3-methoxyflavanone

[CAS No.] 97231-20-4

[化合物分類] フラボノイド (Dihydroflavonols; 4 × O-置換基)

[構造式]

[分子式]  $C_{16}H_{14}O_6$



[分子量]302.283

[基原] *Ambrosia artemisioides*, *Eucalyptus* sp., *Prunus domestica*

[性状] 黄色の塊

[融点] Mp 182-184 °C

-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 374; 583; 1635, (生育)

§ 2',4',6'-Trihydroxyacetophenone

[化学名・別名] 1-(2,4,6-Trihydroxyphenyl) ethanone (CAS名). 2-Acetyl-1,3,5-benzenetriol. Phloracetophenone. Acetophloroglucinol. Acetylphloroglucinol. Phloroacetophenone

[CAS No.] 480-66-0

[関連 CAS No.] 4547-84-6

[化合物分類] 単環芳香族 (Simple aryl ketones)

[構造式]

[分子式] C<sub>8</sub>H<sub>8</sub>O<sub>4</sub>

[分子量] 168.149

[基原] 次の植物の樹皮から分離: *Prunus domestica*. また *Pseudomonas fluorescens* から得られる

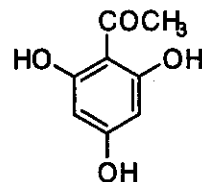
[用途] 胆汁分泌促進剤

[性状] 針状結晶 (H<sub>2</sub>O)

[融点] Mp 219 °C (無水物)

UV: [neutral] λ<sub>max</sub> 228 (ε 14500); 288 (ε 16200) (EtOH) (Berdy)

[販売元] Aldrich:T6460-2; Fluka:91930; Rare Chemicals Library:S3916-1



-----文献-----

Reddi, T.K. et al., *Khim. Prir. Soedin.*, 1968, 5, 133; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, 5, 116, (分離)

Chou, C.J. et al., *J. Nat. Prod.*, 1992, 55, 795, (Geranyloxydihydroxyacetophenones)

Singh, A.K. et al., *Phytochemistry*, 1997, 44, 555, (Annphenone)

§ 2',4',6'-Trihydroxyacetophenone; 4'-Me ether

[化学名・別名] 2',6'-Dihydroxy-4'-methoxyacetophenone. 4-O-Methylphloracetophenone

[CAS No.] 7507-89-3

[化合物分類] 単環芳香族 (Simple aryl ketones)

[構造式]

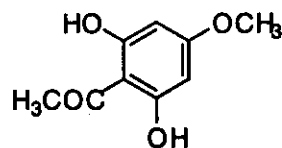
[分子式] C<sub>9</sub>H<sub>10</sub>O<sub>4</sub>

[分子量] 182.176

[基原] 次の植物の樹皮から分離: *Prunus domestica*

[用途] 抗カビ剤

[融点] Mp 141-142 °C



-----文献-----

Reddi, T.K. et al., *Khim. Prir. Soedin.*, 1968, 5, 133; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, 5, 116, (分離)

Ahsan, M. et al., *J. Nat. Prod.*, 1994, 57, 63, (4'-farnesyl ether)

§ 2',4',6'-Trihydroxyacetophenone; 4'-Me ether, O-β-D-glucopyranoside

[化学名・別名] Pleoside. Domesticoside

[CAS No.] 24587-97-1

[化合物分類] 単環芳香族 (Simple aryl ketones)

[構造式]

[分子式] C<sub>15</sub>H<sub>20</sub>O<sub>9</sub>

[分子量] 344.318

[基原] 次の植物から分離: *Prunus domestica* の樹皮, シダ類: *Pleopeltis*

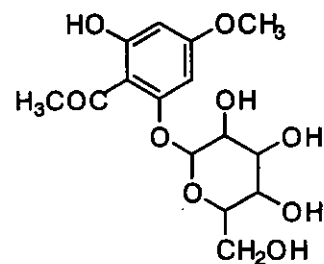
*thunbergiana*

[性状] 針状結晶 (MeOH)

[融点] Mp 189-191 °C (焼結温度: 183 °C). Mp 200-203 °C

[比旋光度]: [α]<sub>D</sub> -41.6 (Py)

[その他のデータ] Identity of samples not apparently establ. 高い融点と比旋光度は Pleoside に似ている



-----文献-----

Hikino, H. et al., Yakugaku Zasshi, 1969, 89, 372, (Pleoside)

Nagarajan, G.R. et al., Indian J. Chem., Sect. B, 1977, 15, 955, (Domesticoside)

§ 3,5,7-Trihydroxy-4',8-dimethoxyflavone

[化学名・別名] 3,5,7-Trihydroxy-8-methoxy-2-(4-methoxyphenyl)-4H-1-benzopyran-4-one.  
5,7-Dihydroxy-4',8-dimethoxyflavonol. Prudomestin

[CAS No.] 3443-28-5

[化合物分類] フラボノイド (Flavonols; 5 × O-置換基)

[構造式]

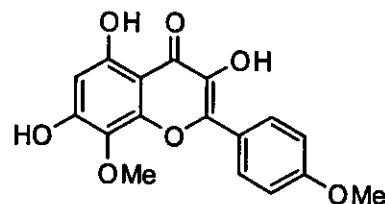
[分子式]  $C_{17}H_{14}O_7$

[分子量] 330.293

[基原] 次の植物から分離: *Prunus domestica* の心材, *Pityrogramma triangularis*

[性状] 黄色の針状結晶 (CHCl<sub>3</sub>/petrol)

[融点] Mp 209-210 °C



-----文献-----

Hasegawa, M., Shokubutsugaku Zasshi, 1969, 82, 148; CA, 71, 67949x, (Prudomenin)

§ 2,2,9-Trimethyldecane

[CAS No.] 62238-00-0

[化合物分類] 脂肪族化合物 (Branched aliphatic hydrocarbons)

[構造式]  $(H_3C)_2CH(CH_2)_6C(CH_3)_2$

[分子式]  $C_{13}H_{28}$

[分子量] 184.364

[基原] *Prunus domestica* の果実

-----文献-----

Etievant, P.X. et al., Sci. Aliments, 1986, 6, 417, (分離)

§ 3,3,4-Trimethyldecane

[CAS No.] 49622-18-6

[化合物分類] 脂肪族化合物 (Branched aliphatic hydrocarbons)

[構造式]  $H_3C(CH_2)_3CH(CH_3)C(CH_3)_2CH_2CH_3$

[分子式]  $C_{13}H_{28}$

[分子量] 184.364

[基原] *Prunus domestica* の果実

-----文献-----

Etievant, P.X. et al., Sci. Aliments, 1986, 6, 417, (分離)

\*\*\*\*\*ブリオニア (Bryonia) \*\*\*\*\*

§ § ウリ科ブリオニア (*Bryonia alba* L.) の根。

§ 4-Methylstigmast-7-en-3-ol; (3 β,4 α,5 α,24R)-form

[化学名・別名] 24-Ethyllophenol

[CAS No.] 36735-29-2

[化合物分類] ステロイド (Stigmastane steroids). (C29).

[構造式]

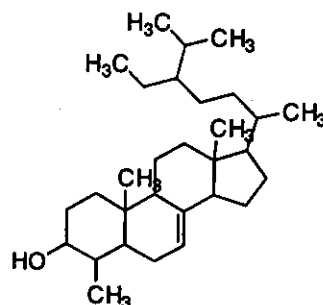
[分子式]  $C_{30}H_{52}O$

[分子量] 428.74

[基原] 次の植物から分離: *Bryonia alba* の種子, *Lycopersicon esculentum*, 多くの野菜のオイル

[性状] 結晶 (Me<sub>2</sub>CO/MeOH)

[融点] Mp 175.5-176.5 °C



-----文献-----

Panosyan, A.G. et al., Khim. Prir. Soedin., 1977, 13, 353; 1980, 16, 781; Chem. Nat. Compd. (Engl. Transl.), 1977, 13, 300; 1980, 16, 554, (分離)

Itoh, T. et al., Fette, Seifen, Anstrichm., 1978, 80, 382  
 Itoh, T. et al., Phytochemistry, 1980, 19, 2491  
 Itoh, T. et al., Yukagaku, 1981, 30, 586, (HPLC)

§ 2,16,20,24,25-Pentahydroxycucurbit-5-ene-3,11,22-trione; (16 $\alpha$ ,20R,24S)-form, 2-Ketone

[化学名・別名] 2,16,20,24,25-Pentahydroxycucurbita-1,5-diene-3,11,22-trione.  
 16,20,24,25-Tetrahydroxycucurbit-5-ene-2,3,11,22-tetron $\acute{e}$ . Cucurbitacin J

[CAS No.] 5979-41-9

[化合物分類] テルペノイド

(Cucurbitane triterpenoids)

[構造式]

[分子式] C<sub>30</sub>H<sub>44</sub>O<sub>8</sub>

[分子量] 532.673

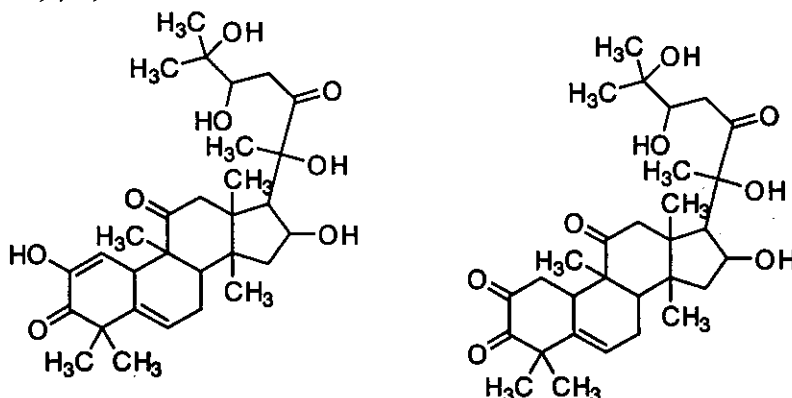
[基原] *Citrullus ecirrhosus* と  
*Bryonia alba* の苦味成分

[性状] 結晶 (MeOH)

[融点] Mp 196-198 °C

[比旋光度]: [α]<sub>D</sub> -36 (c, 1.0 in  
 CHCl<sub>3</sub>)

[その他のデータ] Exists in enol  
 form



Tautomeric astructures

-----文献-----

Pohlmann, J. et al., Phytochemistry, 1975, 14, 1587-1589, (Cucurbitacin J, Cucurbitacin K)

Fujita, S. et al., Phytochemistry, 1995, 38, 465-472, (C13-NMR)

§ 9,10,13-Trihydroxy-11,15-octadecadienoic acid; (9R,10S,11E,13R,15Z)-form

[CAS No.] 95341-37-0

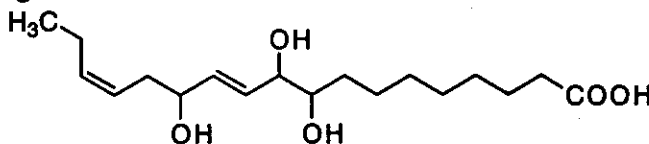
[化合物分類] 脂肪族化合物 (Oxylipins (including Eicosanoids)), 脂肪族化合物 (Unbranched alkenic  
 carboxylic acids and lactones)

[構造式]

[分子式] C<sub>19</sub>H<sub>32</sub>O<sub>5</sub>

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)

Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 9,10,13-Trihydroxy-11,15-octadecadienoic acid; (9S,10R,11E,13R,15Z)-form

[CAS No.] 95341-33-6

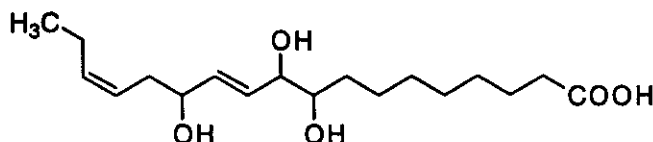
[化合物分類] 脂肪族化合物 (Oxylipins (including Eicosanoids)), 脂肪族化合物 (Unbranched alkenic  
 carboxylic acids and lactones)

[構造式]

[分子式] C<sub>18</sub>H<sub>32</sub>O<sub>5</sub>

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)

Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 9,10,13-Trihydroxy-11,15-octadecadienoic acid; (9S,10R,11E,13S,15Z)-form

[CAS No.] 95341-40-5

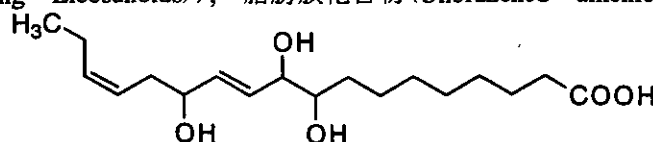
[化合物分類] 脂肪族化合物 (Oxylipins (including Eicosanoids)), 脂肪族化合物 (Unbranched alkenic  
 carboxylic acids and lactones)

[構造式]

[分子式] C<sub>18</sub>H<sub>32</sub>O<sub>5</sub>

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)  
 Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 9,10,13-Trihydroxy-11,15-octadecadienoic acid; (9S,10S,11E,13R,15Z)-form

[CAS No.] 211236-20-3

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

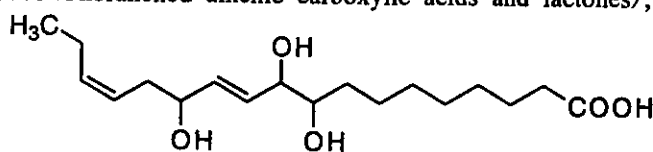
(including

[構造式]

[分子式] C<sub>18</sub>H<sub>32</sub>O<sub>5</sub>

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)  
 Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 9,10,13-Trihydroxy-11,15-octadecadienoic acid; (9S,10S,11E,13S,15Z)-form

[CAS No.] 95341-42-7

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

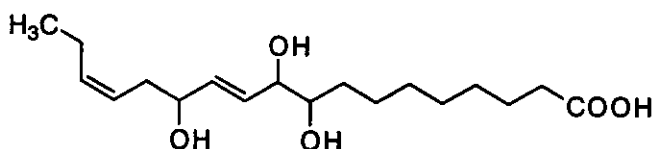
[構造式]

(9S,10S,11E,13S,  
15Z)-form

[分子式] C<sub>18</sub>H<sub>32</sub>O<sub>5</sub>

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)  
 Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 9,12,13-Trihydroxy-10,15-octadecadienoic acid; (9R,10E,12R,13S,15Z)-form

[CAS No.] 95341-35-8

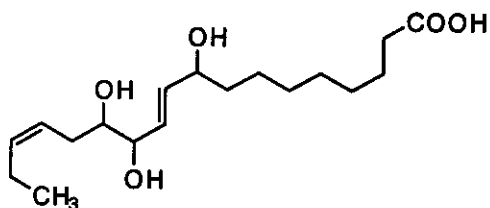
[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones), 脂肪族化合物 (Oxylipins (including Eicosanoids))

[構造式]

[分子式] C<sub>18</sub>H<sub>32</sub>O<sub>5</sub>

[分子量] 328.448

[基原] 次の植物の根から分離: *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Khim. Prir. Soedin., 1980, 825, (分離)  
 Cardellina, J.H. et al., Tetrahedron, 1980, 36, 993, (分離)  
 Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126, (分離, 構造決定)  
 Herz, W. et al., Phytochemistry, 1985, 24, 89; 1986, 25, 1481; 1913, (分離)  
 Kato, T. et al., Tet. Lett., 1985, 26, 2357, (分離)  
 Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 9,12,13-Trihydroxy-10,15-octadecadienoic acid; (9R,10E,12S,13S,15Z)-form

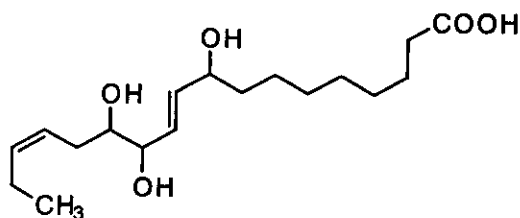
[CAS No.] 95341-38-1

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

[構造式]

[分子式] C<sub>18</sub>H<sub>32</sub>O<sub>5</sub>

[分子量] 328.448



[基原] *Bryonia alba*

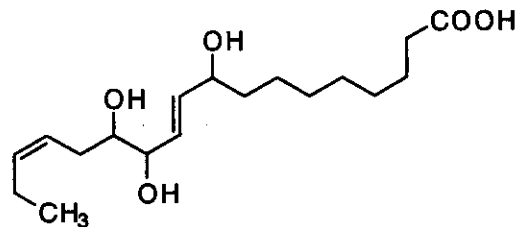
文献

- Panosyan, A.G. et al., *Khim. Prir. Soedin.*, 1980, 825, (分離)  
Cardellina, J.H. et al., *Tetrahedron*, 1980, 36, 993, (分離)  
Panosyan, A.G. et al., *Bioorg. Khim.*, 1985, 11, 126, (分離, 構造決定)  
Herz, W. et al., *Phytochemistry*, 1985, 24, 89; 1986, 25, 1481; 1913, (分離)  
Kato, T. et al., *Tet. Lett.*, 1985, 26, 2357, (分離)  
Karageuzyan, K.G. et al., *Planta Med.*, 1998, 64, 417-422, (分離)

§ 9,12,13-Trihydroxy-10,15-octadecadienoic acid; (9*S*,10*E*,12*R*,13*R*,15*Z*)-form

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

[構造式]



[分子式]  $C_{18}H_{32}O_5$

[分子量] 328.448

[基原] *Bryonia alba*

文献

- Panosyan, A.G. et al., *Khim. Prir. Soedin.*, 1980, 825, (分離)  
Cardellina, J.H. et al., *Tetrahedron*, 1980, 36, 993, (分離)  
Panosyan, A.G. et al., *Bioorg. Khim.*, 1985, 11, 126, (分離, 構造決定)  
Herz, W. et al., *Phytochemistry*, 1985, 24, 89; 1986, 25, 1481; 1913, (分離)  
Kato, T. et al., *Tet. Lett.*, 1985, 26, 2357, (分離)  
Karageuzyan, K.G. et al., *Planta Med.*, 1998, 64, 417-422, (分離)

§ 9,12,13-Trihydroxy-10,15-octadecadienoic acid; (9*S*,10*E*,12*R*,13*S*,15*Z*)-form

[化学名・別名] Malyngic acid

[CAS No.] 74923-93-6

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

[構造式]

[分子式]  $C_{18}H_{32}O_5$

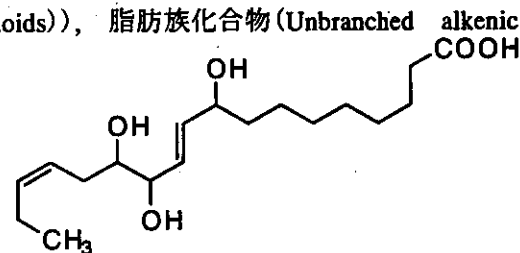
[分子量] 328.448

[基原] 次の植物から分離: *Lyngbya majuscula*; *Bryonia alba* と *Wedelia pinetorum* の根

[性状] ワックス様の塊

[融点] Mp 48.5-51 °C

[比旋光度]:  $[\alpha]_D +7.7$  (MeOH)



文献

- Panosyan, A.G. et al., *Khim. Prir. Soedin.*, 1980, 825, (分離)  
Cardellina, J.H. et al., *Tetrahedron*, 1980, 36, 993, (分離)  
Panosyan, A.G. et al., *Bioorg. Khim.*, 1985, 11, 126, (分離, 構造決定)  
Herz, W. et al., *Phytochemistry*, 1985, 24, 89; 1986, 25, 1481; 1913, (分離)  
Kato, T. et al., *Tet. Lett.*, 1985, 26, 2357, (分離)  
Karageuzyan, K.G. et al., *Planta Med.*, 1998, 64, 417-422, (分離)

§ 9,12,13-Trihydroxy-10,15-octadecadienoic acid; (9*S*,10*E*,12*S*,13*R*,15*Z*)-form

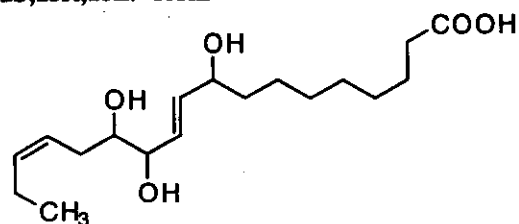
[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones), 脂肪族化合物 (Oxylipins (including Eicosanoids))

[構造式]

[分子式]  $C_{18}H_{32}O_5$

[分子量] 328.448

[基原] *Bryonia alba*



文献

- Panosyan, A.G. et al., *Khim. Prir. Soedin.*, 1980, 825, (分離)

Cardellina, J.H. et al., Tetrahedron, 1980, 36, 993, (分離)  
 Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126, (分離, 構造決定)  
 Herz, W. et al., Phytochemistry, 1985, 24, 89; 1986, 25, 1481; 1913, (分離)  
 Kato, T. et al., Tet. Lett., 1985, 26, 2357, (分離)  
 Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 9,12,13-Trihydroxy-10,15-octadecadienoic acid; (9S,10E,12S,13S,15Z)-form

[化学名・別名] Corchorifatty acid F

[CAS No.] 95341-44-9

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

[構造式]

[分子式]  $C_{18}H_{32}O_5$

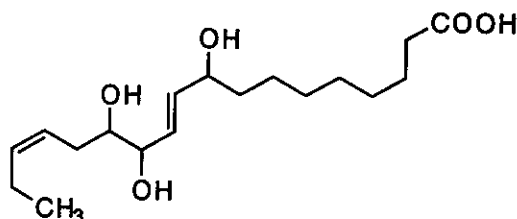
[分子量] 328.448

[基原] 次の植物から分離: *Bryonia alba*, *Helianthus heterophyllus*, *Corchorus olitorius* and rice infected with blast disease

[用途] Confers activity against rice blast disease

[比旋光度]:  $[\alpha]_D^{24} -10.5$  (c, 0.7 in MeOH)

[その他のデータ] Unnatural stereoisomers also synthesised



-----文献-----

Panosyan, A.G. et al., Khim. Prir. Soedin., 1980, 825, (分離)  
 Cardellina, J.H. et al., Tetrahedron, 1980, 36, 993, (分離)  
 Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126, (分離, 構造決定)  
 Herz, W. et al., Phytochemistry, 1985, 24, 89; 1986, 25, 1481; 1913, (分離)  
 Kato, T. et al., Tet. Lett., 1985, 26, 2357, (分離)  
 Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 12,13,16-Trihydroxy-9,14-octadecadienoic acid; (9Z,12R,13R,14E,16S)-form

[CAS No.] 211236-15-6

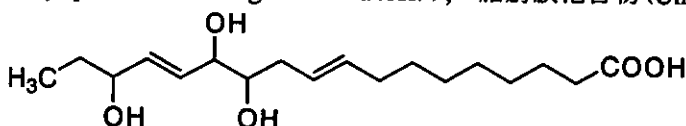
[化合物分類] 脂肪族化合物 (Oxylipins (including Eicosanoids)), 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones)

[構造式]

[分子式]  $C_{18}H_{32}O_5$

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)  
 Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 12,13,16-Trihydroxy-9,14-octadecadienoic acid; (9Z,12R,13S,14E,16S)-form

[CAS No.] 211236-16-7

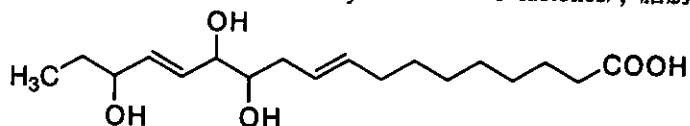
[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones), 脂肪族化合物 (Oxylipins (including Eicosanoids))

[構造式]

[分子式]  $C_{18}H_{32}O_5$

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)  
 Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

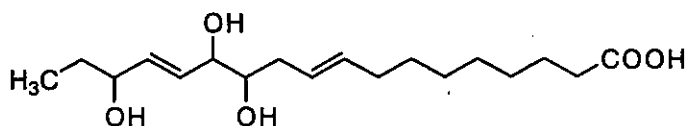
§ 12,13,16-Trihydroxy-9,14-octadecadienoic acid; (9Z,12S,13R,14E,16R)-form

[CAS No.] 95341-32-5

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

[構造式]

[分子式]  $C_{18}H_{32}O_5$   
[分子量] 328.448  
[基原] *Bryonia alba*



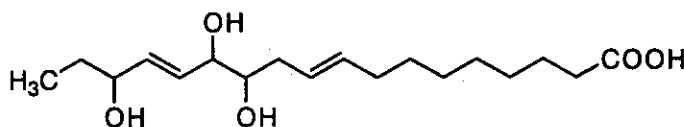
-----文献-----

Panosyan, A.G. et al., *Bioorg. Khim.*, 1985, 11, 126-131, (分離)  
Karageuzyan, K.G. et al., *Planta Med.*, 1998, 64, 417-422, (分離)

§ 12,13,16-Trihydroxy-9,14-octadecadienoic acid; (9Z,12S,13R,14E,16S)-form

[CAS No.] 95341-39-2  
[化合物分類] 脂肪族化合物 (Oxylipins (including Eicosanoids)), 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones)  
[構造式]

[分子式]  $C_{18}H_{32}O_5$   
[分子量] 328.448  
[基原] *Bryonia alba*



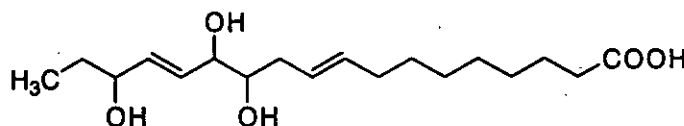
-----文献-----

Panosyan, A.G. et al., *Bioorg. Khim.*, 1985, 11, 126-131, (分離)  
Karageuzyan, K.G. et al., *Planta Med.*, 1998, 64, 417-422, (分離)

§ 12,13,16-Trihydroxy-9,14-octadecadienoic acid; (9Z,12S,13S,14E,16R)-form

[CAS No.] 95341-36-9  
[化合物分類] 脂肪族化合物 (Oxylipins (including Eicosanoids)), 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones)  
[構造式]

[分子式]  $C_{18}H_{32}O_5$   
[分子量] 328.448  
[基原] *Bryonia alba*



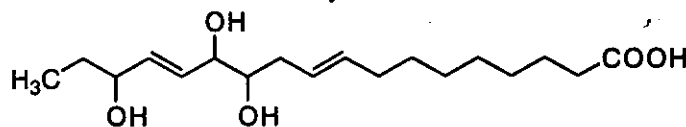
-----文献-----

Panosyan, A.G. et al., *Bioorg. Khim.*, 1985, 11, 126-131, (分離)  
Karageuzyan, K.G. et al., *Planta Med.*, 1998, 64, 417-422, (分離)

§ 12,13,16-Trihydroxy-9,14-octadecadienoic acid; (9Z,12S,13S,14E,16S)-form

[CAS No.] 95341-43-8  
[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones), 脂肪族化合物 (Oxylipins (including Eicosanoids))  
[構造式]

[分子式]  $C_{18}H_{32}O_5$   
[分子量] 328.448  
[基原] *Bryonia alba*



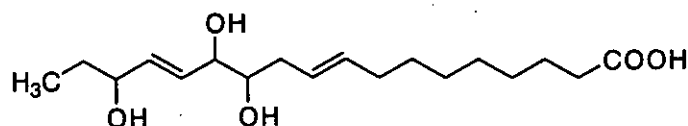
-----文献-----

Panosyan, A.G. et al., *Bioorg. Khim.*, 1985, 11, 126-131, (分離)  
Karageuzyan, K.G. et al., *Planta Med.*, 1998, 64, 417-422, (分離)

§ 12,15,16-Trihydroxy-9,13-octadecadienoic acid; (9Z,12R,13E,15R,16S)-form

[CAS No.] 95341-34-7  
[化合物分類] 脂肪族化合物 (Oxylipins (including Eicosanoids)), 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones)  
[構造式]

[分子式]  $C_{18}H_{32}O_5$   
[分子量] 328.448  
[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., *Bioorg. Khim.*, 1985, 11, 126-131, (分離)  
Karageuzyan, K.G. et al., *Planta Med.*, 1998, 64, 417-422, (分離)



§ 12,15,16-Trihydroxy-9,13-octadecadienoic acid; (9Z,12R,13E,15S,16S)-form

[CAS No.] 95588-21-9

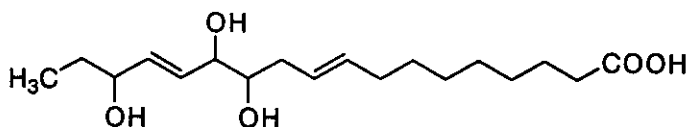
[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones), 脂肪族化合物 (Oxylipins (including Eicosanoids))

[構造式]

[分子式]  $C_{18}H_{32}O_5$

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)

Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 12,15,16-Trihydroxy-9,13-octadecadienoic acid; (9Z,12S,13E,15R,16S)-form

[CAS No.] 95588-22-0

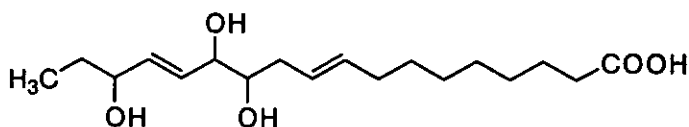
[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones), 脂肪族化合物 (Oxylipins (including Eicosanoids))

[構造式]

[分子式]  $C_{18}H_{32}O_5$

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)

Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ 12,15,16-Trihydroxy-9,13-octadecadienoic acid; (9Z,12S,13E,15S,16S)-form

[CAS No.] 95341-41-6

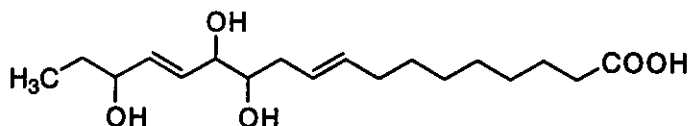
[化合物分類] 脂肪族化合物 (Oxylipins (including Eicosanoids)), 脂肪族化合物 (Unbranched alkenic carboxylic acids and lactones)

[構造式]

[分子式]  $C_{18}H_{32}O_5$

[分子量] 328.448

[基原] *Bryonia alba*



-----文献-----

Panosyan, A.G. et al., Bioorg. Khim., 1985, 11, 126-131, (分離)

Karageuzyan, K.G. et al., Planta Med., 1998, 64, 417-422, (分離)

§ § ウリ科 (*Bryonia dioica* Jacquin) の根。

§ Alliaroside

[化合物分類] フラボノイド (Flavonoids 構造は一部又は全てが未知)

[分子式]  $C_{22}H_{22}O_{11}$

[分子量] 486.431

[一般的性質] 構造は未知. Flavonoid. Prob. a Vicenin (4',5,7-trihydroxyflavone 6,8-di- C -glucoside)

[基原] 次の植物の葉から分離: *Alliaria officinalis*, *Bryonia dioica*

[性状] 淡黄色の針状結晶 + 2·1/2H<sub>2</sub>O

[融点] Mp 260-262 °C

-----文献-----

Paris, R.R. et al., C. R. Hebd. Seances Acad. Sci., 1962, 254, 928, (分離, IR, UV)

Paris, R.R. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1966, 262, 1372, (分離)

Seikel, M.K. et al., Phytochemistry, 1966, 5, 439, (構造決定)

§ Cucurbitacin S

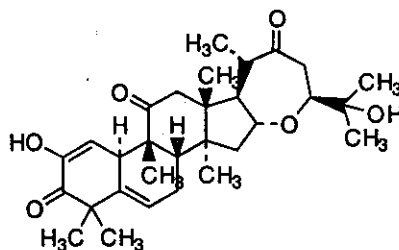
[化学名・別名] 16 α,24S-Epoxy-2,25-dihydroxycucurbita-1,5-diene-3,11,22-trione

[CAS No.] 60137-06-6

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

[構造式]

[分子式]  $C_{30}H_{42}O_6$   
 [分子量] 498.658  
 [基原] *Bryonia dioica*  
 [性状] 黄色の結晶 (EtOAc/petrol)  
 [融点] Mp 128-130 °C

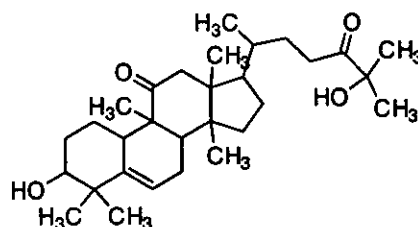


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Hylands, P.J. et al., *Phytochemistry*, 1976, 15, 559, (分離)  
 Hylands, P.J. et al., *Phytochemistry*, 1982, 21, 2703, (分離, 構造決定)  
 Ahmad, M.U. et al., *Phytochemistry*, 1994, 36, 421, (分離)

§ 3,25-Dihydroxycucurbit-5-ene-11,24-dione; 3  $\beta$ -form

[化学名・別名] Bryosigenin  
 [CAS No.] 5532-38-7  
 [化合物分類] テルペノイド (Cucurbitane triterpenoids)  
 [構造式]  
 [分子式]  $C_{30}H_{48}O_4$   
 [分子量] 472.707  
 [基原] *Bryonia dioica*  
 [性状] 結晶 (MeOH)  
 [融点] Mp 188-191 °C  
 [比旋光度]:  $[\alpha]_D^{20} +144$  (c, 0.405 in  $CHCl_3$ )

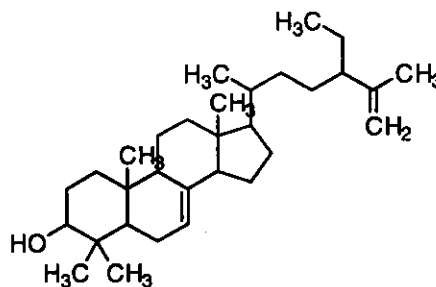


-----文献-----

Tunmann, P. et al., *Naturwissenschaften*, 1965, 52, 661, (Bryosigenin)  
 Nakano, K. et al., *Phytochemistry*, 1995, 39, 209, (Cabenoside H)

§ 4,4-Dimethylstigmasta-7,25-dien-3-ol; (3  $\beta$ , 24S)-form

[化学名・別名] 4,4-Dimethylporiferasta-7,25-dien-3-ol  
 [化合物分類] テルペノイド (Lanostane triterpenoids),  
 ステロイド (Ergostane steroids; excluding withanolides and  
 brassinolides). (C28).  
 [構造式]



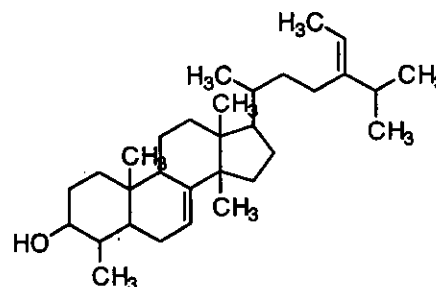
[分子式]  $C_{31}H_{52}O$   
 [分子量] 440.751  
 [基原] *Bryonia dioica*

-----文献-----

Akihisa, T. et al., *Chem. Pharm. Bull.*, 1996, 44, 1202-1207, (分離, H-NMR, Mass)

§ 4,14-Dimethylstigmasta-7,24(28)-dien-3-ol; (3  $\beta$ , 4  $\alpha$ , 5  $\alpha$ , 24(28)E)-form

[CAS No.] 178275-57-5  
 [化合物分類] ステロイド (Stigmastane steroids). (C29), テルペノイド (Lanostane triterpenoids)  
 [構造式]



[分子式]  $C_{31}H_{52}O$   
 [分子量] 440.751  
 [基原] *Bryonia dioica*  
 [性状] 結晶  
 [融点] Mp 161-162 °C

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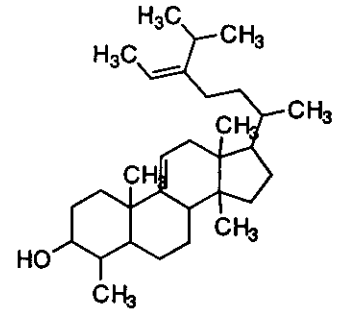
Akihisa, T. et al., *Chem. Pharm. Bull.*, 1996, 44, 1202-1207, (分離, H-NMR, C13-NMR, Mass)

§ 4,14-Dimethylstigmasta-9(11),24(28)-dien-3-ol; (3  $\beta$ , 4  $\alpha$ , 5  $\alpha$ , 24(28)E)-form

[CAS No.] 178275-58-6

[化合物分類] ステロイド (Stigmastane steroids). (C29). ,  
テルペノイド (Lanostane triterpenoids)

[構造式]



[分子式]  $C_{31}H_{52}O$

[分子量] 440.751

[基原] *Bryonia dioica*

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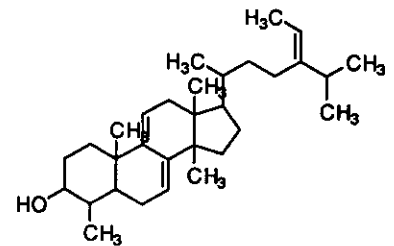
Akihisa, T. et al., *Phytochemistry*, 1989, 28, 1219

Akikisa, T. et al., *Chem. Pharm. Bull.*, 1996, 44, 1202, (分離, H-NMR, Mass)

§ 4,14-Dimethylstigmasta-7,9(11),24(28)-trien-3-ol; (3 $\beta$ ,4 $\alpha$ ,5 $\alpha$ ,24(28)*E*)-form

[化合物分類] テルペノイド (Lanostane triterpenoids),  
ステロイド (Stigmastane steroids). (C29).

[構造式]



[分子式]  $C_{31}H_{50}O$

[分子量] 438.735

[基原] *Bryonia dioica*

-----文献-----

Akihisa, T. et al., *Chem. Pharm. Bull.*, 1996, 44, 1202-1207, (分離, H-NMR, C13-NMR, Mass)

§ 3-Hydroxycucurbit-5-ene-11,24-dione; 3 $\beta$ -form

[化学名・別名] Bryogenin

[CAS No.] 2361-10-6

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

[構造式]

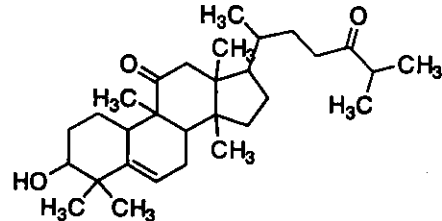
[分子式]  $C_{30}H_{48}O_3$

[分子量] 456.707

[基原] *Bryonia dioica* の配糖体

[性状] 結晶

[融点] Mp 157 °C



-----文献-----

Biglino, G. et al., *Tet. Lett.*, 1963, 1651, (分離, 構造決定)

Audier, H.E. et al., *Tet. Lett.*, 1966, 2205, (Mass)

§ *N*'-(2-Hydroxyethyl)asparagine; (*S*)-form

[化学名・別名] L-form

[CAS No.] 7175-33-9

[化合物分類] アミノ酸とペプチド (Non-protein  $\alpha$ -aminoacids)

[構造式]

[分子式]  $C_6H_{12}N_2O_4$

[分子量] 176.172

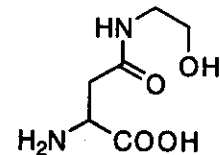
[基原] 次の植物に存在する: the vegetative parts and seeds of the squirting cucumber (*Ecballium elaterium*) and bryony (*Bryonia dioica*)

[性状] 結晶 (EtOH)

[融点] Mp 199-200 °C

[比旋光度]:  $[\alpha]_D^{20} +2.9$  (c, 5 in H<sub>2</sub>O)

[PKa 値] pK<sub>a1</sub> 2.32; pK<sub>a2</sub> 8.92



-----文献-----

Fowden, L. et al., *Biochem. J.*, 1961, 81, 154, (分離)

Fowden, L. et al., *Phytochemistry*, 1965, 4, 933  
Fowden, L. et al., *J.C.S. (C)*, 1971, 833, (絶対構造)

§ 3-Hydroxy-7,9(11)-multifloradien-29-oic acid; 3  $\alpha$ -form

[CAS No.] 74513-34-1

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

[構造式]

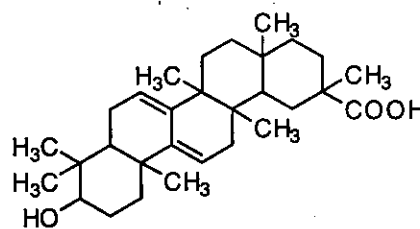
[分子式]  $C_{30}H_{46}O_3$

[分子量] 454.682

[基原] *Bryonia dioica*

[性状] 結晶 (EtOAc)

[融点] Mp 204-206 °C



-----文献-----

Hylands, P.J. et al., *Phytochemistry*, 1979, 18, 1843

Hylands, P.J. et al., *J.C.S. Perkin 1*, 1980, 2933

§ 3-Hydroxy-7,9(11)-multifloradien-29-oic acid; 3  $\alpha$ -form, 3-(4-Hydroxycinnamoyl)

[化学名・別名] Bryocoumaric acid

[CAS No.] 76475-14-4

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

[構造式]

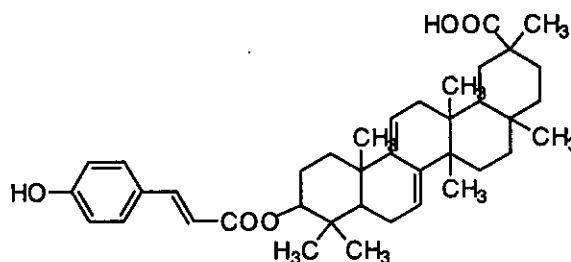
[分子式]  $C_{35}H_{52}O_5$

[分子量] 600.837

[基原] *Bryonia dioica*

[性状] Foam

[融点] Mp 143-145 °C



-----文献-----

Hylands, P.J. et al., *Phytochemistry*, 1979, 18, 1843

Hylands, P.J. et al., *J.C.S. Perkin 1*, 1980, 2933

§ 3-Hydroxy-8-multifloren-29-oic acid; 3  $\beta$ -form

[化学名・別名] Bryonolic acid

[CAS No.] 24480-45-3

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

[構造式]

[分子式]  $C_{30}H_{48}O_3$

[分子量] 456.707

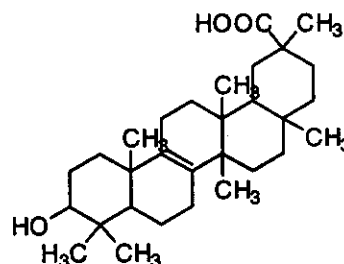
[基原] *Bryonia dioica*, *Sandoricum indicum*

[用途] 抗アレルギー薬

[性状] 結晶 (EtOAc)

[融点] Mp 300-303 °C

[比旋光度]:  $[\alpha]_D^{25} +24$  (c, 2.53 in Py)



-----文献-----

Cho, H.J. et al., *Phytochemistry*, 1992, 31, 3893, (生育)

Tabata, M. et al., *J. Nat. Prod.*, 1993, 56, 165, (分離, 用途)

Cho, H.J. et al., *Phytochemistry*, 1993, 33, 1407, (生合成)

Kosela, S. et al., *Phytochemistry*, 1995, 38, 691, (Bryononic acid, H-NMR, C13-NMR, 結晶構造)

§ 3-Hydroxy-8-multifloren-29-oic acid; 3  $\beta$ -form, Ac

[CAS No.] 24480-46-4

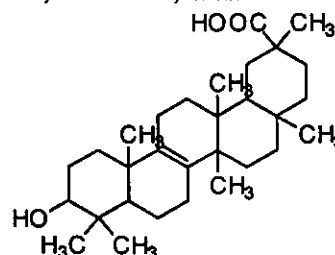
[化合物分類]テルペノイド (Multiflorane triterpenoids)

[構造式]

[分子式]  $C_{32}H_{50}O_4$

[分子量] 498.745

[基原] *Bryonia dioica* の発芽中の種子



-----文献-----