

\*\*\*\*\*ブルーベリー (Blueberry) \*\*\*\*\*

§ § ツツジ科クロマメノキ (*Vaccinium uliginosum* L.) の果実。

本調査研究では、成分に関する文献はなかった。

§ § ツツジ科ビルベリー (*Vaccinium myrtillus* L.) の果実。

§ Avicularin

[化学名・別名] 3-( $\alpha$ -L-Arabinofuranosyloxy)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one (CAS 名). Quercetin 3- $\alpha$ -L-arabinofuranoside. Avicularoside. Fenicularin

[CAS No.] 572-30-5

[関連 CAS No.] 119786-64-0

[化合物分類] フラボノイド (Flavonols; 5 × O-置換基), 炭水化物 (Miscellaneous carbohydrate antibiotics)

[構造式]

[分子式]  $C_{20}H_{18}O_{11}$

[分子量] 434.356

[基原] *Polygonum aviculare*, *Vaccinium myrtillus*, *Juglans regia*, 等

[性状] 黄色の針状結晶 + H<sub>2</sub>O (EtOH 溶液)

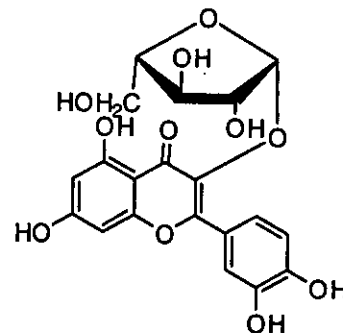
[融点] Mp 217 °C (無水物 222 °C)

[比旋光度]:  $[\alpha]_D^{20}$  -241 (c, 0.138 in MeOH) → -116 (24 hr)

[溶解性] BERDY SOL: エタノール, 塩基に可溶; エーテルに易溶; 水, ヘキサンに難溶

UV: [neutral]  $\lambda_{max}$  260 ( $\epsilon$  20900); 360 ( $\epsilon$  17400) (EtOH) (Berdy)

[その他のデータ] Identity of Fenicularin from *Foeniculum vulgare* with Avicularin not fully establ. (same struct. assigned but higher Mp. (256 °C) given)



----- 文献 -----

Ohta, T., Hoppe Seyler's Z. Physiol. Chem., 1940, 263, 221, (分離, 構造決定)

El Khadem, H. et al., J.C.S., 1958, 3320, (分離)

§ *p*-Menth-1-en-9-ol

[CAS No.] 18479-68-0

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

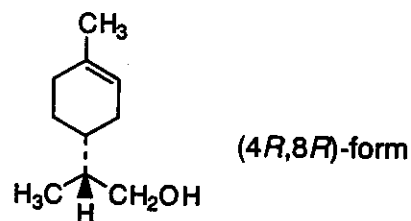
[構造式]

[分子式]  $C_{10}H_{18}O$

[分子量] 154.252

[基原] *Vaccinium myrtillus* (bilberry) and tangerine oil

[販売元] Aldrich:18374-1



----- 文献 -----

Schulte-Elte, K.H. et al., Helv. Chim. Acta, 1966, 49, 2150

Pawson, B.A. et al., J.A.C.S., 1970, 92, 336, (合成法, H-NMR)

§ Octahydro-4-methyl-2H-quinolizin-2-one; (4*R*,9*aR*)-form

[化学名・別名] Myrtine

[CAS No.] 66835-10-7

[化合物分類] アルカロイド化合物 (Quinolizidine alkaloids; 2 × rings)

[構造式]

[分子式]  $C_{10}H_{17}NO$

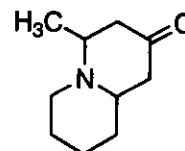
[分子量] 167.25

[基原] 次の植物から得られるアルカロイド: *Vaccinium myrtillus* の地上部 (ツツジ科)

[性状] オイル

[比旋光度]:  $[\alpha]_D^{20}$  +3.1 (c, 2.1 in CHCl<sub>3</sub>) (天然物).  $[\alpha]_D^{23}$  +11.3 (c, 2.7 in CHCl<sub>3</sub>) (合成品)

[その他のデータ] Isol. sample has only 25% opt. purity. This is not due to isom. during isol.



----- 文献 -----

Slosse, P. et al., Tetrahedron, 1981, 37, 4287, (分離, IR, Mass, H-NMR, C13-NMR, 合成法, 分割)

§ Octahydro-4-methyl-2H-quinolizin-2-one; (4*R*,9*aS*)-form

[化学名・別名] Epimyrtine

[CAS No.] 82111-02-2

[化合物分類] アルカロイド化合物 (Quinolizidine alkaloids; 2 × rings)

[構造式]

[分子式] C<sub>10</sub>H<sub>17</sub>NO

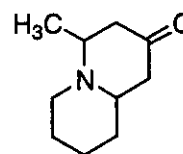
[分子量] 167.25

[基原] 次の植物から得られるアルカロイド: *Vaccinium myrtillus* (ツツジ科)

[性状] オイル

[比旋光度]: [α]<sub>D</sub><sup>20</sup> -2.5 (c, 1.2 in CHCl<sub>3</sub>) (天然物). [α]<sub>D</sub><sup>23</sup> -18 (c, 5.2 in CHCl<sub>3</sub>) (合成品)

[その他のデータ] Low opt. purity



-----文献-----

Slosse, P. et al., *Tetrahedron*, 1981, 37, 4287, (分離, IR, Mass, H-NMR, C13-NMR, 合成法, 分割)  
Pilli, R.A. et al., *J.O.C.*, 1995, 60, 717, (合成法)

§ § ツツジ科ローブッシュ・ブルーベリー (*Vaccinium angustifolium* Aiton) の果実。

本調査研究では、成分に関する文献はなかった。

\*\*\*\*\*ブレッドフルーツ (Breadfruit) \*\*\*\*\*

§ § クワ科パンノキ (*Artocarpus altilis* Fosb.) の果実または材。

§ **Cudraflavone A**

[化学名・別名] Isocyclomorusin

[CAS No.] 96843-73-1

[化合物分類] フラボノイド (Cyclised C-isopentenylated flavonoids),  
フラボノイド (Flavones; 3 × O-置換基)

[構造式]

[分子式] C<sub>25</sub>H<sub>22</sub>O<sub>6</sub>

[分子量] 418.445

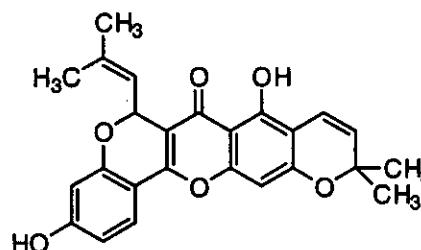
[基原] *Cudrania tricuspidata*. また *Artocarpus altilis* から分離される

[性状] 結晶

[融点] Mp 265-272 °C (244-245 °C)

[比旋光度]: [α]<sub>D</sub><sup>19</sup> +27.3 (c, 0.147 in CHCl<sub>3</sub>). [α]<sub>D</sub><sup>25</sup> +30 (c, 0.29 in Me<sub>2</sub>CO)

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



-----文献-----

Fujimoto, T. et al., *Planta Med.*, 1984, 50, 218, (分離, 構造決定)  
Messana, I. et al., *Planta Med.*, 1987, 53, 541, (誘導体)  
Chen, C.-C. et al., *J. Nat. Prod.*, 1993, 56, 1594, (分離, H-NMR, C13-NMR)

§ **Cycloartocarpin; O-De-Me**

[化学名・別名] Cyclocommunin. Isocyclomulberrin

[CAS No.] 145682-71-9

[化合物分類] フラボノイド (Cyclised C-isopentenylated  
flavonoids), フラボノイド (Flavones; 4 × O-置換基)

[構造式]

[分子式] C<sub>25</sub>H<sub>24</sub>O<sub>6</sub>

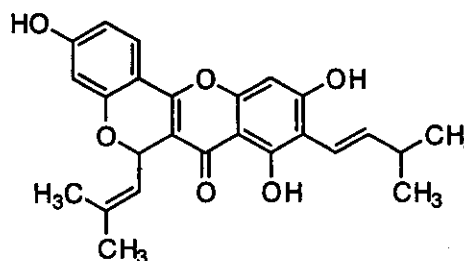
[分子量] 420.461

[基原] 次の植物から分離: *Artocarpus communis* の根皮,  
*Artocarpus altilis* の茎

[性状] 黄色の粉末 (C<sub>6</sub>H<sub>6</sub>)

[融点] Mp 277-279 °C (270-271 °C)

[比旋光度]: [α]<sub>D</sub><sup>25</sup> +53 (c, 0.31 in Me<sub>2</sub>CO)



-----文献-----

Lin, C.N. et al., *Phytochemistry*, 1992, 31, 2922, (Cyclocommunin)  
Chen, C.C. et al., *J. Nat. Prod.*, 1993, 56, 1594, (Isocyclomulberrin)

### § Cyclomorusin

[化学名・別名] 6,11-Dihydroxy-3,3-dimethyl-8-(2-methyl-1-propenyl)-3*H*,7*H*,8*H*-bis[1] benzopyrano [4,3-*b*:6',5'-*e*] pyran-7-one (CAS名). Cyclomulberochromene

[CAS No.] 62596-34-3

[化合物分類] フラボノイド (Cyclised C-isopentenylated flavonoids), フラボノイド (Flavones; 4 × O-置換基)

[構造式]

[分子式] C<sub>25</sub>H<sub>22</sub>O<sub>6</sub>

[分子量] 418.445

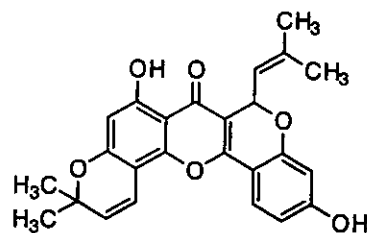
[基原] 次の植物の根皮から分離: *Morus alba*. また *Artocarpus altilis* から得られる

[性状] 淡黄色のプリズム結晶 (MeOH)

[融点] Mp 256-257 °C (233-234 °C)

[比旋光度]: [α]<sub>D</sub><sup>20</sup> +20 (c, 0.15 in MeOH)

UV: [neutral] λ<sub>max</sub> 223 (ε 28300); 283 (ε 27000); 353 (ε 15400) (MeOH) (Berdy)



-----文献-----

Deshpande, V.H. et al., Indian J. Chem., 1974, 12, 431, (分離)

Nomura, T. et al., Chem. Pharm. Bull., 1976, 24, 2898; 1978, 26, 1394, (分離)

Nomura, T. et al., Heterocycles, 1979, 12, 1289, (構造決定)

Nomura, T. et al., Planta Med., 1983, 49, 90, (分離)

Chen, C.-C. et al., J. Nat. Prod., 1993, 56, 1594, (分離, H-NMR)

Lin, C.-N. et al., Phytochemistry, 1996, 41, 1215, (C13-NMR)

### § Cyclomulberrin

[化学名・別名] 3,8,10-Trihydroxy-11-(3-methyl-2-butenyl)-6-(2-methyl-1-propenyl)-6*H*,7*H*-[1] benzopyrano [4,3-*b*] [1] benzopyran-7-one (CAS名)

[CAS No.] 19275-51-5

[化合物分類] フラボノイド (Cyclised C-isopentenylated flavonoids), フラボノイド (Flavones; 4 × O-置換基)

[構造式]

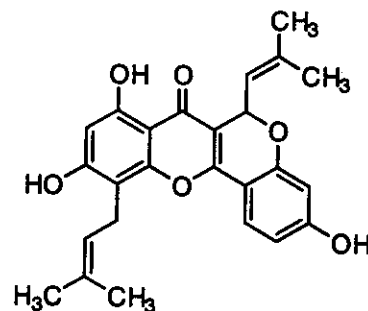
[分子式] C<sub>25</sub>H<sub>24</sub>O<sub>6</sub>

[分子量] 420.461

[基原] 次の植物の樹皮から分離: *Morus* spp. また *Artocarpus altilis* から分離される

[融点] Mp 231-232 °C. Mp 245-246 °C

UV: [neutral] λ<sub>max</sub> 214 (ε 39600); 274 (ε 21000); 370 (ε 16000) (EtOH) (Berdy)



-----文献-----

Deshpande, V.H. et al., Tet. Lett., 1968, 1715, (分離)

Deshpande, V.H. et al., Indian J. Chem., 1972, 10, 681; 1974, 12, 431, (分離)

Nomura, T. et al., Heterocycles, 1979, 12, 1289, (構造決定)

Lin, C.-N. et al., Phytochemistry, 1992, 31, 2922, (Dihydroisocycloartomunin)

Chen, C.-C. et al., J. Nat. Prod., 1993, 56, 1594, (Cycloaltilisin)

Lin, C.-N. et al., Phytochemistry, 1996, 41, 1215, (C13-NMR, Dihydroisocycloartomunin)

### § Cyclomulberrin; 5'-Hydroxy, 4'-Me ether

[化学名・別名] Cycloaltilisin

[CAS No.] 152130-62-6

[化合物分類] フラボノイド (Flavones; 5 × O-置換基), フラボノイド (Cyclised C-isopentenylated flavonoids)

[構造式]

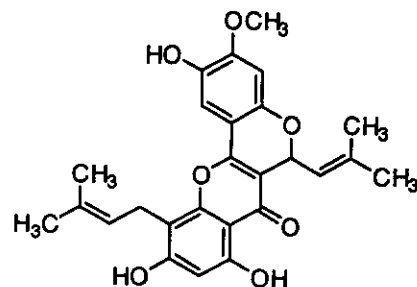
[分子式] C<sub>26</sub>H<sub>26</sub>O<sub>7</sub>

[分子量] 450.487

[基原] *Artocarpus altilis*

[融点] Mp 186-188 °C

[比旋光度]: [α]<sub>D</sub><sup>25</sup> +99 (c, 0.36 in Me<sub>2</sub>CO)



-----文献-----

Chen, C.-C. et al., J. Nat. Prod., 1993, 56, 1594, (Cycloaltilisin)

§ 2',4',5,5',7-Pentahydroxy-3,8-diprenylflavone

[化学名・別名] 5,7-Dihydroxy-3,8-bis(3-methyl-2-butenyl)-2-(2,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one (CAS名). Artonin V

[CAS No.] 158642-43-4

[化合物分類] フラボノイド (Flavones; 5 × O-置換基)

[構造式]

[分子式] C<sub>23</sub>H<sub>26</sub>O<sub>7</sub>

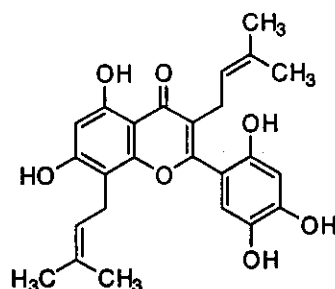
[分子量] 438.476

[基原] *Artocarpus altilis* (クワ科) の根皮

[性状] 青白い黄色の針状結晶 (hexane/Et<sub>2</sub>O)

[融点] Mp 85-87 °C

UV: [neutral] λ<sub>max</sub> 206; 263; 301; 341 (MeOH)



-----文献-----

Hano, Y. et al., J. Chem. Res., Synop., 1994, 348, (分離, IR, UV, H-NMR, C13-NMR)

§ § クワ科パラミツ (*Artocarpus heterophylla* Lam.) の果実または材。

§ Chaplashin

[化学名・別名] 6,7-Dihydro-3,9-dihydroxy-6-(1-hydroxy-1-methylethyl)-11-methoxy-10-(3-methyl-1-butenyl)-8H-1-benzopyrano[3,2-d][1]benzoxepin-8-one (CAS名). Artonin S

[CAS No.] 40413-47-6

[化合物分類] フラボノイド (Flavones; 4 × O-置換基), フラボノイド (Cyclised C-isopentenylated flavonoids)

[構造式]

[分子式] C<sub>26</sub>H<sub>28</sub>O<sub>7</sub>

[分子量] 452.503

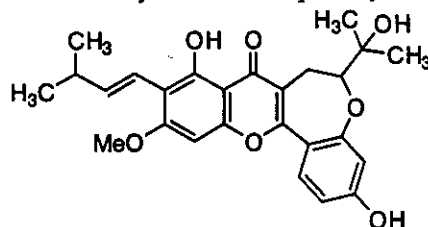
[一般的性質] Stereochemical identity of Chaplashin and Artonin S not demonstrated

[基原] *Artocarpus chaplasha* と *Artocarpus heterophylla* の心材

[性状] 黄色の針状結晶 (MeOH or EtOAc)

[融点] Mp 250 °C (236-238 °C)

[比旋光度]: [α]<sub>D</sub><sup>25</sup> +10 (c, 0.2 in MeOH)



-----文献-----

Rao, A.V.R. et al., Indian J. Chem., 1972, 10, 905; 989, (Chaplashin)

Aida, M. et al., Heterocycles, 1994, 39, 847, (Artonin S)

Hakim, E.H. et al., J. Nat. Prod., 1999, 62, 613-615, (Artoindonesianin B)

\*\*\*\*\*ヘイ (Hay) \*\*\*\*\*

§ § セリ科セリ (*Prangos pabularia* Lindl.) の果実

§ Aviprin; (R)-form, 3'-O-β-D-Glucopyranoside

[CAS No.] 73485-83-3

[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>22</sub>H<sub>26</sub>O<sub>11</sub>

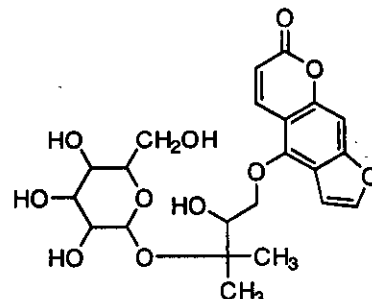
[分子量] 466.441

[基原] *Prangos pabularia*

[性状] 結晶

[融点] Mp 250-253 °C

[比旋光度]: [α]<sub>D</sub><sup>30</sup> -30 (H<sub>2</sub>O)



-----文献-----

Nielsen, B.E. et al., Acta Chem. Scand., 1964, 18, 1379; 1969, 23, 962, (構造決定, 絶対構造)

Gupta, B.D. et al., Indian J. Chem., 1964, 2, 464, (分離)

- Nikonov, G.K. et al., Zh. Obshch. Khim., 1964, 34, 1353; J. Gen. Chem. USSR (Engl. Transl.), 1964, 34, 1353, (分離)  
 Méndez, J. et al., Experientia, 1973, 29, 371, (分離, UV)  
 Atkinson, E. et al., Phytochemistry, 1974, 13, 853, (分離)  
 Khaled, S.A. et al., Phytochemistry, 1975, 14, 1461, (分離)  
 Reisch, J. et al., Phytochemistry, 1975, 14, 1889, (分離)  
 Ivie, G.W. et al., J. Agric. Food Chem., 1978, 26, 1394, (分離, H-NMR, Mass, 誘導體)  
 Kerimov, S.S. et al., Khim. Prir. Soedin., 1978, 14, 396; 1979, 15, 92; Chem. Nat. Compd. (Engl. Transl.), 1978, 14, 331; 1979, 15, 77, (分離)  
 Koul, S.K. et al., Phytochemistry, 1979, 18, 1762, (配糖体)  
 Harkar, S. et al., Phytochemistry, 1984, 23, 419, (分離, IR, H-NMR, C13-NMR)

### § Heraclenol; (±)-form

[化合物分類] ベンゾピラノイド (7,8-Dioxygenated coumarins), ベンゾピラノイド (Furanocoumarins)  
 [構造式] とるに足らない誘導體. 有効な構造式はない  
 [基原] 次の植物から分離: *Prangos pabularia*, *Prangos serawschanica*  
 [性状] 結晶 (Et<sub>2</sub>O/petrol)  
 [融点] Mp 128-129 °C

#### ----- 文献 -----

- Gupta, B.D. et al., Indian J. Chem., 1964, 2, 464, (分離)  
 Sharma, Y.N. et al., Naturwissenschaften, 1964, 51, 537, (分離)  
 Nielsen, B.E. et al., Acta Chem. Scand., 1969, 23, 962, (構造)  
 Sokolova, A.I. et al., Khim. Prir. Soedin., 1969, 5, 359; Chem. Nat. Compd. (Engl. Transl.), 1969, 5, 299, (Tomasin)  
 Bandopadhyay, M. et al., Indian J. Chem., 1970, 8, 855; 1146; 1973, 11, 530, (分離, 合成法)  
 González, A.G., An. Quim., 1974, 70, 856; 1976, 72, 584; 1977, 73, 858, (誘導體)  
 Ivie, G.W. et al., J. Agric. Food Chem., 1978, 26, 1394, (分離)  
 Razdan, T.K. et al., Phytochemistry, 1982, 21, 923, (分離, IR, UV, H-NMR, Mass)  
 Harkar, S. et al., Phytochemistry, 1984, 23, 419, (分離, IR, Mass)  
 Sun, H. et al., Pharmazie, 1986, 41, 888  
 Elgmal, M.H.A. et al., Phytochemistry, 1993, 34, 819, (2'-Ac)  
 Trani, M. et al., Gazz. Chim. Ital., 1997, 127, 415-418, (分離, S-form)  
 Zhou, P. et al., Phytochemistry, 2000, 53, 689-697, (Fesumtuorin B)

### § 7-Hydroxy-6-prenylcoumarin; Me ether

[化学名・別名] 7-Methoxy-6-(3-methyl-2-butenyl)-2H-1-benzopyran-2-one (CAS名).  
 7-Methoxy-6-prenylcoumarin. Suberosin

[CAS No.] 581-31-7

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

[構造式]

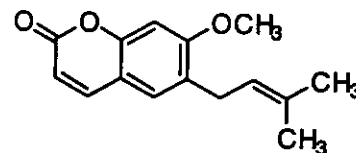
[分子式] C<sub>15</sub>H<sub>16</sub>O<sub>3</sub>

[分子量] 244.29

[基原] 次の植物から分離: *Zanthoxylum* spp., *Hesperethusa crenulata*, *Prangos pabularia*, *Seseli indicum*, *Platitenia absinthifolia*

[性状] プリズム結晶 (MeOH)

[融点] Mp 87-88 °C



#### ----- 文献 -----

- Mali, R.S. et al., Chem. Comm., 1994, 251, (合成法, Suberosin)  
 Masuda, T. et al., Phytochemistry, 1998, 47, 13-16, (分離, UV, H-NMR, C13-NMR)

### § Pabularinone

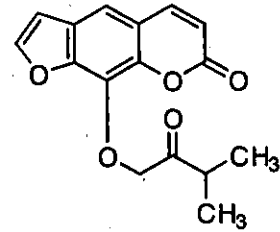
[化学名・別名] 9-(3-Methyl-2-oxobutoxy)-7H-furo[3,2-g][1]-benzopyran-7-one (CAS名). 9-(3-Methyl-2-oxobutoxy)-7-oxofuro[3,2-g]chromene. Isoheraclenin. Isoprangenin. Prangenone. Isooxyimperatorin

[CAS No.] 4889-31-0

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

[構造式]

[分子式]  $C_{16}H_{14}O_5$   
 [分子量] 286.284  
 [基原] *Prangos pabularia*, *Heracleum candicans*, *Heracleum pyrenaicum*,  
*Peucedanum stenocarpum*  
 [性状] プリズム結晶 ( $C_6H_6$ /petrol)  
 [融点] Mp 131-132 °C

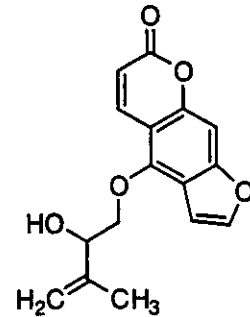


----- 文献 -----

Chatterjee, A. et al., *Tetrahedron*, 1972, 28, 5175, (分離, Mass, UV, H-NMR)  
 Bandopadhyay, M. et al., *Indian J. Chem.*, 1973, 11, 410, (分離)  
 González, A. et al., *An. Quim.*, 1976, 72, 584; *CA*, 85, 174282; 1977, 73, 1015; 88, 133243; 73, 1188; 89, 193816; 1978, 74, 637; 89, 176305, (分離)

§ Pabulenol; (S)-form

[CAS No.] 33889-70-2  
 [化合物分類] ベンゾピラノイド (5,7-Dioxygenated coumarins), ベンゾピラノイド (Furanocoumarins)  
 [構造式]  
 [分子式]  $C_{16}H_{14}O_5$   
 [分子量] 286.284  
 [基原] *Angelica apaensis*, *Cachrys sicula*, *Peucedanum ostruthium*, *Prangos pabularia*  
 [融点] Mp 134-135 °C  
 [比旋光度]:  $[\alpha]_D^{25}$  -3.8 (EtOH)

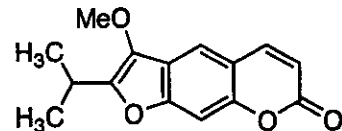


----- 文献 -----

Neilsen, B.E. et al., *Acta Chem. Scand.*, 1965, 19, 1810, (分離)  
 Abyshev, A.Z. et al., *Khim. Prir. Soedin.*, 1965, 5, 3; 1971, 7, 522; 1972, 8, 49; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, 5, 3; 1971, 7, 498; 1972, 8, 43, (分離, 合成法)  
 Ognyanov, I. et al., *Dokl. Bolg. Akad. Nauk*, 1971, 24, 315, (分離)  
 Basa, S.C. et al., *Tet. Lett.*, 1971, 1977, (分離)  
 Chatterjee, A. et al., *Tetrahedron*, 1972, 28, 5175, (分離)  
 Reisch, J. et al., *Phytochemistry*, 1975, 14, 1889, (分離)  
 Babu, K. et al., *Chem. Pharm. Bull.*, 1981, 29, 2565, (分離)  
 Méndez, J. et al., *Phytochemistry*, 1983, 22, 2599, (分離)  
 Grande, M. et al., *Phytochemistry*, 1986, 25, 505, (分離)

§ Peucedanin

[化学名・別名] 3-Methoxy-2-(1-methylethyl)-7H-furo[3,2-g][1]benzopyran-7-one (CAS 名).  
 2-Isopropyl-3-methoxy-7H-furo[3,2-g][1]benzopyran-7-one  
 [CAS No.] 133-26-6  
 [化合物分類] ベンゾピラノイド (7-Oxygenated coumarins, 6-substituted), ベンゾピラノイド (Furanocoumarins)  
 [構造式]  
 [分子式]  $C_{15}H_{14}O_4$   
 [分子量] 258.273  
 [基原] *Peucedanum officinale* とその他の *Peucedanum* spp. の根, *Prangos pabularia*  
 [性状] プリズム結晶もしくは板状結晶 ( $C_6H_6$ /petrol)  
 [融点] Mp 109 °C  
 [溶解性] BERDY SOL: メタノール, エーテルに可溶; 水に難溶  
 UV: [neutral]  $\lambda_{max}$  255 ( $\epsilon$  25120); 295 ( $\epsilon$  11220); 340 ( $\epsilon$  5010) (MeOH) (Berdy) [neutral]  $\lambda_{max}$  219 ( $\epsilon$  18620); 257 ( $\epsilon$  28840); 299 ( $\epsilon$  14120) (EtOH) (Berdy)  
 [その他のデータ] Toxic to fish  
 [傷害・毒性] BERDY HAZD: 50% 致死量 ( $LD_{50}$ ) (マウス, 経口) 315 mg/kg  
 [化学物質毒性データ総覧 (RTECS) 登録番号] LV1225000



----- 文献 -----

Spaumlth, E., *Ber.*, 1939, 72, 52, (構造決定, 成書)

Schmid, H. et al., Helv. Chim. Acta, 1951, 34, 1982, (合成法)

Gupta, B.K. et al., Indian J. Chem., 1964, 2, 464, (分離)

\*\*\*RTECS (化学物質毒性データ)\*\*\*

生体影響物質 : 医薬品.

\*\*\*健康障害に関するデータ\*\*\*

\*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 経口投与.

被験動物 : げっ歯類-マウス.

投与量・期間: 315 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

Voprosy Onkologii. Problems of Oncology. For English translation, see PONCAU. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) 43,1959

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 皮下投与.

被験動物 : げっ歯類-マウス.

投与量・期間: 100 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

Voprosy Onkologii. Problems of Oncology. For English translation, see PONCAU. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) 43,1959

### § Prangosine

[化学名・別名] 2-(1-Amino-1-methylethyl)-7H-furo[3,2-g][1]benzopyran-7-one (CAS 名)

[CAS No.] 15399-67-4

[化合物分類] アルカロイド化合物 (Miscellaneous acyclic alkaloids), ベンゾピラノイド (Furanocoumarins), ベンゾピラノイド (7-Oxygenated coumarins, 6-substituted)

[構造式]

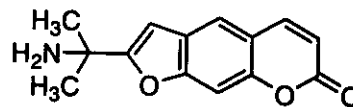
[分子式]  $C_{14}H_{13}NO_3$

[分子量] 243.262

[基原] 次の植物から得られるアルカロイド: *Prangos pabularia* (セリ科)

[性状] 結晶

[融点] Mp 131-132 °C



### ----- 文献 -----

Mukhamedova, K.S. et al., Khim. Prir. Soedin., 1967, 3, 117; 357; Chem. Nat. Compd. (Engl. Transl.), 1967, 3, 97; 303, (構造決定, Mass)

Akramov, S.T. et al., Khim. Prir. Soedin., 1967, 3, 287; Chem. Nat. Compd. (Engl. Transl.), 1967, 3, 243, (H-NMR)

### § *Prangos pabularia* Substance E

[化合物分類] 構造未知の天然物

[分子式]  $C_{16}H_{14}O_4$

[分子量] 270.284

[一般的性質] 構造式は未知. A coumarin

[基原] 次の植物の種子から分離: *Prangos pabularia*

[融点] Mp 109 °C

UV: [neutral]  $\lambda_{max}$  252 ; 312 (溶媒に関する報告はない)

[その他のデータ] Shows similar uv spectral props. to Osthol (Osthenol 参照)

### ----- 文献 -----

Markman, A.L. et al., Khim. Prir. Soedin., 1965, 1, 202; Chem. Nat. Compd. (Engl. Transl.), 1965, 1, 155

### § § イネ科ハルガヤ (*Anthoxanthum odoratum* L.) の全草

本調査研究では、成分に関する文献はなかった。

§ § イネ科コウボウ (*Hierochloa odorata* (L.) Beauvois var. *pabescens* Krylov.) の全草 (地上部)。  
本調査研究では、成分に関する文献はなかった。

\*\*\*\*\*ベイ (Bay) \*\*\*\*\*

§ § フトモ科ヤセイチョウジ (*Pimenta racemosa* (Miller) J. W. Moore (*Caryophyllus racemosus* Miller ; *P. acris* Kostel)) の枝葉, 果実。  
本調査研究では、成分に関する文献はなかった。

\*\*\*\*\*ヘザー (Heather) \*\*\*\*\*

§ § ツツジ科ギョウリュウモドキ (*Calluna vulgaris* Hull.) の花、葉及び樹皮。

§ Astragalin; 6''-O-(2,3,4-Tri-O-acetyl- $\alpha$ -L-arabinopyranosyl)

[CAS No.] 151193-58-7

[化合物分類] フラボノイド (Flavonols; 4 × O-置換基)

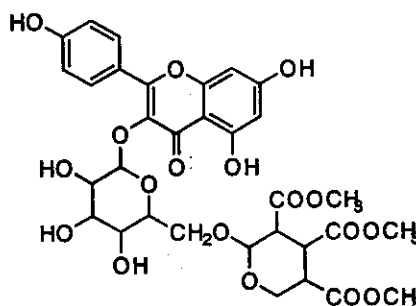
[構造式]

[分子式]  $C_{32}H_{34}O_{18}$

[分子量] 706.61

[基原] *Calluna vulgaris*

[性状] 青白い黄色の粉末



-----文献-----

The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

§ 5,7-Dihydroxy-4H-1-benzopyran-4-one; 7-O- $\beta$ -Glucopyranoside

[CAS No.] 60444-96-4

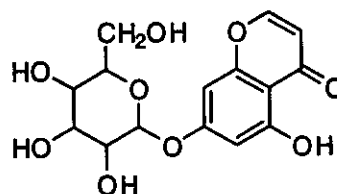
[化合物分類] ベンゾピラノイド (1-Benzopyrans)

[構造式]

[分子式]  $C_{15}H_{16}O_9$

[分子量] 340.286

[基原] *Calluna vulgaris*



-----文献-----

Pendse, R. et al., *Phytochemistry*, 1973, 12, 2033, (分離)

Simon, A. et al., *Phytochemistry*, 1994, 36, 1043, (7-glucoside)

Vasconcelos, J.M.J. et al., *Phytochemistry*, 1998, 49, 1421-1424, (分離, H-NMR, C13-NMR)

§ Hyperin; 6''-O-(2,3,4-Tri-O-acetyl- $\alpha$ -L-arabinopyranosyl)

[CAS No.] 157072-31-6

[化合物分類] フラボノイド (Flavonols; 5 × O-置換基)

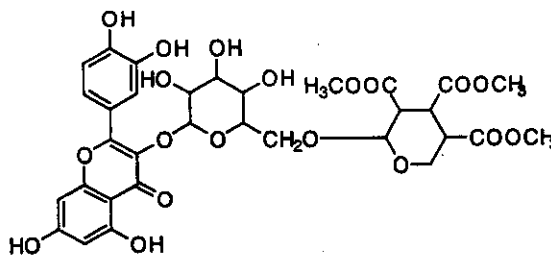
[構造式]

[分子式]  $C_{32}H_{34}O_{19}$

[分子量] 722.609

[基原] *Calluna vulgaris* の花

[性状] 青白い黄色の粉末



-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1531, (生育)

Hiller, K. et al., *Pharmazie*, 1979, 34, 192; 1981, 36, 377, (6''-arabinoside)

Riess-Maurer, I. et al., *Tetrahedron*, 1982, 38, 1269, (Quercetin 3-rhamnoside)

Hiller, K. et al., *Pharmazie*, 1984, 39, 51, (6''-glucoside)

Brasseur, T. et al., *Phytochemistry*, 1986, 25, 563, (6''-rhamnoside)



Finger, A. et al., *Phytochemistry*, 1991, 30, 2057, (6''-glucosylrhamnoside)  
El-Mousallamy, A.M.D., *Phytochemistry*, 1998, 48, 759-761, (6''-rhamnosylglucoside)

§ Isoquercitrin; 6''-O-(2,3,4-Tri-O-acetyl- $\alpha$ -L-arabinopyranosyl)

[CAS No.] 149507-87-9

[化合物分類] フラボノイド (Flavonols; 5 × O-置換基)

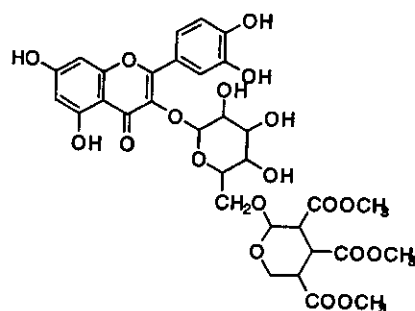
[構造式]

[分子式]  $C_{32}H_{34}O_{19}$

[分子量] 722.609

[基原] *Calluna vulgaris*

[性状] 黄色の粉末



----- 文献 -----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1531, (生育)

Kofinas, C. et al., *Phytochemistry*, 1998, 48, 637-641, (6''-diacetylramnosyl)

El-Sayed, N.H. et al., *Rev. Latinoam. Quim.*, 1998, 26, 30-35, (2''-glucuronosyl Et ester)

Beck, M.-A. et al., *Phytochemistry*, 1999, 50, 329-332, (6''-rhamnosylramnosyl)

§ Isoquercitrin; 6''-O-(2,3,5-Tri-O-acetyl- $\alpha$ -L-arabinofuranosyl)

[化合物分類] フラボノイド

(Flavonols; 5 × O-置換基)

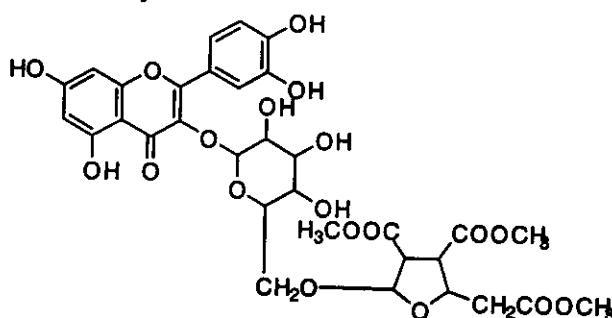
[構造式]

[分子式]  $C_{32}H_{34}O_{19}$

[分子量] 722.609

[基原] *Calluna vulgaris*

[性状] 黄色の無定型の塊



----- 文献 -----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1531, (生育)

Kofinas, C. et al., *Phytochemistry*, 1998, 48, 637-641, (6''-diacetylramnosyl)

Beck, M.-A. et al., *Phytochemistry*, 1999, 50, 329-332, (6''-rhamnosylramnosyl)

§ 5-Methyl-1,3-benzenediol; O- $\beta$ -D-Glucopyranoside

[化学名・別名] Sakakin

[CAS No.] 21082-33-7

[化合物分類] 単環芳香族 (Simple phenols)

[構造式]

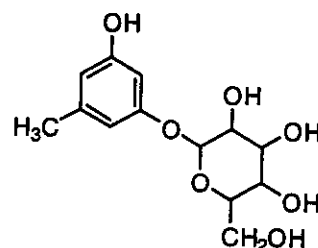
[分子式]  $C_{13}H_{16}O_7$

[分子量] 286.281

[基原] *Calluna vulgaris*, *Cleyera ochraceae*, *Curculigo orchoides*

[性状] 微細板状結晶 (MeOH/EtOH)

[融点] Mp 138 °C



----- 文献 -----

Yamada, T. et al., *Agric. Biol. Chem.*, 1968, 32, 599, (Sakakin)

§ 3,4,5,7,8-Pentahydroxyflavanone; (2R,3R)-form, 8-O- $\beta$ -D-Glucopyranoside

[化学名・別名] Callunin

[CAS No.] 83905-64-0

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

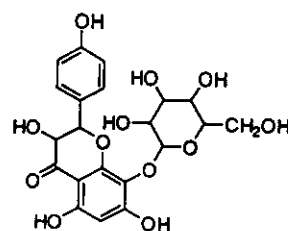
[構造式]

[分子式]  $C_{21}H_{22}O_{12}$

[分子量] 466.398

[基原] 次の植物から分離: *Calluna vulgaris*

[性状] 長針状結晶 (H<sub>2</sub>O)



[融点] Mp 187-188 °C

文献

Proksch, P. et al., *Planta Med.*, 1987, 53, 334, (誘導体)  
Parmar, V.S. et al., *Phytochemistry*, 1992, 31, 2185, (4',8-di-Me ether)  
Allais, D.P. et al., *Phytochemistry*, 1995, 39, 427, (2"-Acetylcallunin)

§ 3,4',5,7,8-Pentahydroxyflavanone; (2*R*,3*R*)-form, 8-*O*-(2-Acetyl-β-D-glucopyranoside)

[化学名・別名] 2"-Acetylcallunin

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

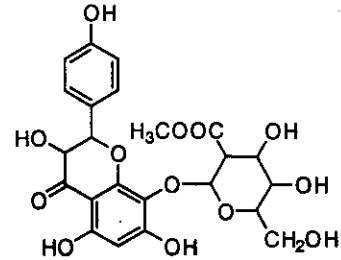
[構造式]

[分子式] C<sub>25</sub>H<sub>24</sub>O<sub>13</sub>

[分子量] 508.435

[基原] *Calluna vulgaris*

[性状] 粉末



文献

Allais, D.P. et al., *Phytochemistry*, 1995, 39, 427, (2"-Acetylcallunin)

§ 3,4',5,7,8-Pentahydroxyflavone; 8-*O*-β-D-Glucopyranoside

[化学名・別名] Herbacin †

[CAS No.] 11021-22-0

[化合物分類] フラボノイド (Flavonols; 5 × O-置換基)

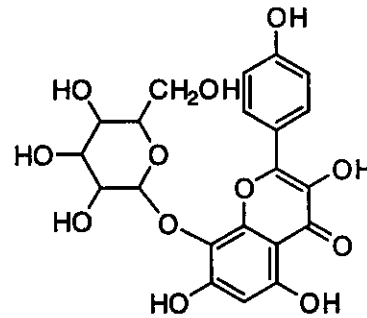
[構造式]

[分子式] C<sub>21</sub>H<sub>20</sub>O<sub>12</sub>

[分子量] 464.382

[基原] 次の植物から分離: *Calluna vulgaris*, *Limonium sinuatum*, *Althaea rosea*, その他の植物属

[融点] Mp 212-214 °C



文献

Parthasarathy, M.R. et al., *CA*, 1967, 66, 46558, (Herbacin)

Ross, S.A. et al., *Planta Med.*, 1980, 39, 187, (Herbacin)

§ 3,4',5,7,8-Pentahydroxyflavone; 8-*O*-[β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranoside]

[化学名・別名] Herbacetin 8-gentiobioside

[CAS No.] 69640-76-2

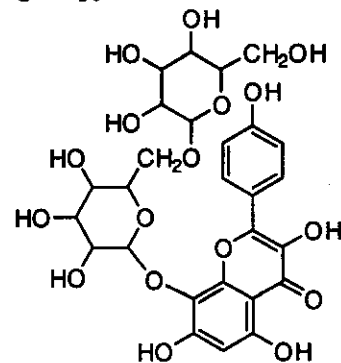
[化合物分類] フラボノイド (Flavonols; 5 × O-置換基)

[構造式]

[分子式] C<sub>27</sub>H<sub>30</sub>O<sub>17</sub>

[分子量] 626.524

[基原] 次の植物から分離: *Calluna vulgaris*



文献

Parthasarathy, M.R. et al., *CA*, 1967, 66, 46558, (Herbacin)

Ross, S.A. et al., *Planta Med.*, 1980, 39, 187, (Herbacin)

The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

§ 4',5,7,8-Tetrahydroxyflavanone; (S)-form, 8-*O*-β-D-Glucopyranoside

[化学名・別名] Isocarthamidin 8-glucoside. 3-Desoxycallunin

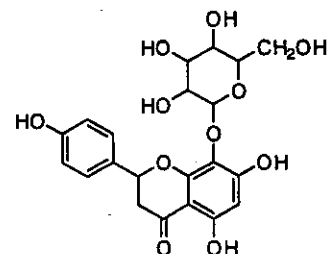
[化合物分類] フラボノイド (Flavanones; 4 × O-置換基)

[構造式]

[分子式] C<sub>21</sub>H<sub>22</sub>O<sub>11</sub>

[分子量] 450.398

[基原] *Calluna vulgaris*



-----文献-----

Allais, D.P. et al., *Phytochemistry*, 1995, 39, 427, (8-glucoside)

§ 4',5,7,8-Tetrahydroxyflavone

[化学名・別名] 5,7,8-Trihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one (CAS 名). Isoscutellarein.  
8-Hydroxyapigenin

[CAS No.] 41440-05-5

[関連 CAS No.] 107347-36-4, 129946-98-1

[化合物分類] フラボノイド (Flavones; 4 × O-置換基)

[構造式]

[分子式] C<sub>15</sub>H<sub>10</sub>O<sub>6</sub>

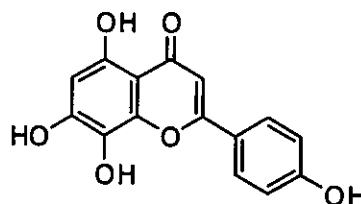
[分子量] 286.24

[基原] 次の植物から分離: *Pinguicula vulgaris*, *Calluna vulgaris*, Dikamali gum

[性状] 黄色の針状結晶 (AcOH 溶液)

[融点] Mp 247-248 °C. Mp 300-301 °C

UV: [neutral] λ<sub>max</sub> 286 ; 339 (MeOH) (Berdy)



-----文献-----

Tatum, J.H. et al., *Phytochemistry*, 1978, 17, 447, (4',5,7,8-Tetramethoxyflavone)

§ 3,5,7-Trihydroxyflavone; 3-Me ether, 7-O-β-D-glucopyranoside

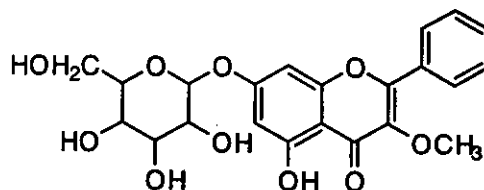
[化合物分類] フラボノイド (Flavonols; 3 × O-置換基)

[構造式]

[分子式] C<sub>22</sub>H<sub>22</sub>O<sub>10</sub>

[分子量] 446.41

[基原] 次の植物から分離: *Calluna vulgaris*



-----文献-----

Khimura et al., *Yakugaku Zasshi*, 1935, 55, 229, (分離)

Franca, N.C. et al., *Phytochemistry*, 1976, 15, 572, (3,5,7-Trimethoxyflavone)

Stepien, W.O. et al., *Pol. J. Chem. (Rocz. Chem.)*, 1978, 52, 2167, (3-Me ether, 7-glucoside)

Parmar, S.V. et al., *Indian J. Chem., Sect. B*, 1993, 32, 244, (合成法, 成書)

Deng, B.-L. et al., *Liebigs Ann./Recl.*, 1997, 2169-2175, (3-Me ether)

§ 4',5,7-Trihydroxyflavone; 7-O-(2-O-Acetyl-6-O-methyl-β-D-glucuronopyranoside)

[化学名・別名] Apigenin 7-(2-acetyl-6-methylglucuronide)

[CAS No.] 137162-04-0

[化合物分類] フラボノイド (Flavones; 3 × O-置換基)

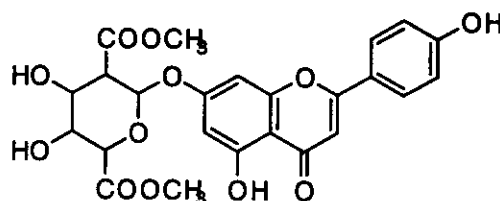
[構造式]

[分子式] C<sub>24</sub>H<sub>22</sub>O<sub>12</sub>

[分子量] 502.431

[基原] 次の植物から分離: *Calluna vulgaris*

[性状] 粉末



-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Jaipetch, T. et al., *Phytochemistry*, 1983, 22, 625, (4',5,7-Trimethoxyflavone)

*The Flavonoids: Advances in Research since 1980*, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

\*\*\*\*\*ヘーゼルナッツ (Hazelnut) \*\*\*\*\*

§ 8 カバノキ科セイヨウハシバミ (*Corylus avellana* L.) の種子 (焙煎)。

§ N<sup>1</sup>,N<sup>10</sup>-Dicoumaroylspermidine; 3' or 3''-Hydroxy, 3' or 3''-methoxy

[化学名・別名] Caffeoylferuloylspermidine

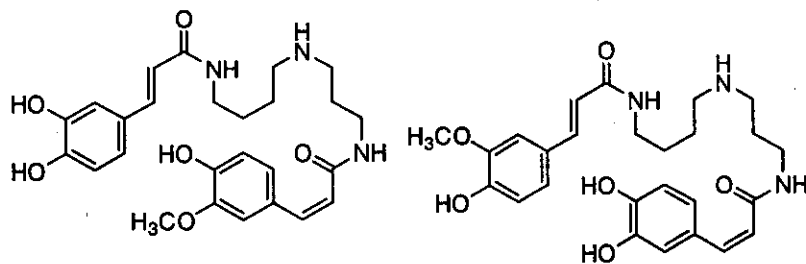
[化合物分類] アルカロイド化合物 (Acyclic spermidine alkaloids)

[構造式]

[分子式]  $C_{26}H_{33}N_3O_6$

[分子量] 483.563

[基原] 次の植物の花粉から得られるアルカロイド: *Corylus avellana* (Corylaceae)



-----文献-----

Delétang, J., Ann. Tab., Sect. 2, 1974, 11, 123; CA, 84, 147656m, (UV, H-NMR, 構造決定, Dicafeoylspermidine)

Cabanne, F. et al., Physiol. Veg., 1977, 15, 429; CA, 88, 86095m, (UV, 構造決定)

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

Meurer, B. et al., Phytochemistry, 1986, 25, 433, (Caffeoylferuloylspermidine, Diferuloylspermidine)

### § $N^1, N^6$ -Dicoumaroylspermidine; 3',3''-Dimethoxy

[化学名・別名]  $N^1, N^6$ -Diferuloylspermidine

[CAS No.] 70185-61-4

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

[構造式]

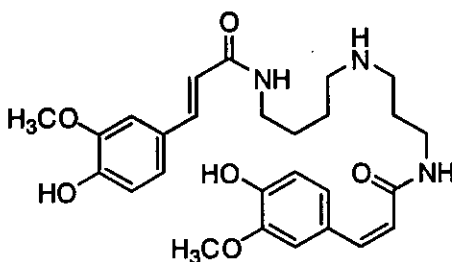
[分子式]  $C_{27}H_{35}N_3O_6$

[分子量] 497.59

[基原] 次の植物から得られるアルカロイド: *Corylus avellana* の花粉, また *Ananas comosus*, *Dianthus caryophyllus*, *Vicia faba*,

*Lunaria esculentum* から得られる (Corylaceae, パイナップル科, ナデシコ科, マメ科, ナス科)

[その他のデータ] Only the alkaloid from *C. avellana* has been shown to have the exact struct. shown. The other isolates are diferuloylspermidine with undefined regioisomerism (i.e. could be  $N^5$ -substituted)



-----文献-----

Delétang, J., Ann. Tab., Sect. 2, 1974, 11, 123; CA, 84, 147656m, (UV, H-NMR, 構造決定, Dicafeoylspermidine)

Meurer, B. et al., Phytochemistry, 1986, 25, 433, (Caffeoylferuloylspermidine, Diferuloylspermidine)

### § Hyperin; 2''-O-β-D-Glucopyranosyl

[CAS No.] 95043-15-5

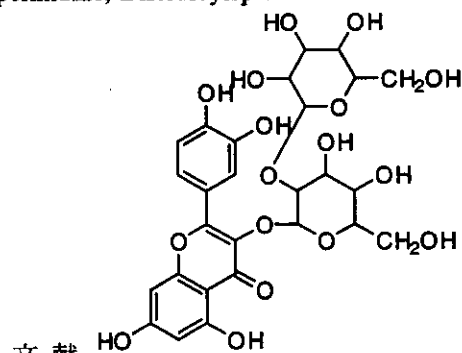
[化合物分類] フラボノイド (Flavonols; 5 × O-置換基)

[構造式]

[分子式]  $C_{27}H_{30}O_{17}$

[分子量] 626.524

[基原] 次の植物の花粉から分離: *Corylus avellana*



-----文献-----

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1531, (生育)

Strack, D. et al., Phytochemistry, 1984, 23, 2970, (2''-glucoside)

### § 20(29)-Lupene-3,28-diol; 3 β-form

[化学名・別名] Betulin. Betulinol (obsol.). Trochol

[CAS No.] 473-98-3

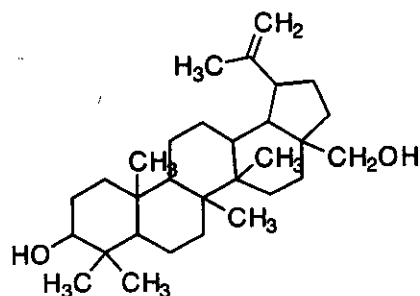
[化合物分類] テルペノイド (Lupane triterpenoids)

[構造式]

[分子式]  $C_{30}H_{50}O_2$

[分子量] 442.724

[基原] 樺の樹皮. また *Trochodendron aralioides*, *Corylus avellana*,



*Vicia faba*, その他多くの植物からも得られる。Isol. as a mixt. of acyl esters from archaeological resins

[性状] 結晶

[融点] Mp 251-252 °C

[比旋光度]:  $[\alpha]_D^{15} +20$  (Py)

[その他のデータ] 薬理的活性な異性体

[販売元] Aldrich:12376-5; Sigma:B9757

-----文献-----

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2024, (生育)

Siddiqui, S. et al., J. Nat. Prod., 1988, 51, 229-233, (Betulin, H-NMR, C13-NMR)

Hayek, E.W.H. et al., Phytochemistry, 1989, 28, 2229-2242, (レビュー)

Fuchino, H. et al., Chem. Pharm. Bull., 1995, 43, 1937-1942, (Betulin caffeate)

Lavoie, S. et al., Synth. Commun., 2001, 31, 1565-1571, (betulin, 分離, H-NMR, Mass)

§ Spermidine; *N*-(3,4-Dihydroxycinnamoyl), *N'*-(4-hydroxy-3-methoxycinnamoyl)

[化学名・別名] *N'*-Caffeoyl-*N''*-feruloylspermidine

[CAS No.] 101164-74-3

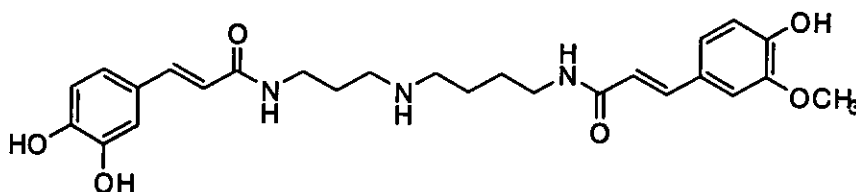
[化合物分類] アルカロイド  
化合物 (Acyclic spermidine  
alkaloids)

[構造式]

[分子式]  $C_{26}H_{31}N_3O_6$

[分子量] 483.563

[基原] 次の植物から得られるアルカロイド: *Corylus avellana* (Corylaceae) の花粉



-----文献-----

Meurer, B. et al., Phytochemistry, 1986, 25, 433, (*N*-Caffeoyl-*N''*-feruloylspermidine)

§ Stigmast-5-ene-3,7,22-triol; (3 $\alpha$ ,7 $\alpha$ ,22 $R$ ,24 $R$ )-form

[化学名・別名] Stigmastentriol

[化合物分類] AJ1550, ステロイド (Stigmastane steroids). (C<sub>29</sub>).

[構造式]

[分子式]  $C_{29}H_{50}O_3$

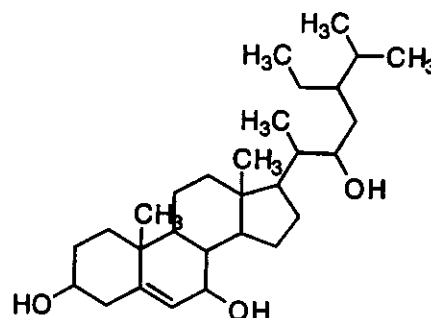
[分子量] 446.712

[基原] 次の植物から分離: *Aesculus hippocastanum* と *Corylus avellana* の葉

[性状] 針状結晶 (Me<sub>2</sub>CO/MeOH)

[融点] Mp 130-140 °C, 176-178 °C (double Mp)

[比旋光度]:  $[\alpha]_D^{20} -61.5$  (CHCl<sub>3</sub>)



-----文献-----

Fischer, F.G. et al., Annalen, 1960, 636, 88, (isol. struct)

Seiler, N. et al., Z. Naturforsch., B, 1966, 21, 78, (分離)

Pettit, G.R. et al., J. Nat. Prod., 2000, 63, 72-78, (Schleicherastatins, 結晶構造)

§ § カバノキ科ハシバミ (*Corylus heterophylla* Fischer) の種子 (焙煎)。

§ 2,3:4,6-Bis( hexahydroxydiphenoyl) glucose; ( *S,S* ) axial- $\beta$

-*D*-pyranose-form, 1-*O*-(3,4,5-Trihydroxybenzoyl)

[化学名・別名] 1-*O*-Galloyl-2,3:4,6-bis-(*S*)-hexahydroxydiphenoyl-

$\beta$ -*D*-glucopyranose. Casuarictin

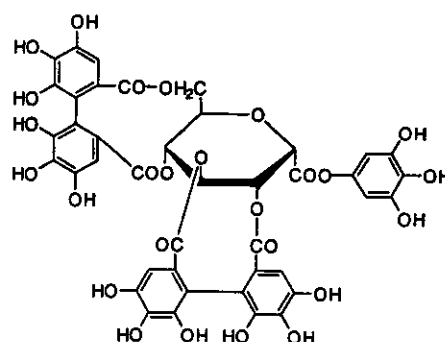
[CAS No.] 79786-00-8

[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] 次の植物から分離: *Casuarina stricta* の葉, *Stachyurus praecox*, *Corylus heterophylla*

[性状] 灰白色の無定型の粉末・六水和物

[比旋光度]:  $[\alpha]_D^{20} +35$  (c, 0.2 in MeOH)

-----文献-----

Okuda, T. et al., J.C.S. Perkin 1, 1983, 1765, (Casuarictin)

### § Casuarinin

[CAS No.] 79786-01-9

[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

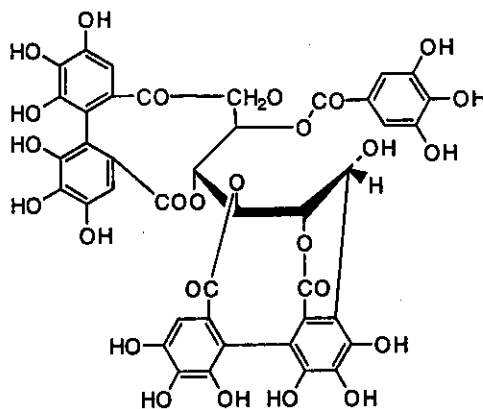
[基原] 次の植物から分離: *Casuarina stricta* の葉, *Stachyurus praecox*, *Corylus heterophylla*

[性状] 青白い黄色の無定型の粉末・七水和物

[比旋光度]:  $[\alpha]_D +43.6$  (c, 1 in MeOH)

UV: [neutral]  $\lambda_{max}$  221 ( $\epsilon$  74130); 267 ( $\epsilon$  32360) (MeOH)

(Berdy)



-----文献-----

Okuda, T. et al., Chem. Pharm. Bull., 1982, 30, 766, (構造決定, UV, H-NMR)

Feng, H. et al., Phytochemistry, 1988, 27, 1185, (Castanin)

Nonaka, G. et al., Chem. Pharm. Bull., 1990, 38, 2151, (構造決定, 絶対構造)

### § Heterophylliin B

[CAS No.] 135329-62-3

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

[分子式]  $C_{62}H_{56}O_{32}$

[分子量] 1873.313

[基原] An ellagitannin constit. of *Corylus heterophylla*

[性状] 灰白色の無定型の粉末・十二水和物

[比旋光度]:  $[\alpha]_D^{20} +141$  (c, 1.0 in MeOH)

-----文献-----

Yoshida, T. et al., Chem. Pharm. Bull., 1991, 39, 49, (構造決定, CD, H-NMR, C13-NMR)

### § Heterophylliin C

[CAS No.] 135308-98-4

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

[構造式]

[分子式]  $C_{67}H_{54}O_{32}$

[分子量] 1871.297

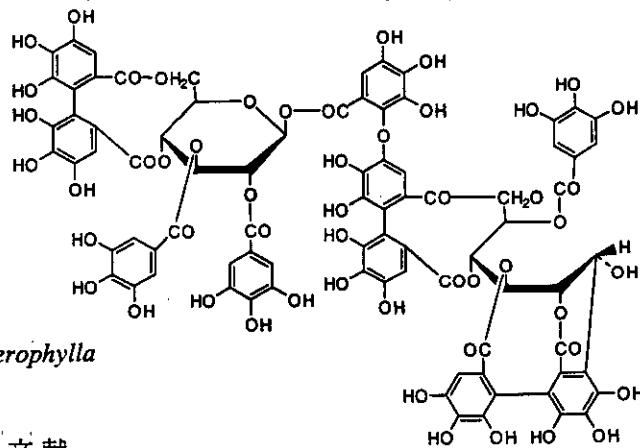
[基原] An ellagitannin from the leaf of *Corylus heterophylla*

[性状] 淡褐色の無定型の粉末・十五水和物

[比旋光度]:  $[\alpha]_D^{20} +101$  (c, 1.0 in MeOH)

-----文献-----

Yoshida, T. et al., Chem. Pharm. Bull., 1991, 39, 49, (構造決定, UV, CD, H-NMR, C13-NMR)

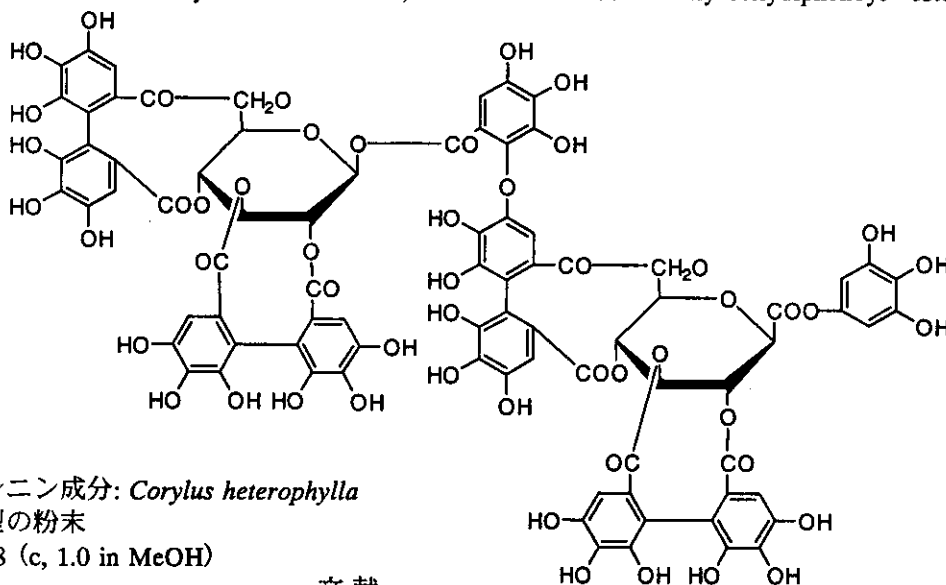


### § Heterophylliin D

[CAS No.] 135308-99-5

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

[構造式]



[分子式]  $C_{82}H_{54}O_{52}$

[分子量] 1871.297

[基原] 次の植物のタンニン成分: *Corylus heterophylla*

[性状] 灰白色の無定型の粉末

[比旋光度]:  $[\alpha]_D^{20} +78$  (c, 1.0 in MeOH)

文献

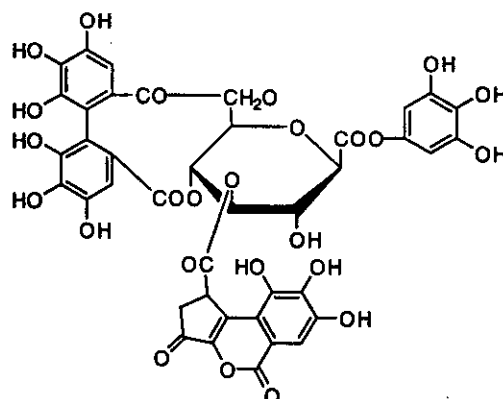
Yoshida, T. et al., Chem. Pharm. Bull., 1987, 35, 1817; 1991, 39, 49, (構造決定, UV, CD, H-NMR, C13-NMR)

### 8 Heterophyllin E

[CAS No.] 135309-00-1

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

[構造式]



[分子式]  $C_{40}H_{28}O_{25}$

[分子量] 908.646

[基原] 次の植物の葉から分離: *Corylus heterophylla*

[性状] 灰白色の無定型の粉末・七水和物

[比旋光度]:  $[\alpha]_D^{20} -36$  (c, 1.0 in MeOH)

文献

Yoshida, T. et al., Chem. Pharm. Bull., 1991, 39, 49, (構造決定, UV, CD, H-NMR, C13-NMR)

### 8 Heterophyllin G

[CAS No.] 211190-41-9

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

[構造式]

[分子式]  $C_{116}H_{78}O_{74}$

[分子量] 2655.848

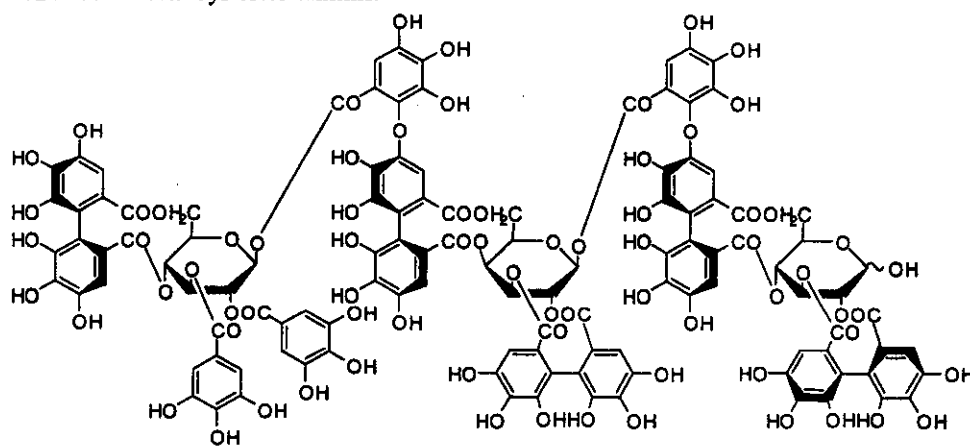
[基原] *Corylus heterophylla*

[性状] 無定型の淡褐色の粉末

[比旋光度]:  $[\alpha]_D +91.7$  (c, 1 in MeOH)

UV: [neutral]  $\lambda_{max}$  210 (log  $\epsilon$  5.58);

285 (log  $\epsilon$  5.24) (MeOH)



文献

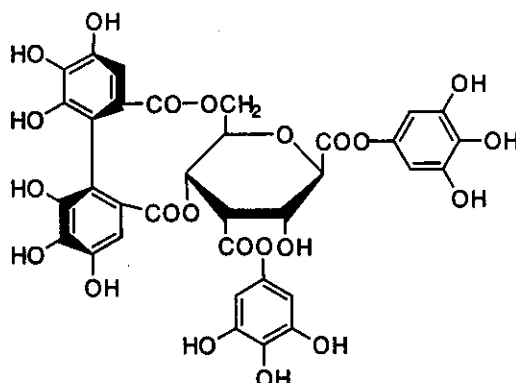
§ 4,6-Hexahydroxydiphenoylglucose; (S)-anti- $\alpha$ -D-Pyranose-form, 1,3-Bis-(3,4,5-trihydroxybenzoyl)

[化学名・別名] 1,3-Di-O-galloyl-4,6-(S)-hexahydroxydiphenoyl- $\alpha$ -D-glucopyranose. Heterophylliin A

[CAS No.] 87687-52-3

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

[構造式]



[分子式]  $C_{34}H_{26}O_{22}$

[分子量] 786.566

[基原] 次の植物の葉から分離: *Corylus heterophylla*

[性状] 灰白色の無定型の粉末・六水和物

[比旋光度]:  $[\alpha]_D^{20} +117$  (c, 0.6 in MeOH)

-----文献-----

Yoshida, T. et al., Chem. Pharm. Bull., 1991, 39, 49-54, (Heterophylliin A)

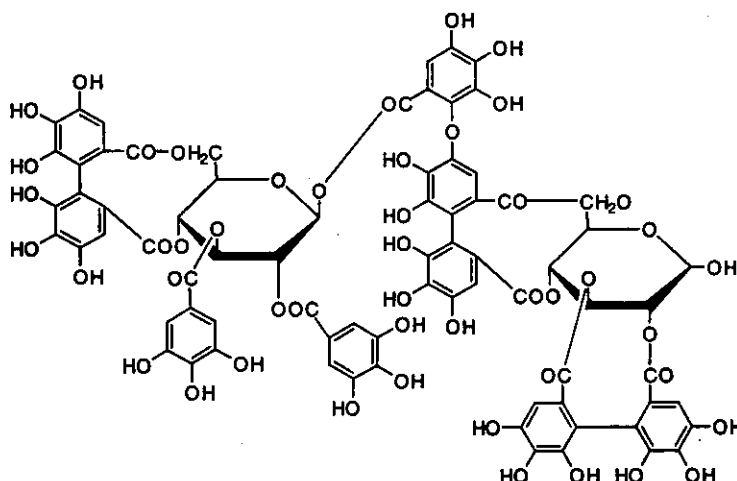
§ Rugosin F; 1-O-Degalloyl

[化学名・別名] Degalloylrugosin F

[化合物分類] タンニン化合物

(Valoneoyl ester tannins)

[構造式]



[分子式]  $C_{75}H_{52}O_{48}$

[分子量] 1721.207

[基原] 次の植物の葉から分離: *Corylus heterophylla*

[性状] 淡褐色の無定型の粉末

[比旋光度]:  $[\alpha]_D^{20} +96$  (c, 1.0 in MeOH)

[その他のデータ] 等量のアノマーの混合物

-----文献-----

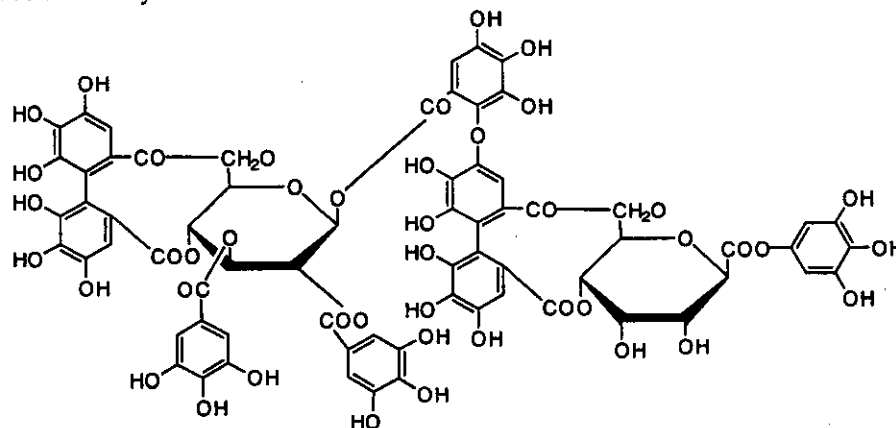
Yoshida, T. et al., Chem. Pharm. Bull., 1991, 39, 49, (Degalloylrugosin F)

§ Rugosin F; 2,3-De-O-(hexahydroxydiphenoyl)

[化学名・別名] Heterophylliin F

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

[構造式]



[分子式]  $C_{68}H_{50}O_{44}$

[分子量] 1571.117

[基原] *Corylus heterophylla*

[性状] 無定型の灰白色の粉末

[比旋光度]:  $[\alpha]_D +75.3$  (c, 1 in MeOH)

UV: [neutral]  $\lambda_{max}$  210 (log  $\epsilon$  5.34); 285 (log  $\epsilon$  4.98) (MeOH)

-----文献-----

Jin, Z.X. et al., Phytochemistry, 1998, 48, 333-338, (Heterophylliin F)



§ § カバノキ科フィルバート (*Corylus maxima* Miller) の種子 (焙煎)。  
本調査研究では、成分に関する文献はなかった。

\*\*\*\*\*ベチパー (Vetiver) \*\*\*\*\*

§ § イネ科ベチベルソウ (*Vetiveria zizanioides* Nash) の根または全草。

§ 3,9-Acoradiene

[CAS No.] 55781-50-5

[関連 CAS No.] 35944-18-4, 38229-83-3, 59573-57-8

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

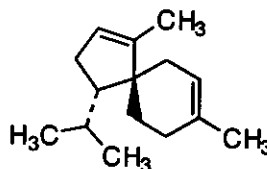
[構造式]

[分子式]  $C_{15}H_{24}$

[分子量] 204.355

[基原] ベチパーオイル (*Vetiveria zizanioides*)

[性状] オイル



----- 文献 -----

Kaiser, R. et al., Tet. Lett., 1972, 2009; 2013, (分離, 構造決定)

Zalkow, L.H. et al., Tet. Lett., 1975, 75, (絶対構造)

§ 3-Cedren-15-ol; (2 $\beta$ ,6 $\beta$ ,7 $\alpha$ ,10 $\alpha$ )-form

[CAS No.] 38229-89-9

[構造式]

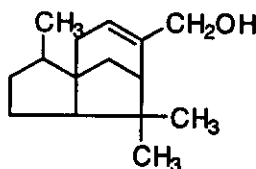
[分子式]  $C_{15}H_{24}O$

[分子量] 220.354

[基原] ベチパーオイル (*Vetiveria zizanioides*)

[性状] オイル

[沸点]  $Bp_{1.5}$  150 °C



----- 文献 -----

Singh, A.N. et al., Tetrahedron, 1969, 3855; 3866, (合成法)

Kaiser, R. et al., Tet. Lett., 1972, 13, 2009-2012, (*Vetiveria zizanioides* constits)

§ 3-Cedren-15-ol; (2 $\beta$ ,6 $\beta$ ,7 $\alpha$ ,10 $\alpha$ )-form, Aldehyde

[CAS No.] 38229-90-2

[構造式]

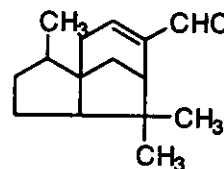
[分子式]  $C_{15}H_{22}O$

[分子量] 218.338

[基原] ベチパーオイル (*Vetiveria zizanioides*)

[性状] オイル

[沸点]  $Bp_{2.5}$  129-130 °C



----- 文献 -----

Kaiser, R. et al., Tet. Lett., 1972, 13, 2009-2012, (*Vetiveria zizanioides* constits)

\*\*\*\*\*ベーター (Betel) \*\*\*\*\*

§ § コシユウ科キンマ (*Piper betle* L.) の葉。

本調査研究では、成分に関する文献はなかった。

\*\*\*\*\*ベニノキ (Annatto) \*\*\*\*\*

§ § ベニノキ科ベニノキ (*Bixa orellana* L.) の種子。

§ 6'-Apo- $\psi$ -caroten-6'-oic acid; (9'Z)-form, Me ester

[化学名・別名] Methyl 6'-apo-9'Z-lycopen-6'-oate

[CAS No.] 174206-07-6

[化合物分類] テルペノイド (Apocarotenoids)

[構造式]

[分子式]  $C_{33}H_{44}O_2$

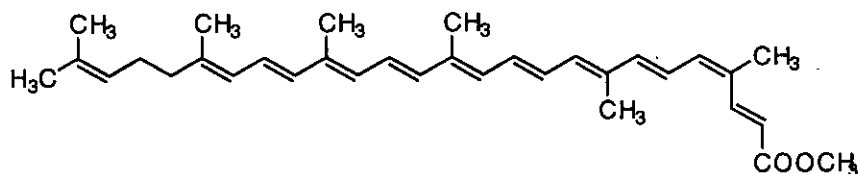
[分子量] 472.409

[基原] *Bixa orellana*

UV: [neutral]  $\lambda_{max}$  342 ; 360

; 439 (sh); 460 ; 493 (sh) (報

告はない)



-----文献-----

Mercadante, A.Z. et al., *Phytochemistry*, 1996, 41, 1201-1203, (分離, H-NMR, UV)

§ 10(14)-Aromadendrene; (1  $\alpha$ , 4  $\alpha$ , 5  $\beta$ , 6  $\alpha$ , 7  $\alpha$ )-form

[化学名・別名] (-)-Aromadendrene.  $\beta$ -Diploalbicene

[CAS No.] 14682-34-9

[その他の CAS No.] 72747-25-2

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

[構造式]

[分子式]  $C_{15}H_{24}$

[分子量] 204.355

[基原] *Bixa orellana*, *Eucalyptus sideroxylon*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{25}$  -11 (EtOH)



-----文献-----

Büchi, G. et al., *J.A.C.S.*, 1969, 91, 6473, (合成法, 絶対構造, 成書)

Tressl, R. et al., *J. Agric. Food Chem.*, 1983, 31, 892, (Aromadendrene epoxide)

Zafra-Polo, M.C. et al., *J. Chromatogr.*, 1990, 518, 230, (Aromadendrene epoxide)

Williams, H.J. et al., *Phytochemistry*, 1995, 40, 1633, (H-NMR, C13-NMR, Mass)

§ 4,8-Dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoic acid; (2E,4Z,6E,8E,10E)-form, Me ester

[CAS No.] 201996-40-9

[化合物分類] 脂肪族化合物 (Branched alkenic methyl esters)

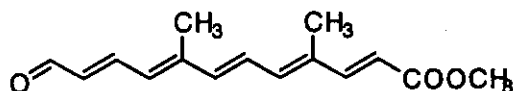
[構造式]

[分子式]  $C_{15}H_{18}O_3$

[分子量] 246.305

[基原] *Bixa orellana* の種子

UV: [neutral]  $\lambda_{max}$  350 ; 367 ; 387 (溶媒に関する報告はない)



-----文献-----

Mercadante, A.Z. et al., *Phytochemistry*, 1997, 46, 1379-1383, (分離, ester, H-NMR, C13-NMR, Mass)

§ Norbixin; (9E)-form, Mono-Me ester

[化学名・別名] Bixin.  $\beta$ -Bixin. Labile bixin

[CAS No.] 39937-23-0

[化合物分類] テルペノイド (Apocarotenoids)

[構造式]

[分子式]  $C_{23}H_{30}O_4$

[分子量] 394.51

[基原] *Bixa orellana* (annatto)

[性状] 結晶 (EtOH)

[融点] Mp 204-206 °C

UV: [neutral]  $\lambda_{max}$  443 ; 475 ; 509 (CHCl<sub>3</sub>) (Berdy) [neutral]  $\lambda_{max}$  475 ( $\epsilon$  130000) (C<sub>6</sub>H<sub>6</sub>) (Berdy)

-----文献-----

Barber, M.S. et al., *J.C.S.*, 1961, 1625, (構造決定)

Reith, J.F. et al., *J. Food Sci.*, 1971, 36, 861, (分離, 構造決定)

Kelly, D.R. et al., *J. Chem. Res., Synop.*, 1996, 446; *J. Chem. Res., Miniprint*, 1996, 2640, (分離, H-NMR, C13-NMR, Mass, 結晶構造)

*Encyclopedia of Food and Color Additives*, (ed. Burdock, G.A.), CRC Press, 1997, 184, (レビュー)

Mercadante, A.Z. et al., *Phytochemistry*, 1999, 52, 135-139, (Phytatetraenyl esters)

§ Norbixin; (9E)-form, Di-Me ester

[化学名・別名] *trans*-Methylbixin. Isomethylbixin

[CAS No.] 62697-46-5

[化合物分類] テルペノイド (Apocarotenoids)

[構造式]

[分子式]  $C_{28}H_{32}O_4$

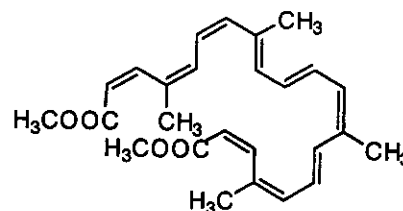
[分子量] 408.536

[基原] *Bixa orellana*

[性状] 青-紫色のプリズム結晶 ( $C_6H_6$ )

[融点] Mp 204-205 °C

UV: [neutral]  $\lambda_{max}$  432 ; 456 ; 490 (petrol) [neutral]  $\lambda_{max}$  446 ; 473 ; 506 ( $C_6H_6$ )



-----文献-----

Reith, J.F. et al., J. Food Sci., 1971, 36, 861, (分離, 構造決定)

Kelly, D.R. et al., J. Chem. Res., Synop., 1996, 446; J. Chem. Res., Miniprint, 1996, 2640, (分離, H-NMR, C13-NMR, Mass, 結晶構造)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 184, (レビュー)

Mercadante, A.Z. et al., Phytochemistry, 1997, 46, 1379-1383, (分離, H-NMR, C13-NMR)

§ Norbixin; (9E)-form, 6-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenyl)-6'-Me ester

[CAS No.] 247030-35-9

[化合物分類] テルペノイド (Apocarotenoids)

[構造式]

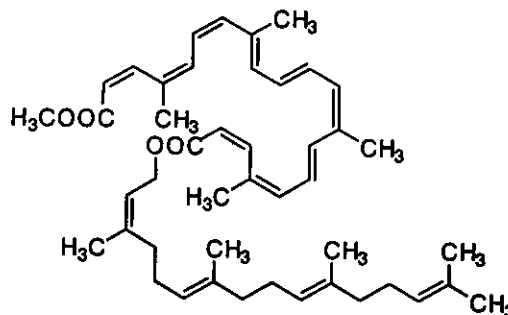
[分子式]  $C_{45}H_{62}O_4$

[分子量] 666.982

[基原] *Bixa orellana* の種子

UV: [neutral]  $\lambda_{max}$  350 ; 432 ; 456 ; 489

(2-methoxy-2-methylpropane)



-----文献-----

Barber, M.S. et al., J.C.S., 1961, 1625, (構造決定)

Reith, J.F. et al., J. Food Sci., 1971, 36, 861, (分離, 構造決定)

Kelly, D.R. et al., J. Chem. Res., Synop., 1996, 446; J. Chem. Res., Miniprint, 1996, 2640, (分離, H-NMR, C13-NMR, Mass, 結晶構造)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 184, (レビュー)

Mercadante, A.Z. et al., Phytochemistry, 1997, 46, 1379-1383, (分離, H-NMR, C13-NMR)

§ Norbixin; (9Z)-form, 6-Me ester

[化学名・別名]  $\alpha$ -Bixin. Isobixin. Stable bixin

[CAS No.] 6983-79-5

[化合物分類] テルペノイド (Apocarotenoids)

[構造式]

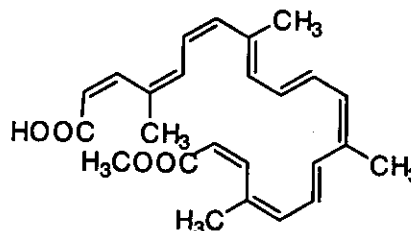
[分子式]  $C_{23}H_{30}O_4$

[分子量] 394.51

[基原] *Bixa orellana* (annatto)

[性状] 結晶 ( $Me_2CO$ )

[融点] Mp 189.5-190.5 °C



-----文献-----

Barber, M.S. et al., J.C.S., 1961, 1625, (構造決定)

Reith, J.F. et al., J. Food Sci., 1971, 36, 861, (分離, 構造決定)

Kelly, D.R. et al., J. Chem. Res., Synop., 1996, 446; J. Chem. Res., Miniprint, 1996, 2640, (分離, H-NMR, C13-NMR, Mass, 結晶構造)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 184, (レビュー)

Mercadante, A.Z. et al., Phytochemistry, 1997, 46, 1379-1383, (分離, H-NMR, C13-NMR)

§ Norbixin; (9Z)-form, Di-Me ester

[化学名・別名] *cis*-Methylbixin. Natural methylbixin

[CAS No.] 26585-94-4

[化合物分類] テルペノイド (Apocarotenoids)

[構造式]

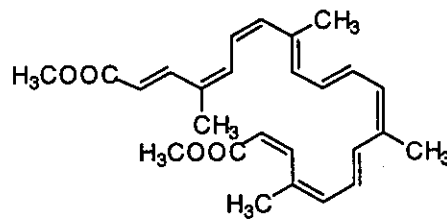
[分子式]  $C_{26}H_{32}O_4$

[分子量] 408.536

[基原] *Bixa orellana* (annatto)

[性状] 結晶

[融点] Mp 164 °C



-----文献-----

Barber, M.S. et al., J.C.S., 1961, 1625, (構造決定)

Reith, J.F. et al., J. Food Sci., 1971, 36, 861, (分離, 構造決定)

Kelly, D.R. et al., J. Chem. Res., Synop., 1996, 446; J. Chem. Res., Miniprint, 1996, 2640, (分離, H-NMR, C13-NMR, Mass, 結晶構造)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 184, (レビュー)

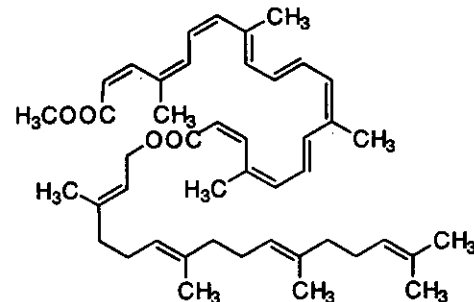
Mercadante, A.Z. et al., Phytochemistry, 1997, 46, 1379-1383, (分離, H-NMR, C13-NMR)

§ Norbixin; (9Z)-form, 6-(3,7,11,5-Tetramethyl-2,6,10,14-hexadecatetraenyl)-6'-Me ester

[CAS No.] 247030-34-8

[化合物分類] テルペノイド (Apocarotenoids)

[構造式]



[分子式]  $C_{45}H_{62}O_4$

[分子量] 666.982

[基原] *Bixa orellana* の種子

UV: [neutral]  $\lambda_{max}$  350 ; 426 ; 452 ; 482 (2-methoxy-2-methylpropane)

-----文献-----

Barber, M.S. et al., J.C.S., 1961, 1625, (構造決定)

Reith, J.F. et al., J. Food Sci., 1971, 36, 861, (分離, 構造決定)

Kelly, D.R. et al., J. Chem. Res., Synop., 1996, 446; J. Chem. Res., Miniprint, 1996, 2640, (分離, H-NMR, C13-NMR, Mass, 結晶構造)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 184, (レビュー)

Mercadante, A.Z. et al., Phytochemistry, 1997, 46, 1379-1383, (分離, H-NMR, C13-NMR)

§ Norbixin; (9Z,9'Z)-form, Di-Me ester

[CAS No.] 201996-34-1

[化合物分類] テルペノイド (Apocarotenoids)

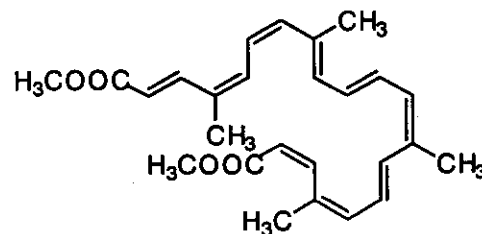
[構造式]

[分子式]  $C_{26}H_{32}O_4$

[分子量] 408.536

[基原] *Bixa orellana* (annatto)

UV: [neutral]  $\lambda_{max}$  350 ; 423 ; 448 ; 476 (2-methoxy-2-methylpropane)



-----文献-----

Barber, M.S. et al., J.C.S., 1961, 1625, (構造決定)

Reith, J.F. et al., J. Food Sci., 1971, 36, 861, (分離, 構造決定)

Kelly, D.R. et al., J. Chem. Res., Synop., 1996, 446; J. Chem. Res., Miniprint, 1996, 2640, (分離, H-NMR, C13-NMR, Mass, 結晶構造)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 184, (レビュー)

Mercadante, A.Z. et al., Phytochemistry, 1997, 46, 1379-1383, (分離, H-NMR, C13-NMR)

§ 6'-Oxo-6,5'-diapo-6-carotenoic acid; (9Z)-form, Me ester

[CAS No.] 201996-49-8

[化合物分類] テルペノイド (Apocarotenoids)

[構造式]