

§ 3,4,5,7-Tetrahydroxyflavylium (1+); 3-O-[4-Hydroxy-E-cinnamoyl-(→ 6) - β-D-glucopyranoside], 5-O-(4,6-di-O-malonyl-β-D-glucopyranoside)

[化学名・別名] Monardein. Monardein

[CAS No.] 73545-87-6

[化合物分類] フラボノイド

(Anthocyanidins and anthocyanins; 4 × O-置換基)

[構造式]

[分子式] C<sub>22</sub>H<sub>41</sub>O<sub>23</sub><sup>(\*)</sup>

[分子量] 913.772

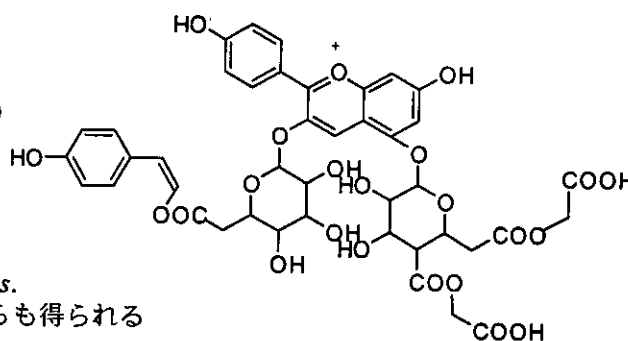
[基原] Colouring matter of golden balm (*Monarda didyma*), of *Salvia coccinea* and of *Salvia splendens*.

また *Gilia coronopifolia*, *Hyacinthus orientalis* から得られる

[性状] 赤色の粉末 (as chloride)

[比旋光度]: [α]<sub>D</sub> -374.5 (0.1% HCl, as chloride)

[その他のデータ] CAS no. は chloride のものである



-----文献-----

Karrer, P. et al., Helv. Chim. Acta, 1927, 10, 67; 1928, 12, 292, (分離, Monardein)

Kondo, T. et al., Tet. Lett., 1985, 26, 5879; 1989, 30, 6729, (構造決定, Monardein, Salvianin)

§ 3,4,5,7-Tetrahydroxyflavylium (1+); 3-O-[4-Hydroxy-3-methoxy-E-cinnamoyl-(→ 6) - β-D-glucopyranoside], 5-O-β-D-glucopyranoside

[化合物分類] フラボノイド

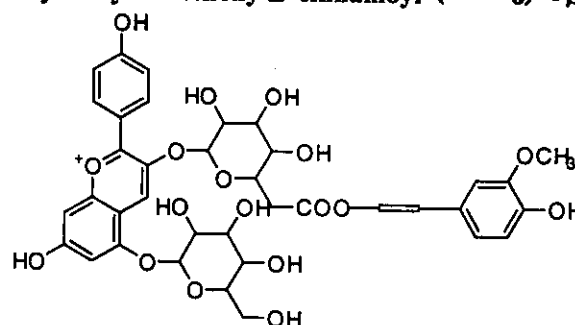
(Anthocyanidins and anthocyanins; 4 × O-置換基)

[構造式]

[分子式] C<sub>37</sub>H<sub>59</sub>O<sub>18</sub><sup>(\*)</sup>

[分子量] 771.704

[基原] *Hyacinthus orientalis*



-----文献-----

Karrer, P. et al., Helv. Chim. Acta, 1927, 10, 67; 1928, 12, 292, (分離, Monardein)

Robertson, A. et al., J.C.S., 1928, 1460; 1533, (分離)

Timberlake, C.F. et al., The Flavonoids, (Eds. Harborne, J.B. et al), Chapman and Hall, London, 1975, 215, (レビュー)

Iacobucci, G.A. et al., Tetrahedron, 1983, 39, 3005, (レビュー)

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

§ 3,4,5,7-Tetrahydroxyflavylium (1+); 3-O-[4-Hydroxy-3-methoxy-E-cinnamoyl-(→ 6) - β-D-glucopyranoside], 5-O-(6-O-malonyl-β-D-glucopyranoside)

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

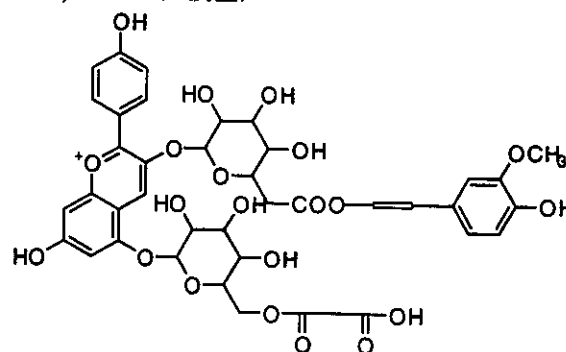
[構造式]

[分子式] C<sub>40</sub>H<sub>47</sub>O<sub>21</sub><sup>(\*)</sup>

[分子量] 857.751

[基原] *Hyacinthus orientalis* の花

[性状] 粉末



-----文献-----

Karrer, P. et al., Helv. Chim. Acta, 1927, 10, 67; 1928, 12, 292, (分離, Monardein)

Robertson, A. et al., J.C.S., 1928, 1460; 1533, (分離)

Timberlake, C.F. et al., The Flavonoids, (Eds. Harborne, J.B. et al), Chapman and Hall, London, 1975, 215, (レビュー)

§ 4',5,7-Trihydroxy-3',5'-dimethoxyflavone; 7-O-[D-Fructosyl-(1 → ?)-D-glucopyranoside]

[CAS No.] 58798-49-5

[化合物分類]フラボノイド (Flavones; 5 × O-置換基), フラボノイド (Flavonoids 構造は一部又は全てが未知)

[構造式]有効な構造式はない

[分子式] C<sub>29</sub>H<sub>34</sub>O<sub>17</sub>

[分子量] 654.577

[基原]次の植物から分離: *Hyacinthus orientalis*

-----文献-----

Kaneta, M. et al., Bull. Chem. Soc. Jpn., 1972, 45, 528, (分離)

Bhattacharyya, J. et al., J. Pharm. Sci., 1978, 67, 1325, (分離, C13-NMR)

Liu, Y.-L. et al., Phytochemistry, 1982, 21, 209, (分離)

Harborne, J.B. et al., Phytochemistry, 1985, 24, 751, (分離)

Rofi, R.D. et al., Phytochemistry, 1985, 24, 2131, (分離)

Hirai, Y. et al., Chem. Pharm. Bull., 1986, 34, 82, (誘導體)

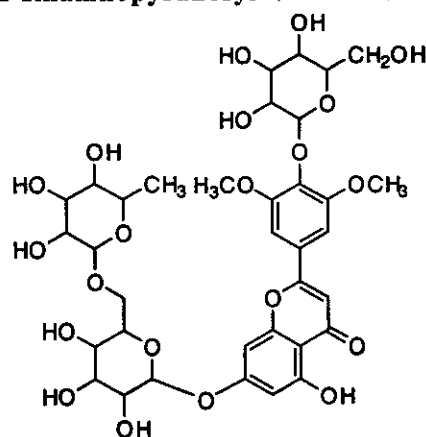
§ 4',5,7-Trihydroxy-3',5'-dimethoxyflavone; 7-O-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], 4'-O-β-D-glucopyranoside

[化学名・別名] Tricin 4'-glucoside 7-rutinoside

[CAS No.] 58795-16-7

[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>33</sub>H<sub>44</sub>O<sub>21</sub>

[分子量] 800.72

[基原]次の植物から分離: *Hyacinthus orientalis*

-----文献-----

Kaneta, M. et al., Bull. Chem. Soc. Jpn., 1972, 45, 528, (分離)

Markham, K.R. et al., Phytochemistry, 1973, 12, 2007, (7-rhamnosylglucuronide)

Desai, H.K. et al., Indian J. Chem., Sect. B, 1976, 14, 473, (分離)

Bhattacharyya, J. et al., J. Pharm. Sci., 1978, 67, 1325, (分離, C13-NMR)

Liu, Y.-L. et al., Phytochemistry, 1982, 21, 209, (分離)

Mabry, T.J. et al., J. Nat. Prod., 1984, 47, 127, (7-rhamnosylgalacturonoside)

Harborne, J.B. et al., Phytochemistry, 1985, 24, 751, (分離)

Rofi, R.D. et al., Phytochemistry, 1985, 24, 2131, (分離)

Rettig, J.H. et al., Biochem. Syst. Ecol., 1990, 18, 393, (7-glucoside)

\*\*\*\*\*ヒヨドリバナ (*Eupatorium*) \*\*\*\*\*

§ § キク科 (*Eupatorium ayapana* Ventenat) の葉、茎及び根。

§ 7-Hydroxy-2H-1-benzopyran-2-one; Me ether

[化学名・別名] 7-Methoxy-2H-1-benzopyran-2-one (CAS 名). 7-Methoxycoumarin. Herniarin. Umbelliferone methyl ether. Ayapanin

[CAS No.] 531-59-9

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

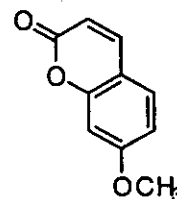
[構造式]

[分子式] C<sub>10</sub>H<sub>8</sub>O<sub>3</sub>

[分子量] 176.171

[基原] *Herniaria* spp., *Eupatorium ayapana*, *Ruta pinnata*, *Prunus mahaleb*, その他の植物

[性状] 葉状結晶 (H<sub>2</sub>O or MeOH)



[融点] Mp 117-118 °C

UV: [neutral]  $\lambda_{\max}$  247 ( $\epsilon$  2240); 320 ( $\epsilon$  14125) (MeOH) (Berdy)

[化学物質毒性データ総覧(RTECS)登録番号] DJ3100380

[販売元] Aldrich:22033-7

-----文献-----

Hata, K. et al., Chem. Pharm. Bull., 1971, 19, 640, (分離)

Gray, A.I. et al., Phytochemistry, 1987, 26, 257, (誘導體)

Ford, R.A. et al., Food Chem. Toxicol., 1988, 26, 375, (レビュー, 毒性, Me ether)

\*\*\*RTECS (化学物質毒性データ)\*\*\*

\*\*\*健康障害に関するデータ\*\*\*

\*\*\*急性毒性に関するデータ\*\*\*

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 経口投与.

被験動物 : げっ歯類-ラット.

投与量・期間 : 4300 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.

参考文献

Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) 26,375,1988

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 皮膚への塗布

被験動物 : げっ歯類-モルモット.

投与量・期間 : >5 gm/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参考文献

Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) 26,375,1988

### § 6,7-Methylenedioxy-2H-1-benzopyran-2-one

[化学名・別名] 6H-1,3-Dioxolo[4,5-g][1] benzopyran-6-one (CAS 名). 6,7-Methylenedioxy coumarin.

Ayapin. Aiapin

[CAS No.] 494-56-4

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

[構造式]

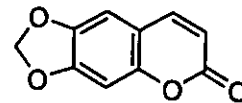
[分子式]  $C_{10}H_6O_4$

[分子量] 190.155

[基原] *Eupatorium ayapana*, *Dendrobium thyrsiflorum*, (おそらく) *Alomia fastigiata*

[性状] 結晶 (MeOH)

[融点] Mp 231-232 °C (224 °C)



-----文献-----

Bose, P.K. et al., Ber., 1937, 70, 702, (分離, 合成法)

Dieterman, L.J. et al., Arch. Biochem. Biophys., 1964, 106, 275, (分離)

\*\*\*\*\*ヒラタケ (Hiratake)\*\*\*\*\*

§ § ヒラタケ科ヒラタケ (*Pleurotus ostreatus* (Jacquin) Q.) の子実体.

### § 3,4-Dihydroxy-5-(hydroxymethyl)-2(5H)-furanone; (R)-form, 1'-O- $\alpha$ -D-Xylopyranoside

[CAS No.] 174339-85-6

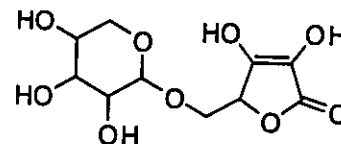
[化合物分類] 炭水化物 (Disaccharides)

[構造式]

[分子式]  $C_{10}H_{14}O_8$

[分子量] 278.215

[基原] *Pleurotus ostreatus*



-----文献-----

Murakawa, S. et al., Agric. Biol. Chem., 1977, 41, 1799-1800, (分離)

Bast, E. et al., Z. Naturforsch., C, 1978, 33, 789-792, (分離, Mass)  
 Liang, Y.T.S. et al., J. Carbohydr. Chem., 1990, 9, 75-84, (D-form, 合成法, 成書)  
 Okamura, M., J. Nutr. Sci. Vitaminol., 1994, 40, 81-94, (分離, 配糖体)  
 Loewus, F.A. et al., Biochem. Biophys. Res. Commun., 1995, 212, 196-203, (分離)  
 Pat. Coop. Treaty (WIPO), 1995, 95 29 928; CA, 124, 212049b, (分離, 配糖体)

§ 3,4-Dihydroxy-5-(hydroxymethyl)-2(5H)-furanone; (R)-form, 1'-O- $\alpha$ -D-Glucopyranoside

[CAS No.] 174339-86-7

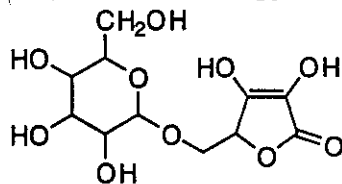
[化合物分類] 炭水化物 (Disaccharides)

[構造式]

[分子式]  $C_{11}H_{16}O_{10}$

[分子量] 308.241

[基原] *Hypsizigus mamoreus*, *Pleurotus ostreatus*



----- 文献 -----

Murakawa, S. et al., Agric. Biol. Chem., 1977, 41, 1799-1800, (分離)  
 Bast, E. et al., Z. Naturforsch., C, 1978, 33, 789-792, (分離, Mass)  
 Okamura, M., J. Nutr. Sci. Vitaminol., 1994, 40, 81-94, (分離, 配糖体)  
 Pat. Coop. Treaty (WIPO), 1995, 95 29 928; CA, 124, 212049b, (分離, 配糖体)

§ Ergosta-7,22-diene-3,5,6,9-tetrol; (3 $\beta$ ,5 $\alpha$ ,6 $\alpha$ ,9 $\alpha$ ,22E,24R)-form, 22,23-Dihydro, 6-ketone

[化学名・別名] 3,5,9-Trihydroxyergosta-7-en-6-one. 3,5,9-Trihydroxy-24-methylcholest-7-en-6-one

[CAS No.] 211486-13-4

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

[構造式]

[分子式]  $C_{28}H_{46}O_4$

[分子量] 446.669

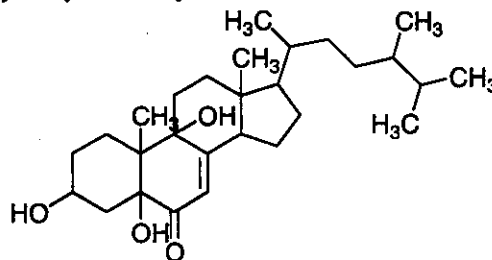
[基原] 次の植物から分離: カビ類: *Lentinus edodes*, *Hypsizigus marmoreus*, *Pleurotus ostreatus*, *Pholiota nameko*

[性状] 無定型の粉末

[比旋光度]:  $[\alpha]_D^{25} -21.5$  (c, 0.09 in  $CHCl_3$ )

UV: [neutral]  $\lambda_{max}$  236 (log  $\epsilon$  3.8) (MeOH)

[その他のデータ] Has 24S-config. (change of Cahn-Ingold-Prelog priorities)



----- 文献 -----

Migliuolo, A. et al., J. Nat. Prod., 1990, 53, 1414-1424, (Spongia officinalis metab, 分離, H-NMR, C13-NMR)  
 Aiello, A. et al., Steroids, 1995, 60, 666-673, (6-sulfates, 分離, H-NMR, C13-NMR)  
 Yaoita, Y. et al., Chem. Pharm. Bull., 1998, 46, 944-950; 1999, 47, 847-851, (mushroom constits)

§ Ergosta-4,6,8,22-tetraen-3-one; (22E,24 $\xi$ )-form

[CAS No.] 194721-75-0

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

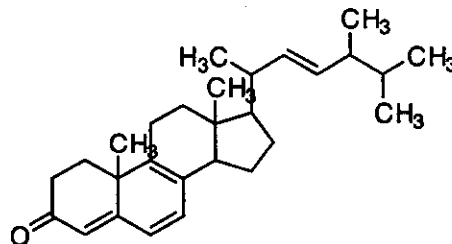
[構造式]

[分子式]  $C_{28}H_{46}O$

[分子量] 392.623

[基原] *Pleurotus ostreatus* (oyster fungus)

UV: [neutral]  $\lambda_{max}$  349 (log  $\epsilon$  4.13) (EtOH)



----- 文献 -----

Chobot, V. et al., Phytochemistry, 1997, 45, 1669-1671, (分離, H-NMR, C13-NMR)

§ 3,5,9,14-Tetrahydroxyergosta-7,22-dien-6-one; (3 $\beta$ ,5 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,22E,24R)-form

[CAS No.] 211486-14-5

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

[構造式]

[分子式]  $C_{28}H_{44}O_5$

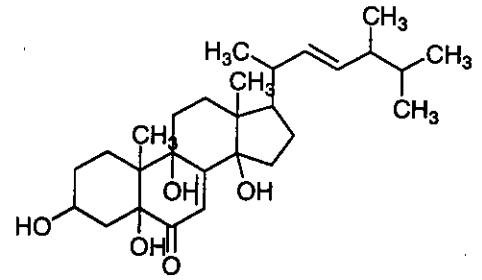
[分子量] 460.653

[基原] *Lentinus edodes*, *Hypsizigus marmoreus*, *Pleurotus ostreatus*, *Pholiota nameko*

[性状] 無定型の粉末

[比旋光度]:  $[\alpha]_D^{19} -22.7$  (c, 0.04 in  $CHCl_3$ )

UV: [neutral]  $\lambda_{max}$  225 (log  $\epsilon$  3.9) (MeOH)



-----文献-----

Yaota, Y. et al., Chem. Pharm. Bull., 1998, 46, 944-950, (分離, H-NMR, C13-NMR)

\*\*\*\*\*ピワ (Biwa, Loquat) \*\*\*\*\*

§ § パラ科ピワ (*Eriobotrya japonica* Lindley) の葉および果実。

§ Cinchonain Ic; 8-Epimer, 9-O- $\beta$ -D-glucopyranoside

[化学名・別名] Cinchonain Id 7-glucoside

[化合物分類] フラボノイド (Neoflavonoids), フラボノイド (Flavan-3-ols)

[構造式]

[分子式]  $C_{30}H_{30}O_{14}$

[分子量] 614.559

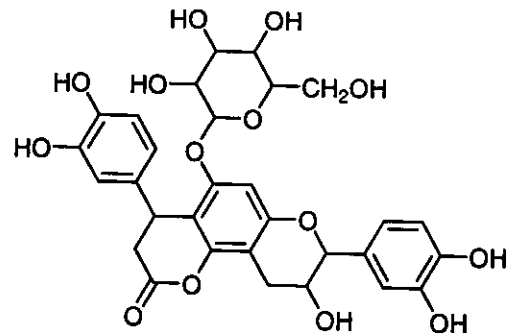
[基原] *Eriobotrya japonica*

[性状] 青白い黄色の粉末

[比旋光度]:  $[\alpha]_D -37.5$  (c, 1 in MeOH)

UV: [neutral]  $\lambda_{max}$  284 (log  $\epsilon$  3.97); 328 (log  $\epsilon$  3.38) (MeOH)

[その他のデータ] Numbering systems vary



-----文献-----

Ito, H. et al., Chem. Pharm. Bull., 2000, 48, 687-693, (Cinchonain Id 7-glucoside)

§ 2,3,4-Dibenzofurantriol; 2,4-Di-Me ether

[化学名・別名] 2,4-Dimethoxy-3-dibenzofuranol (CAS 名). 3-Hydroxy-2,4-dimethoxydibenzofuran. Eriobofuran

[CAS No.] 97218-06-9

[化合物分類] 単環芳香族 (Dibenzofurans)

[構造式]

[分子式]  $C_{14}H_{12}O_4$

[分子量] 244.246

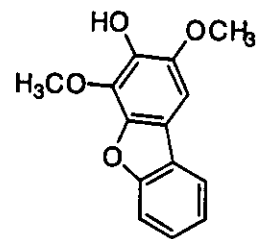
[基原] 次の植物から得られるファイトアレキシン: *Eriobotrya japonica* の葉

[用途] 抗カビ剤

[性状] 結晶

[融点] Mp 157-158 °C

UV: [neutral]  $\lambda_{max}$  260 ; 294 ; 302 (MeOH) (Berdy) [base]  $\lambda_{max}$  333 (MeOH-NAOH) (Berdy)



-----文献-----

Miyakado, M. et al., Nippon Noyaku Gakkaishi, 1985, 10, 101; CA, 103, 66221z, (Eriobofuran)

§ 6,9-Dihydroxy-4,7-megastigmadien-3-one; (6S,7E,9R)-form, 9-O- $[\beta$ -D-Apiofuranosyl-(1  $\rightarrow$  6)- $\beta$ -D-glucopyranoside]

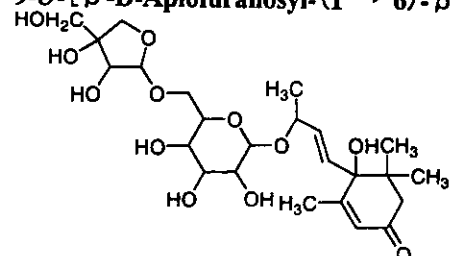
[化合物分類] テルペノイド (Megastigmane norterenoids)

[構造式]

[分子式]  $C_{24}H_{38}O_{12}$

[分子量] 518.557

[基原] 次の植物の茎皮から分離: *Albizia julibrissin*, *Eriobotrya japonica*



[性状]粉末

[比旋光度]: $[\alpha]_D^{25} +15$  (c, 0.14 in MeOH)

-----文献-----

Higuchi, H. et al., Chem. Pharm. Bull., 1992, 40, 534-535, (9-apiosylglucoside)

De Tommasi, N. et al., J. Nat. Prod., 1992, 55, 1025, (9-apiosylglucoside)

Sefton, M.A. et al., Phytochemistry, 1992, 31, 1813-1815, (9-glucoside)

§ 1,6,10-Farnesatrien-3-ol; (S)-form, O-[ $\alpha$ -L-Rhamnopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-glucopyranoside]

[CAS No.] 130466-30-7

[化合物分類]テルペノイド

(Simple farnesane sesquiterpenoids)

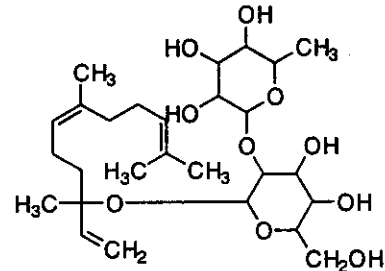
[構造式]

[分子式]  $C_{27}H_{46}O_{10}$

[分子量] 530.654

[基原] *Eriobotrya japonica* (loquat)

[比旋光度]: $[\alpha]_D^{25} -25.4$  (c, 1 in MeOH)



-----文献-----

Borges, J. et al., Tet. Lett., 1966, 3731, (分離)

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 124, (生育)

Opdyke, D.L.J., Food Cosmet. Toxicol., 1975, 13, 887, (レビュー, 毒性)

Weyerstahl, P. et al., Annalen, 1992, 1325, (構造決定)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, (レビュー)

Donath, J. et al., Phytochemistry, 1995, 39, 785, (生合成)

§ 1,6,10-Farnesatrien-3-ol; (S)-form, O-[ $\alpha$ -L-Rhamnopyranosyl-(1 $\rightarrow$ 4)- $\alpha$ -L-rhamnopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-glucopyranoside]

[化合物分類]テルペノイド

(Simple farnesane sesquiterpenoids)

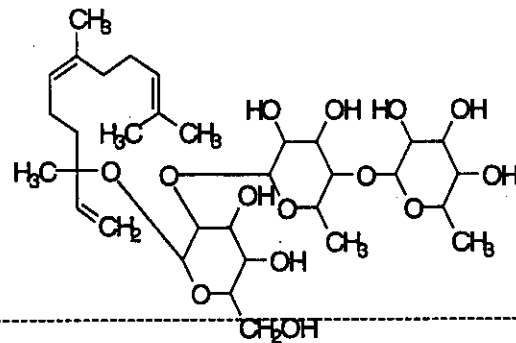
[構造式]

[分子式]  $C_{33}H_{56}O_{14}$

[分子量] 676.797

[基原] *Eriobotrya japonica* (loquat)

[比旋光度]: $[\alpha]_D^{25} -41$  (c, 1 in MeOH)



-----文献-----

Borges, J. et al., Tet. Lett., 1966, 3731, (分離)

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 124, (生育)

Opdyke, D.L.J., Food Cosmet. Toxicol., 1975, 13, 887, (レビュー, 毒性)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, (レビュー)

§ 1,6,10-Farnesatrien-3-ol; (S)-form, O-[ $\alpha$ -L-Rhamnopyranosyl-(1 $\rightarrow$ 4)- $\alpha$ -L-rhamnopyranosyl-(1 $\rightarrow$ 6)- $\beta$ -D-glucopyranoside]

[CAS No.] 130466-33-0

[化合物分類]テルペノイド

(Simple farnesane sesquiterpenoids)

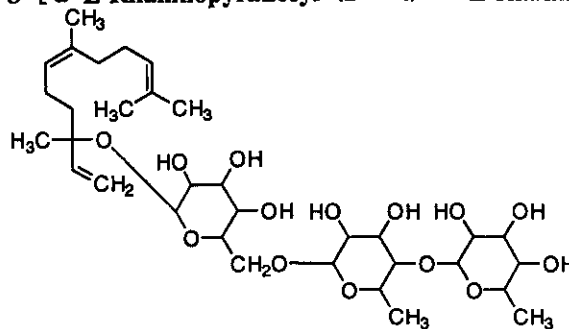
[構造式]

[分子式]  $C_{33}H_{56}O_{14}$

[分子量] 676.797

[基原] *Eriobotrya japonica* (loquat)

[比旋光度]: $[\alpha]_D^{25} -40$  (c, 1 in MeOH)



-----文献-----

Borges, J. et al., Tet. Lett., 1966, 3731, (分離)

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 124, (生育)  
 Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1975, 13, 887, (レビュー, 毒性)  
 Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NCN700  
 Fenaroli's *Handbook of Flavor Ingredients*, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, (レビュー)  
 Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, NCN800

§ 1,6,10-Farnesatrien-3-ol; (S)-form, O-[α-L-Rhamnopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside]

[CAS No.] 130466-32-9

[化合物分類]テルペノイド

(Simple farnesane sesquiterpenoids)

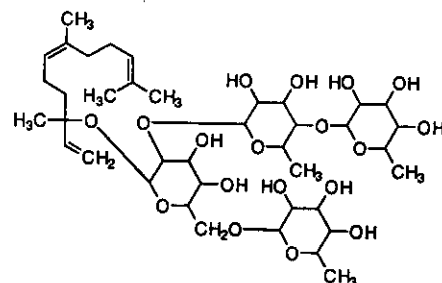
[構造式]

[分子式] C<sub>39</sub>H<sub>66</sub>O<sub>18</sub>

[分子量] 822.94

[基原] *Eriobotrya japonica* (loquat)

[比旋光度]: [α]<sub>D</sub><sup>25</sup> -50 (c, 1 in MeOH)



-----文献-----

Borges, J. et al., *Tet. Lett.*, 1966, 3731, (分離)

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 124, (生育)

Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1975, 13, 887, (レビュー, 毒性)

Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NCN700

Fenaroli's *Handbook of Flavor Ingredients*, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, (レビュー)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, NCN800

§ 1,6,10-Farnesatrien-3-ol; (S)-form, O-[α-L-Rhamnopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[4-(4-hydroxy-3-methoxycinnamoyl)-(E)-α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside]

[CAS No.] 143376-48-1

[化合物分類]テルペノイド

(Simple farnesane sesquiterpenoids)

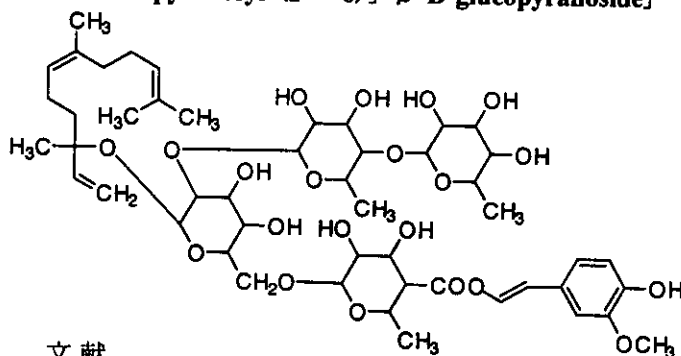
[構造式]

[分子式] C<sub>49</sub>H<sub>74</sub>O<sub>21</sub>

[分子量] 999.111

[基原] *Eriobotrya japonica* (loquat)

[比旋光度]: [α]<sub>D</sub><sup>25</sup> -70 (c, 1 in MeOH)



-----文献-----

Borges, J. et al., *Tet. Lett.*, 1966, 3731, (分離)

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 124, (生育)

Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1975, 13, 887, (レビュー, 毒性)

Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NCN700

Fenaroli's *Handbook of Flavor Ingredients*, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, (レビュー)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, NCN800

§ 1,6,10-Farnesatrien-3-ol; (S)-form, O-[α-L-Rhamnopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside]

[化学名・別名] Loquatifolin A

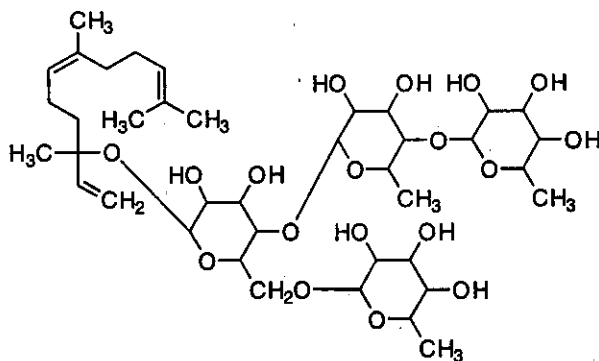
[CAS No.] 116174-69-7

[化合物分類]テルペノイド

(Simple farnesane sesquiterpenoids)

[構造式]

[分子式]  $C_{39}H_{66}O_{18}$   
 [分子量] 822.94  
 [基原] *Eriobotrya japonica* (loquat)  
 [性状] 結晶 + 1·1/2H<sub>2</sub>O  
 [融点] Mp 128-130 °C  
 [比旋光度]:  $[\alpha]_D^{22} -79.7$  (EtOH)

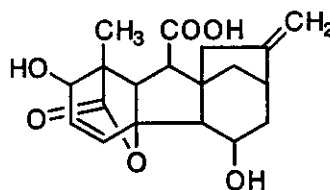


----- 文献 -----

Yanagisawa, H. et al., Chem. Pharm. Bull., 1988, 36, 1270, (Loquatifolin A)

§ Gibberellin A; 11 β-Hydroxy

[化学名・別名] 11 β-Hydroxygibberellin A  
 [CAS No.] 128053-62-3  
 [化合物分類] テルペノイド (Gibberellins)  
 [構造式]  
 [分子式]  $C_{19}H_{22}O_6$   
 [分子量] 346.379  
 [基原] *Lolium temulentum*, *Eriobotrya japonica*

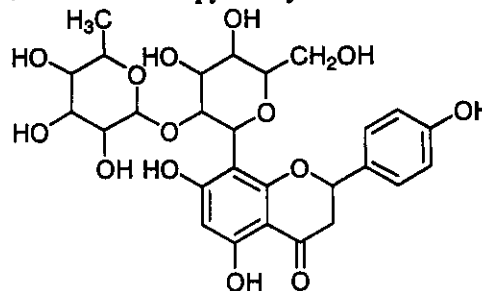


----- 文献 -----

Cross, B.E. et al., Tetrahedron, 1962, 18, 451, (構造決定)  
 Aldridge, D.C. et al., J.C.S., 1965, 3539, (構造決定)  
 Hasegawa, M. et al., Phytochemistry, 1994, 37, 629, (誘導体)

§ 8-Glucopyranosyl-4',5,7-trihydroxyflavanone; (R)-form, 2''-O-α-L-Rhamnopyranosyl

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



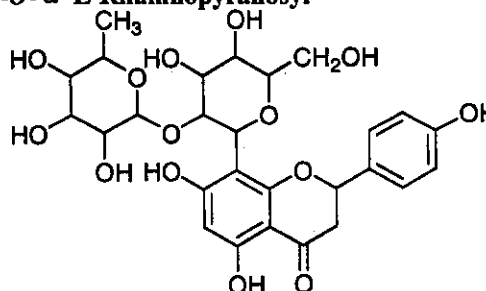
[分子式]  $C_{27}H_{32}O_{14}$   
 [分子量] 580.541  
 [基原] *Eriobotrya japonica*  
 [性状] 青白い黄色の粉末  
 [比旋光度]:  $[\alpha]_D +5.3$  (c, 1 in MeOH)  
 UV: [neutral]  $\lambda_{max}$  218 (log ε 4.43); 290 (log ε 4.2); 328 (sh) (log ε 3.63) (MeOH)

----- 文献 -----

Hillis, W.E. et al., Aust. J. Chem., 1963, 16, 147; 1965, 18, 531, (分離, H-NMR)  
 Lorente, F.T. et al., An. Quim., Ser. C, 1983, 79, 456, (分離)  
 Ito, H. et al., Chem. Pharm. Bull., 2000, 48, 687-693, (2''-rhamnosyl derivs)

§ 8-Glucopyranosyl-4',5,7-trihydroxyflavanone; (S)-form, 2''-O-α-L-Rhamnopyranosyl

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



[分子量] 580.541  
 [基原] *Eriobotrya japonica*  
 [性状] 青白い黄色の粉末  
 [比旋光度]:  $[\alpha]_D +25.3$  (c, 1 in MeOH)  
 UV: [neutral]  $\lambda_{max}$  214 (log ε 4.39); 225 (sh) (log ε 4.36);  
 290 (log ε 4.12); 325 (sh) (log ε 3.64) (MeOH)

----- 文献 -----

Hillis, W.E. et al., Aust. J. Chem., 1963, 16, 147; 1965, 18, 531, (分離, H-NMR)  
 Lorente, F.T. et al., An. Quim., Ser. C, 1983, 79, 456, (分離)  
 Ito, H. et al., Chem. Pharm. Bull., 2000, 48, 687-693, (2''-rhamnosyl derivs)



§ 3,3',4,4',5,7-Hexahydroxyflavan; (2 ξ, 3 ξ, 4 ξ)-form, 3-O-α-L-Arabinopyranoside

[化学名・別名] Loquatoside

[CAS No.] 74046-15-4

[化合物分類] フラボノイド (Leucoanthocyanidins)

[構造式]

[分子式] C<sub>20</sub>H<sub>22</sub>O<sub>11</sub>

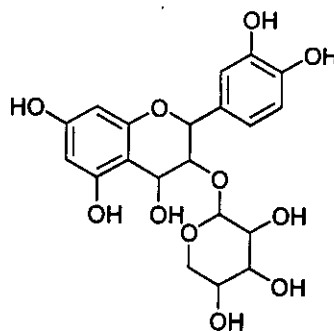
[分子量] 438.387

[基原] *Eriobotrya japonica* の果実

[性状] 結晶 (EtOAc/petrol)

[融点] Mp 208 °C

[比旋光度]: [α]<sub>D</sub><sup>25</sup> -22 (EtOH)



-----文献-----

Agrawal, S. et al., *Planta Med.*, 1980, 38, 277, (Loquatoside)

§ 4-(Hydroxymethyl)-2-pyrrolidinecarboxylic acid; (2R,4S)-form

[化学名・別名] D-trans-form

[CAS No.] 36149-81-2

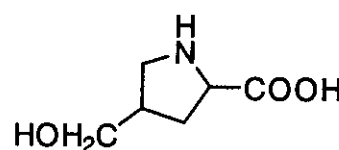
[化合物分類] アミノ酸とペプチド (Non-protein α-aminoacids)

[構造式]

[分子式] C<sub>5</sub>H<sub>11</sub>NO<sub>3</sub>

[分子量] 145.158

[基原] *Eriobotrya japonica* の種子



-----文献-----

Abraham, R.J. et al., *Nature (London)*, 1961, 192, 1150, (H-NMR, conformn)

Welter, A. et al., *Phytochemistry*, 1978, 17, 131, (生育, 分離)

§ 4-(Hydroxymethyl)-2-pyrrolidinecarboxylic acid; (2S,4S)

[化学名・別名] L-cis-form

[CAS No.] 2370-39-0

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

[構造式]

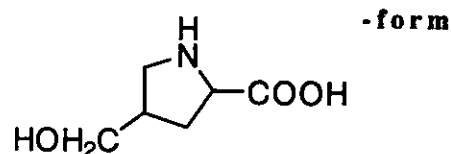
[分子式] C<sub>5</sub>H<sub>11</sub>NO<sub>3</sub>

[分子量] 145.158

[基原] リンゴ, *Eriobotrya japonica*, *Azelia bella* の種子

[融点] Mp 257-258 °C で分解

[比旋光度]: [α]<sub>D</sub><sup>19.5</sup> -75.6 (H<sub>2</sub>O)



-form

-----文献-----

Abraham, R.J. et al., *Nature (London)*, 1961, 192, 1150, (H-NMR, conformn)

Kenner, G.W. et al., *J.C.S.*, 1965, 3850, (合成法)

Welter, A. et al., *Phytochemistry*, 1978, 17, 131, (生育, 分離)

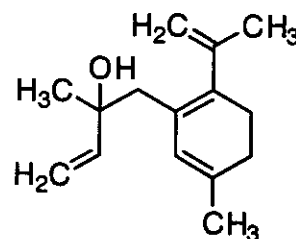
§ Isohumbertiol; (3 ξ, 5 ξ, 10 ξ)-form, 9,10-Didehydro

[化学名・別名] Isohumbertiol †

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

[構造式]

[基原] 次の植物の配糖体として見つかる: *Eriobotrya japonica*



-----文献-----

Weyerstahl, P. et al., *Annalen*, 1992, 1325, (分離, H-NMR, C13-NMR, 合成法)

De Tommasi, N. et al., *J. Nat. Prod.*, 1992, 55, 1025, (配糖体)

§ Isohumbertiol; (3 ξ, 5 ξ, 10 ξ)-form, 9,10-Didehydro, O-[α-L-rhamnopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside]

[CAS No.] 143376-49-2

[化合物分類] テルペノイド

(Humbertiane sesquiterpenoids)

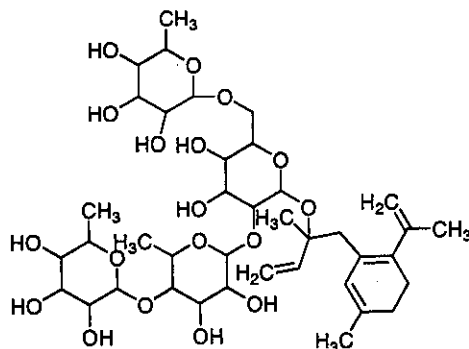
[構造式]

[分子式]  $C_{39}H_{62}O_{18}$

[分子量] 818.908

[基原] *Eriobotrya japonica*

[比旋光度]:  $[\alpha]_D^{25} -40$  (c, 1 in MeOH)



----- 文献 -----

Weyerstahl, P. et al., *Annalen*, 1992, 1325, (分離, H-NMR, C13-NMR, 合成法)

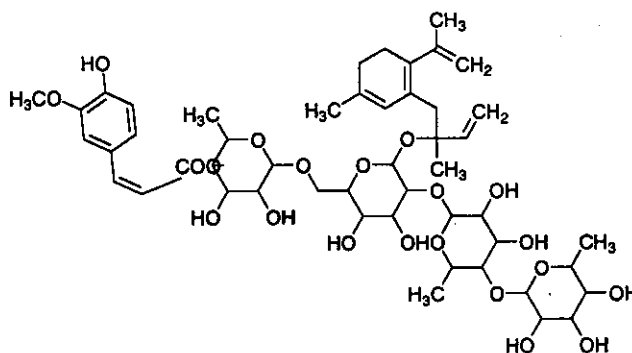
De Tommasi, N. et al., *J. Nat. Prod.*, 1992, 55, 1025, (配糖体)

§ **Isohumbertiol; (3 ξ, 5 ξ, 10 ξ)-form, 9,10-Didehydro, O-[α-L-rhamnopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[(4-hydroxy-3-methoxycinnamoyl (E))-(→ 4)-α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside]**

[CAS No.] 143363-61-5

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

[構造式]



[分子式]  $C_{49}H_{70}O_{21}$

[分子量] 995.079

[基原] *Eriobotrya japonica*

[比旋光度]:  $[\alpha]_D^{25} -72$  (c, 1 in MeOH)

----- 文献 -----

Weyerstahl, P. et al., *Annalen*, 1992, 1325, (分離, H-NMR, C13-NMR, 合成法)

De Tommasi, N. et al., *J. Nat. Prod.*, 1992, 55, 1025, (配糖体)

§ **4,7-Megastigmadiene-3,9-diol; (3S,7E,9R)-form, 3-Ketone, 9-O-[β-D-apiofuranosyl-(1 → 6)-β-D-glucopyranoside]**

[CAS No.] 143363-62-6

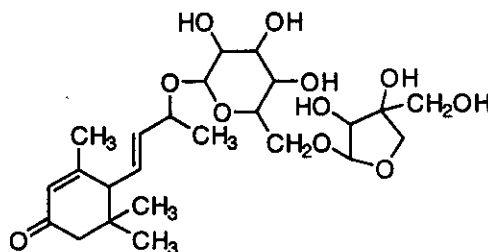
[化合物分類] テルペノイド (Megastigmane norterenoids)

[構造式]

[分子式]  $C_{24}H_{38}O_{11}$

[分子量] 502.558

[基原] *Eriobotrya japonica*



----- 文献 -----

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

Pabst, A. et al., *Phytochemistry*, 1992, 31, 1649, (分離, H-NMR, C13-NMR, 絶対構造)

De Tommasi, N. et al., *J. Agric. Food Chem.*, 1996, 44, 1676, (分離, H-NMR, C13-NMR)

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

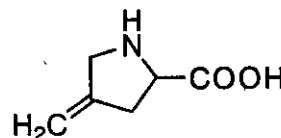
§ **4-Methylene-2-pyrrolidinecarboxylic acid; (±)-form**

[CAS No.] 2370-38-9

[化合物分類] アミノ酸とペプチド (Non-protein α-aminoacids),  
アミノ酸とペプチド (Unsaturated aminoacids)

[構造式]

[分子式]  $C_4H_7NO_2$



[分子量] 127.143

[基原] Present in Loquat seeds (*Eriobotrya japonica*)

[融点] Mp 224-245 (225 °C) °Cで分解

-----文献-----

Gray, D.O. et al., *Phytochemistry*, 1972, 11, 745, (分離, 構造決定)

§ 2,3,19,23-Tetrahydroxy-12-ursen-28-oic acid; (2  $\alpha$ , 3  $\beta$ )-form, 23-(4-Hydroxy-*E*-cinnamoyl)

[化学名・別名] 23-*trans-p*-Coumaroyloxytormentenic acid

[CAS No.] 144604-14-8

[化合物分類] テルペノイド (Ursane triterpenoids)

[構造式]

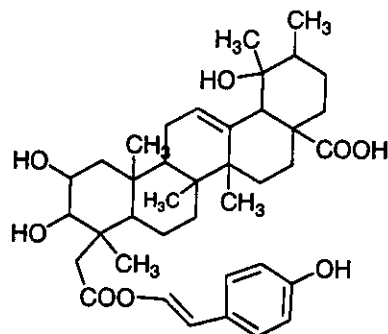
[分子式]  $C_{39}H_{54}O_8$

[分子量] 650.851

[基原] *Eriobotrya japonica*

[比旋光度]:  $[\alpha]_D^{25} +18.2$  (c, 1 in MeOH)

[その他のデータ] Incorrectly named as 23-*trans-p*-Coumaroyltormentenic acid in ref.



-----文献-----

De Tommasi, N. et al., *J. Nat. Prod.*, 1992, 55, 1067, (*p*-coumaroyl esters)

§ 2,3,19,23-Tetrahydroxy-12-ursen-28-oic acid; (2  $\alpha$ , 3  $\beta$ )-form, 23-(4-Hydroxy-*Z*-cinnamoyl)

[化学名・別名] 23-*cis-p*-Coumaroyloxytormentenic acid

[CAS No.] 144604-15-9

[化合物分類] テルペノイド (Ursane triterpenoids)

[構造式]

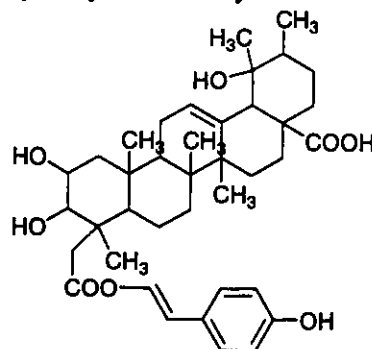
[分子式]  $C_{39}H_{54}O_8$

[分子量] 650.851

[基原] *Eriobotrya japonica*

[比旋光度]:  $[\alpha]_D^{25} +13.3$  (c, 1 in MeOH)

[その他のデータ] Incorrectly named as 23-*cis-p*-Coumaroyltormentenic acid in ref.



-----文献-----

De Tommasi, N. et al., *J. Nat. Prod.*, 1992, 55, 1067, (*p*-coumaroyl esters)

§ 2,3,19-Trihydroxy-12-ursen-28-oic acid; (2  $\alpha$ , 3  $\alpha$ , 19  $\alpha$ )-form, 3-*O*-(4-Hydroxy-3-methoxy-*E*-cinnamoyl)

[化学名・別名] 3-*O-trans*-Feruloylouscaphic acid

[化合物分類] テルペノイド (Ursane triterpenoids)

[構造式]

[分子式]  $C_{40}H_{56}O_8$

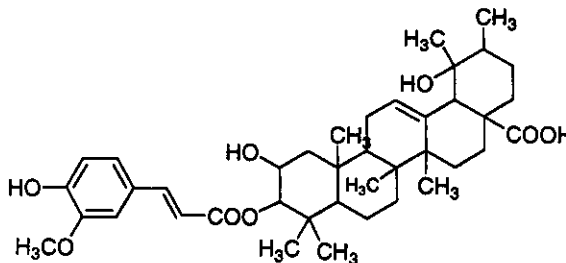
[分子量] 664.878

[基原] *Eriobotrya japonica*

[性状] 無定型の塊

[融点] Mp 185-190 °Cで分解

UV: [neutral]  $\lambda_{max}$  290 ; 320 (MeOH)



-----文献-----

Shimizu, M. et al., *Chem. Pharm. Bull.*, 1996, 44, 2181, (Feruloylouscaphic acid)

§ 2,3,19-Trihydroxy-12-ursen-28-oic acid; (2  $\alpha$ , 3  $\beta$ , 19  $\alpha$ )-form, 3-*O*-(3,4-Dihydroxy-*E*-cinnamoyl)

[化学名・別名] 3-*trans*-Caffeoyltormentenic acid

[CAS No.] 144604-16-0

[化合物分類] テルペノイド

(Ursane triterpenoids)

[構造式]

[分子式]  $C_{39}H_{54}O_8$

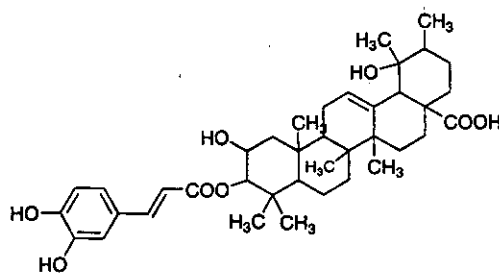
[分子量] 650.851

[基原] *Eriobotrya japonica*

[比旋光度]:  $[\alpha]_D^{25} +1.2$  (c, 1 in MeOH)

UV: [base]  $\lambda_{max}$  217 ( $\epsilon$ ); 380 ( $\epsilon$ ) (EtOH/NaOH) (Derep)

[neutral]  $\lambda_{max}$  221 ( $\epsilon$  20900); 235 ( $\epsilon$ ); 246 ( $\epsilon$ ); 302 ( $\epsilon$ ); 333 ( $\epsilon$ ) (EtOH) (Derep)



----- 文献 -----

De Tommasi, N. et al., J. Nat. Prod., 1992, 55, 1067, (caffeoyl ester)

Yang, M.-H. et al., Planta Med., 1992, 58, 227, (Tormentenic acid, C13-NMR)

### § 3,6,19-Trihydroxy-12-ursen-28-oic acid; (3 $\beta$ , 6 $\alpha$ , 19 $\alpha$ )-form

[CAS No.] 130289-31-5

[化合物分類] テルペノイド (Ursane triterpenoids)

[構造式]

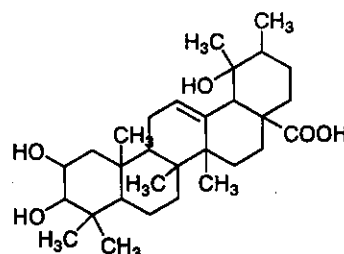
[分子式]  $C_{30}H_{48}O_5$

[分子量] 488.706

[基原] 次の植物の葉から分離: *Eriobotrya japonica*

[融点] Mp 270 °C

[比旋光度]:  $[\alpha]_D^{25} +69$  (c, 1 in MeOH)



----- 文献 -----

Herath, W.H.M.W. et al., Phytochemistry, 1978, 17, 1978, (分離)

Aimi, N. et al., Tetrahedron, 1989, 45, 4125, (分離)

Aquino, R. et al., J. Nat. Prod., 1990, 53, 559, (分離, H-NMR, C13-NMR)

Liang, Z. et al., Planta Med., 1990, 56, 330, (分離, H-NMR, C13-NMR, Mass)

Diyabalange, T.K.K. et al., Phytochemistry, 1995, 40, 1311, (Uncaric acid, 構造決定)

### § 3,19,23-Trihydroxy-12-ursen-28-oic acid; (3 $\beta$ , 19 $\alpha$ )-form, 3-O-(4-Hydroxy-E-cinnamoyl)

[化学名・別名] 3-*trans-p*-Coumaroylrotundic acid

[CAS No.] 144624-03-3

[化合物分類] テルペノイド (Ursane triterpenoids)

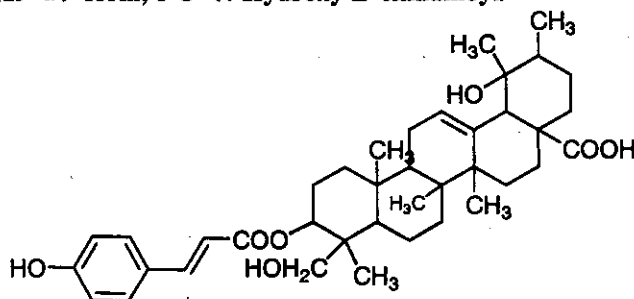
[構造式]

[分子式]  $C_{39}H_{54}O_7$

[分子量] 634.851

[基原] *Eriobotrya japonica*

[比旋光度]:  $[\alpha]_D^{25} +5.2$  (c, 1 in MeOH)



----- 文献 -----

De Tommasi, N. et al., J. Nat. Prod., 1992, 55, 1067, (*p*-coumaroyl ester)

### § Violaxanthin; (all-E)-form, Monodeoxy

[化学名・別名] 5,5',6,6'-Diepoxy-5,5',6,6'-tetrahydro- $\beta$ , $\beta$ -caroten-3-ol (CAS 名). Cryptoxanthin diepoxide

[CAS No.] 2086-87-5

[化合物分類] テルペノイド (Tetraterpenoids)

[構造式]

[分子式]  $C_{40}H_{56}O_3$

[分子量] 584.881

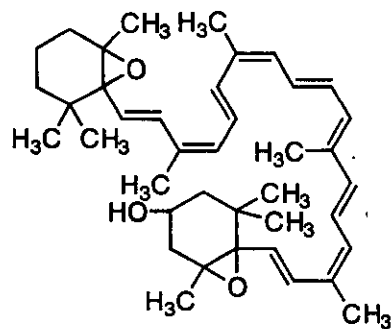
[基原] Prepared by oxidation of Cryptoxanthin; isol. from the algae of Xanthophyceae, the loquat fruit *Eriobotrya japonica* and *Prunus persica* fruit

[性状] 結晶 ( $C_6H_6$ /petrol)

[融点] Mp 194 °C

UV: [neutral]  $\lambda_{max}$  473 ; 503 (CS 2) [neutral]  $\lambda_{max}$  415 ; 438 ; 468

(溶媒の報告はない) [neutral]  $\lambda_{max}$  442 ; 472 (EtOH)



----- 文献 -----

de Ville, T.E. et al., Chem. Comm., 1969, 1311, (絶対構造)  
 Stransky, H. et al., Arch. Microbiol., 1970, 71, 164, (分離, deoxy)  
 Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag,  
 Sapozhnikov, D.I., Pure Appl. Chem., 1973, 35, 47, (レビュー)  
 Lessertois, D. et al., Phytochemistry, 1978, 17, 411, (分離, deoxy)  
 Straub, O. et al., Key to Carotenoids, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 259, (成書)  
 Baumeler, A. et al., Helv. Chim. Acta, 1992, 75, 773, (15,15'-didehydro)

\*\*\*\*\*ピンピネラ (Burnet) \*\*\*\*\*

§ § セリ科 (*Pimpinella saxifraga* L.) の全草及び種子。

§ 5,6-Dihydroxy-2*H*-furo [2,3-*h*]-1-benzopyran-2-one; Di-Me ether

[化学名・別名] 5,6-Dimethoxy-2*H*-furo [2,3-*h*]-1-benzopyran-2-one (CAS 名). Pimpinellin

[CAS No.] 131-12-4

[化合物分類] ベンゾピラノイド (5,6,7-Trioxxygenated coumarins), ベンゾピラノイド (Furanocoumarins),  
 薬物: GABA 拮抗薬 (GABA antagonists)

[構造式]

[分子式] C<sub>13</sub>H<sub>10</sub>O<sub>5</sub>

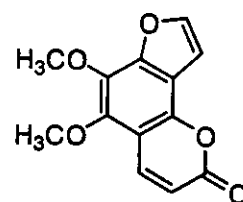
[分子量] 246.219

[基原] *Pimpinella saxifraga*. また *Pimpinella magna*, 数多くの *Heracleum* spp.

[用途] GABA 受容体拮抗薬, ファイトアレキシン

[性状] 結晶 (EtOAc/hexane)

[融点] Mp 117-119 °C



-----文献-----

Dreyer, D.L., J.O.C., 1970, 35, 2294-2297, (Isopentenylxybergapten)

Komisarenko, N.F. et al., Khim. Prir. Soedin., 1978, 14, 184-187; Chem. Nat. Compd. (Engl. Transl.), 1978,  
 14, 149-151, (Heraclesol)

Reed, M.W. et al., J.O.C., 1988, 53, 4166-4171, (合成法)

§ 1 (10),4-Germacradiene-2,6,11-triol; (1 (10)*E*,2 β,4*E*,6 β)-form, 6-*O*-β-D-Glucopyranoside

[CAS No.] 220698-74-8

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

[構造式]

[分子式] C<sub>21</sub>H<sub>34</sub>O<sub>8</sub>

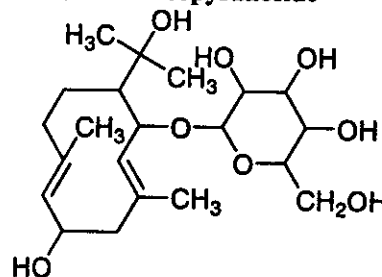
[分子量] 416.511

[基原] *Pimpinella saxifraga*

[性状] 針状結晶 (MeOH) (as penta-Ac)

[融点] Mp 178-180 °C (penta-Ac)

[比旋光度]: [α]<sub>D</sub><sup>21</sup> -16.8 (c, 1 in MeOH) (penta-Ac)



-----文献-----

Kisiel, W. et al., Phytochemistry, 1998, 49, 2031-2033, (分離, H-NMR, C13-NMR)

§ 6-Hydroxy-2*H*-furo [2,3-*h*]-1-benzopyran-2-one; Me ether

[化学名・別名] 6-Methoxy-2*H*-furo [2,3-*h*]-1-benzopyran-2-one (CAS 名). Sphondin

[CAS No.] 483-66-9

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

[構造式]

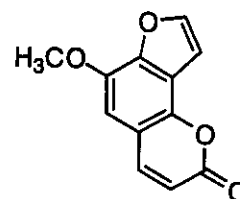
[分子式] C<sub>12</sub>H<sub>8</sub>O<sub>4</sub>

[分子量] 216.193

[基原] *Heracleum sphondylium* の種子, *Heracleum lanatum*, その他の *Heracleum*  
 spp., *Ruta pinnata*, *Pimpinella saxifraga*

[性状] 針状結晶 (EtOAc)

[融点] Mp 192-193 °C



-----文献-----

Späth, E. et al., Monatsh. Chem., 1936, 67, 344, (分離)

Späth, E. et al., Ber., 1941, 74, 595, (構造決定)

Wessely, F. et al., *Monatsh. Chem.*, 1953, 84, 217, (分離)  
Fujita, M. et al., *CA*, 1955, 49, 9241; 1956, 50, 12999, (分離)  
Gupta, B.D. et al., *Phytochemistry*, 1976, 15, 1319, (分離)

### § Isobergaptol; Me ether

[化学名・別名] 5-Methoxy-2*H*-furo[2,3-*h*]-1-benzopyran-2-one (CAS 名) (旧 CAS 名). Isobergapten

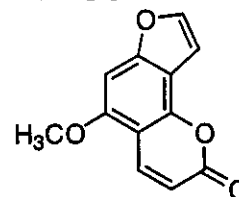
[CAS No.] 482-48-4

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

[構造式]

[分子式]  $C_{13}H_{10}O_4$

[分子量] 216.193



[基原] *Heracleum* spp. と *Pimpinella saxifraga* の根. また *Pimpinella magna*, *Ruta*

*pinnata*

[融点] Mp 222 °C

----- 文献 -----

Gupta, B.D. et al., *Phytochemistry*, 1975, 14, 2533, (分離)  
Gupta, B.D. et al., *Indian J. Chem., Sect. B*, 1978, 16, 38, (分離)

### § Isopimpinellin

[化学名・別名] 4,9-Dimethoxy-7*H*-furo[3,2-*g*] [1] benzopyran-7-one (CAS 名). 4,9-Dimethoxy-7-oxofuro[3,2-*g*] chromene. 4,9-Dimethoxypsoralen

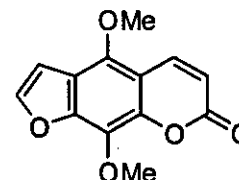
[CAS No.] 482-27-9

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

[構造式]

[分子式]  $C_{13}H_{10}O_5$

[分子量] 246.219



[基原] 次の植物に存在する: *Pimpinella saxifraga* と *Heracleum* spp. の根, *Skimmia laureola* の葉, *Ruta pinnata* の果実, *Archangelica officinalis*, *Pastinaca* spp., その他

[性状] 黄金色の針状結晶 (MeOH)

[融点] Mp 147-148 °C. Mp 151 °C

UV: [neutral]  $\lambda_{max}$  222 ( $\epsilon$  25120); 240 ( $\epsilon$  13490); 248 ( $\epsilon$  15850); 268 ( $\epsilon$  20900); 311 ( $\epsilon$  13800) (EtOH) (Berdy)

----- 文献 -----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1378, (生育)  
Austin, D.J. et al., *Phytochemistry*, 1973, 12, 1657, (合成)  
Innocenti, G. et al., *Phytochemistry*, 1983, 22, 2207-2209, (合成)

### § 2-(3-Methyl-2-oxiranyl)-1,4-benzenediol; 4-Me ether, 1-O-(2-methylpropanoyl)

[化学名・別名] Epoxypseudoisoengenol isobutanoate

[CAS No.] 97164-70-0

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

[構造式]

[分子式]  $C_{14}H_{18}O_4$

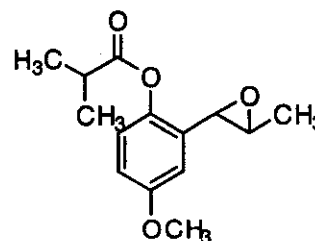
[分子量] 250.294

[基原] *Pimpinella diversifolia*, *Pimpinella major*, *Pimpinella saxifraga*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{25}$  436 +56 (c, 0.8 in  $CHCl_3$ )

[その他のデータ] *trans*-Isomer

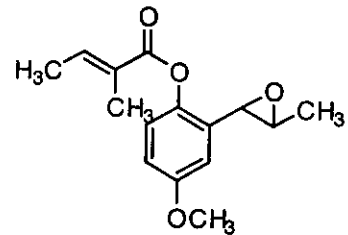


----- 文献 -----

Martin, R. et al., *Planta Med.*, 1985, 51, 198-202, (分離, 合成法, H-NMR, C13-NMR)  
Reichling, J. et al., *Z. Naturforsch., C*, 1985, 40, 465-468, (分離)  
Bottini, A.T. et al., *Phytochemistry*, 1986, 25, 207-211, (分離)  
Macias, M.J. et al., *Phytochemistry*, 1994, 37, 539, (分離, IR, H-NMR, C13-NMR)

### § 2-(3-Methyl-2-oxiranyl)-1,4-benzenediol; 4-Me ether, 1-O-tigloyl

[CAS No.]97164-71-1  
[その他の CAS No.]115016-19-8, 115016-20-1  
[化合物分類]単環芳香族 (Simple phenylpropanoids)  
[構造式]



[分子式]  $C_{13}H_{16}O_4$   
[分子量] 262.305  
[基原] *Pimpinella major*, *Pimpinella saxifraga*

----- 文献 -----

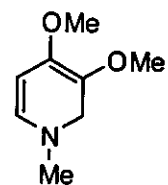
Martin, R. et al., *Planta Med.*, 1985, 51, 198-202, (分離, 合成法, H-NMR, C13-NMR)  
Reichling, J. et al., *Z. Naturforsch., C*, 1985, 40, 465-468, (分離)  
Bottini, A.T. et al., *Phytochemistry*, 1986, 25, 207-211, (分離)  
Macias, M.J. et al., *Phytochemistry*, 1994, 37, 539, (分離, IR, H-NMR, C13-NMR)

\*\*\*\*\*ピンロウ (Areca nut, Betel nut) \*\*\*\*\*

§ § ヤシ科ピンロウ (*Areca catechu* L.) の種子。

§ **Arecolidine**

[化学名・別名] 1,2-Dihydro-3,4-dimethoxy-1-methylpyridine (CAS 名)  
[CAS No.] 57680-57-6  
[化合物分類] アルカロイド化合物 (Miscellaneous pyridine alkaloids)  
[構造式]



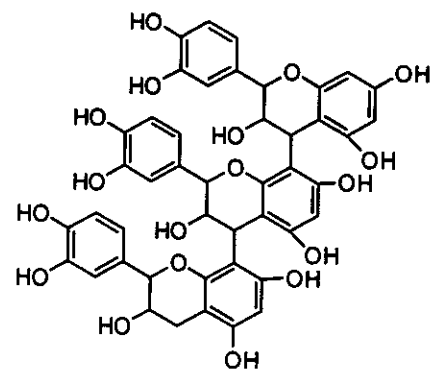
[分子式]  $C_8H_{13}NO_2$   
[分子量] 155.196  
[基原] 次の植物に含まれるアルカロイド微量成分: *Areca catechu* (キンマ) ナッツ (ヤシ科)  
[性状] 針状結晶 (Et<sub>2</sub>O or by subl.)  
[融点] Mp 110 °C

----- 文献 -----

Emde, H., *Chem. Zentralbl.*, 1915, 1381, (分離)  
Dehmlow, E.V. et al., *Heterocycles*, 1994, 37, 355

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

[化学名・別名] [Epicatechin (4 β → 8)]<sub>2</sub>-catechin. Arecatannin A<sub>1</sub>  
[CAS No.] 79813-67-5  
[化合物分類] フラボノイド (Proanthocyanidin flavonoids)  
[構造式]



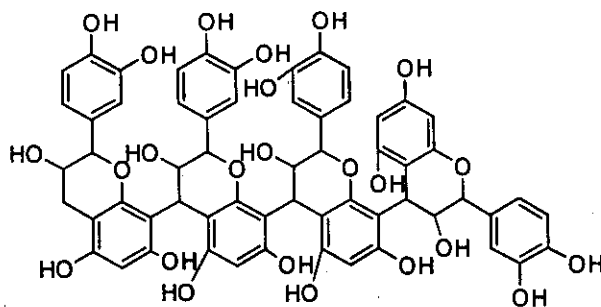
[分子式]  $C_{25}H_{32}O_{18}$   
[分子量] 866.784  
[基原] 次の植物から分離: *Areca catechu*, *Pinus taeda*, その他の植物属.  
[比旋光度]:  $[\alpha]_D +74$  (H<sub>2</sub>O)

----- 文献 -----

Nonaka, G. et al., *Chem. Comm.*, 1981, 781, (分離)  
Hemingway, R.W. et al., *J.C.S. Perkin 1*, 1982, 1209, (分離)  
Hsu, F.L. et al., *Chem. Pharm. Bull.*, 1985, 33, 3293, (分離)  
Delcour, J.A. et al., *J. Inst. Brewing*, 1986, 92, 244, (誘導體)  
Kolodziej, H., *Phytochemistry*, 1986, 25, 1209; 1989, 28, 3487; 1990, 29, 955, (合成法, 分離)  
Morimoto, S. et al., *Phytochemistry*, 1988, 27, 907, (分離)  
Foo, L.Y. et al., *Phytochemistry*, 1989, 28, 1743, (分離)  
Geiss, F. et al., *Phytochemistry*, 1995, 39, 635, (分離)

§ [ 3,3',4',5,7-Pentahydroxyflavan (4 → 8) ] : -3,3',4',5,7-pentahydroxyflavan; (3''S)-form  
[化学名・別名] [Epicatechin (4 β → 8)]<sub>2</sub> catechin. Arecatannin A<sub>2</sub>

[CAS No.] 79763-29-4  
 [化合物分類] フラボノイド  
 (Proanthocyanidin flavonoids)  
 [構造式]



[分子式]  $C_{60}H_{50}O_{24}$   
 [分子量] 1155.041  
 [基原] 次の植物の種子から分離: *Areca catechu*  
 [比旋光度]:  $[\alpha]_D +98.6$  (Me<sub>2</sub>CO)

----- 文献 -----

Nonaka, G. et al., Chem. Comm., 1981, 781, (分離)  
 Delcour, J.A. et al., J.C.S. Perkin 1, 1983, 1711; 1985, 669, (合成法)  
 Kolodziej, H. et al., J.C.S. Perkin 1, 1984, 343, (分離)  
 Ezaki-Furuichi, E. et al., Agric. Biol. Chem., 1986, 50, 2061, (分離)  
 Morimoto, S. et al., Chem. Pharm. Bull., 1986, 34, 633, (分離)

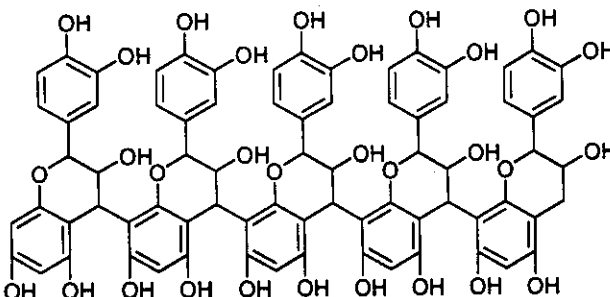
§ [3,3',4',5,7-Pentahydroxyflavan(4 → 8)]<sub>4</sub> -3,3',4',5,7-pentahydroxyflavan; (3''''S)-form

[化学名・別名] [Epicatechin(4 β → 8)]<sub>4</sub> catechin. Arecatannin A<sub>3</sub>

[CAS No.] 86588-85-4

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

[構造式]



[分子式]  $C_{75}H_{60}O_{30}$

[分子量] 1443.297

[基原] 次の植物から分離: *Areca catechu*

[性状] 物理化学的性質に関する報告はない

----- 文献 -----

Morimoto, S. et al., Chem. Pharm. Bull., 1986, 34, 633, (分離)  
 Gujer, R. et al., Phytochemistry, 1986, 25, 1431, (分離)  
 Foo, L.Y. et al., Phytochemistry, 1991, 30, 667, (分離)

§ [3,3',4',5,7-Pentahydroxyflavan(4 → 8)]<sub>2</sub> -3,3',4',5,7-pentahydroxyflavan(4 → 6)  
 -3,3',4',5,7-pentahydroxyflavan; (2R,2'R,2''R,2'''R,3R,3'R,3''R,3'''S,4'R)-form

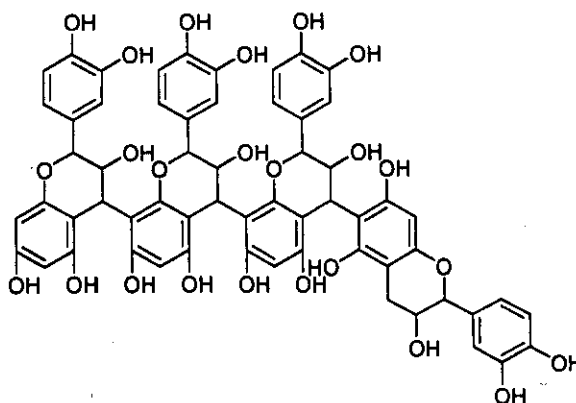
[化学名・別名] [Epicatechin(4 β → 8)]<sub>2</sub> epicatechin(4 β → 6) catechin

[CAS No.] 79763-27-2

[化合物分類] フラボノイド

(Proanthocyanidin flavonoids)

[構造式]



[分子式]  $C_{60}H_{50}O_{24}$

[分子量] 1155.401

[基原] 次の植物の種子から分離: *Areca catechu*

[比旋光度]:  $[\alpha]_D +134.8$  (Me<sub>2</sub>CO)

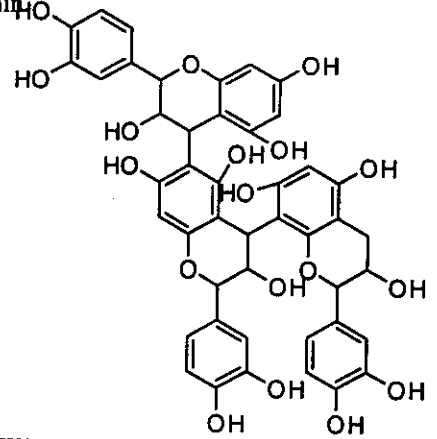
----- 文献 -----

Nonaka, G. et al., Chem. Comm., 1981, 781, (分離)  
 Ezaki-Furuichi, E. et al., Agric. Biol. Chem., 1986, 50, 2061, (分離)

§ 3,3',4',5,7-Pentahydroxyflavan(4 → 6) -3,3',4',5,7-pentahydroxyflavan(4 → 8)  
 -3,3',4',5,7-pentahydroxyflavan; (2R,2'R,2''R,3R,3'R,3''S,4R,4'R)-form



[化学名・別名]Epicatechin-(4 $\beta$ →6)-epicatechin-(4 $\beta$ →8)-catechin  
[CAS No.] 82801-35-2  
[化合物分類]フラボノイド (Proanthocyanidin flavonoids)  
[構造式]



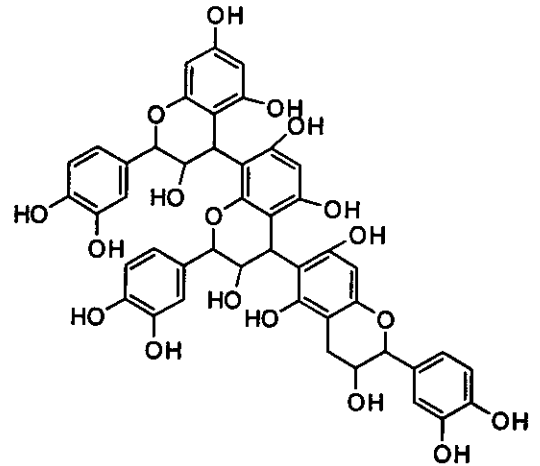
[分子式] C<sub>45</sub>H<sub>36</sub>O<sub>18</sub>  
[分子量] 866.784  
[基原] 次の植物から分離: *Areca catechu*, *Dioscorea cirrhosa*,  
*Kandelia candel*, *Pinus taeda*, その他の植物属.  
[性状] 灰白色の無定型の粉末  
[比旋光度]:  $[\alpha]_D^{25} +138.2$  (c, 0.5 in Me<sub>2</sub>CO)

-----文献-----

Hsu, F.L. et al., Chem. Pharm. Bull., 1985, 33, 3142; 3293, (分離)  
Ezaki-Furuichi, E. et al., Agric. Biol. Chem., 1986, 50, 2061, (分離)  
Foo, L.Y. et al., Phytochemistry, 1989, 28, 1743, (分離)  
Kolodziej, H., Phytochemistry, 1990, 29, 955, (分離)

§ 3,3',4',5,7-Pentahydroxyflavan(4→8)-3,3',4',5,7-pentahydroxyflavan(4→6)-3,3',4',5,7-pentahydroxyflavan; (2*R*,2'*R*,2''*R*,3*R*,3'*R*,3''*S*,4*R*,4'*R*)-form

[化学名・別名]Epicatechin(4 $\beta$ →8)epicatechin(4 $\beta$ →6)catechin. Arecatannin B<sub>1</sub>  
[CAS No.] 79763-28-3  
[化合物分類]フラボノイド (Proanthocyanidin flavonoids)  
[構造式]



[分子式] C<sub>45</sub>H<sub>36</sub>O<sub>18</sub>  
[分子量] 866.784  
[基原] 次の植物から分離: *Areca catechu*, *Betula* spp.,  
*Illicium anisatum*, *Pinus taeda*, *Thujopsis dolabrata*  
[性状] Off-white 無定型の塊 + 1/2H<sub>2</sub>O  
[比旋光度]:  $[\alpha]_D +207$  (c, 0.11 in H<sub>2</sub>O)

-----文献-----

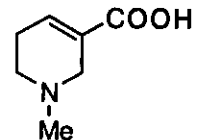
Nonaka, G. et al., Chem. Comm., 1981, 781, (分離)  
Hemingway, R.W. et al., J.C.S. Perkin 1, 1982, 1209, (分離)  
Ezaki-Furuichi, E. et al., Agric. Biol. Chem., 1986, 50, 2061, (分離)  
Nonaka, G. et al., Chem. Pharm. Bull., 1987, 35, 1105, (分離)  
Kolodziej, H., Phytochemistry, 1989, 28, 3487; 1990, 29, 955, (分離)  
Cui, C.-B. et al., Chem. Pharm. Bull., 1992, 40, 889, (分離, H-NMR, C13-NMR)

§ 1,2,5,6-Tetrahydro-1-methyl-3-pyridinecarboxylic acid (CAS 名)

[化学名・別名]Arecidine. Arecaine  
[CAS No.] 499-04-7  
[化合物分類]アルカロイド化合物 (Nicotinic acid derived alkaloids), 薬物: 駆虫薬 (Anthelmintics)  
[構造式]

[分子式] C<sub>7</sub>H<sub>11</sub>NO<sub>2</sub>  
[分子量] 141.169

[基原] 次の植物のナッツから得られるアルカロイド: *Areca catechu* (betel nuts) (ヤシ科)



[用途] Cholinergic and anthelmintic agent  
[融点] Mp 223-224 °C で分解 (無水物は 232 °C で分解)  
[PKa 値] pK<sub>a</sub> 9.07 (25 °C)  
[Log P 計算値] Log P -1.74 (計算値)

[その他のデータ]強い塩基性  
[化学物質毒性データ総覧(RTECS)登録番号]QT2070800

-----文献-----

Jahns, E., Ber., 1888, 21, 3404, (分離)  
Wohl, A. et al., Ber., 1907, 40, 4712, (構造決定, 合成法)  
Chemnitius, F., J. Prakt. Chem., 1927, 117, 147, (分離, 誘導體)  
Nery, R., Biochem. J., 1971, 122, 503, (代謝, 毒性, 成書)  
Burrows, R.B., Prog. Drug Res., 1973, 17, 108, (レビュー)  
Strunz, G.M. et al., Alkaloids (N.Y.), 1985, 26, 89, (レビュー)  
Hollander, E. et al., Br. Med. Bull., 1986, 42, 97, (薬理)

\*\*\*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\*\*\*

\*\*\*変異原性に関するデータ\*\*\*

<<試験方法>> 姉妹染色分体交換.  
曝露経路 : 腹腔内投与.  
試験系 : げっ歯類-マウス.  
投与量・期間 : 1 gm/kg/5 日間 (間欠的)

参考文献

Cancer Letters (Shannon, Ireland). (Elsevier Scientific Pub. Ireland Ltd., POB 85, Limerick, Ireland)  
23,189,1984

<<試験方法>> 形態的形質変換.  
試験系 : げっ歯類-ハムスター腎臓.  
投与量・期間 : 2500 ug/L

参考文献

Lancet. (7 Adam St., London WC2N 6AD, UK) 1,112,1979

<<試験方法>> ほ乳類の体細胞突然変異試験  
試験系 : げっ歯類-ハムスター肺.  
投与量・期間 : 10 mg/L

参考文献

Carcinogenesis (London). (Oxford Univ. Press, Pinkhill House, Southfield Road, Eynsham, Oxford OX8 1JJ,  
UK) 5,501,1984

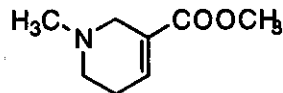
§ 1,2,5,6-Tetrahydro-1-methyl-3-pyridinecarboxylic acid; Me ester

[化学名・別名] Arecoline

[CAS No.] 63-75-2

[化合物分類] 薬物: 駆虫薬 (Anthelmintics), 薬物: 緩下剤 (Laxatives), 薬物: 血圧降下薬 (Hypotensive agents), アルカロイド化合物 (Nicotinic acid derived alkaloids)

[構造式]



[分子式] C<sub>8</sub>H<sub>13</sub>NO<sub>2</sub>

[分子量] 155.196

[基原] 次の植物から得られるアルカロイド: *Areca catechu* (ヤシ科)

[用途] しゃ下剤, 駆虫作用, 血圧降下作用等. 一般にコリン作用物質として用いる; 獣医分野では血圧降下, 条虫駆除薬として用いる

[性状] 液体

[沸点] Bp<sub>17</sub> 94 °C. Bp<sub>7</sub> 74 °C

[PKa 値] pK<sub>a</sub> 7.64 (25 °C)

[Log P 計算値] Log P 1.05 (計算値)

[傷害・毒性] 50%致死量 (LD<sub>50</sub>) (イヌ, 皮下) 5 mg/kg, 50%致死量 (LD<sub>50</sub>) (ラット, 経口) 2500 mg/kg

[化学物質毒性データ総覧(RTECS)登録番号] QT2100000

-----文献-----

Jahns, E., Ber., 1888, 21, 3404, (分離)  
Wohl, A. et al., Ber., 1907, 40, 4712, (構造決定, 合成法)  
Chemnitius, F., J. Prakt. Chem., 1927, 117, 147, (分離, 誘導體)  
Nery, R., Biochem. J., 1971, 122, 503, (代謝, 毒性, 成書)  
Burrows, R.B., Prog. Drug Res., 1973, 17, 108, (レビュー)  
Strunz, G.M. et al., Alkaloids (N.Y.), 1985, 26, 89, (レビュー)

Hollander, E. et al., Br. Med. Bull., 1986, 42, 97, (薬理)

\*\*\*RTECS (化学物質毒性データ)\*\*\*

生体影響物質 : 催腫瘍物質, 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 : 経口投与.

被験動物 : げっ歯類-ラット.

投与量・期間 : 2500 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.

参考文献

European Journal of Medicinal Chemistry--Chimie Therapeutique. (Editions Scientifiques Elsevier, 29 rue Buffon, F-75005, Paris, France) 26,853,1991

<<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 : 40 mg/kg

毒性影響 : [知覚組織と特異感覚] (視覚) 流涙.  
[行動] 痙攣または発作閾値への影響.  
[血管] 収縮(分離した組織).

参考文献

Biochemical Journal. (Biochemical Soc. Book Depot, POB 32, Commerce Way, Colchester, Essex CO2 8HP, UK) 113,123,1969

<<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 : 550 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.

参考文献

European Journal of Medicinal Chemistry--Chimie Therapeutique. (Editions Scientifiques Elsevier, 29 rue Buffon, F-75005, Paris, France) 26,853,1991

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 腹腔内投与.

被験動物 : げっ歯類-マウス.

投与量・期間 : 190 mg/kg

毒性影響 : [栄養と総代謝] 体温低下.

参考文献

Archives Internationales de Pharmacodynamie et de Therapie. (Heymans Institute of Pharmacology, De Pintelaan 185, B-9000 Ghent, Belgium) 192,88,1971

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 静脈内投与.

被験動物 : げっ歯類-マウス.

投与量・期間 : 36 mg/kg

毒性影響 : [行動] 傾眠(全身活動度の低下).  
[行動] 痙攣または発作閾値への影響.  
[行動] 興奮.

参考文献

Farmakologiya i Toksikologiya (Moscow). For English translation, see PHTXA6 and RPTOAN. (V/O Mezhdunarodnaya Kniga, 113095 Moscow, USSR) 28,33,1965

<<試験方法>> 認知されている最低致死量に関する試験

曝露経路 : 報告なし.

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.

参考文献

"Abderalden's Handbuch der Biologischen Arbeitsmethoden." (Leipzig, Ger. Dem. Rep.) 4,1289,1935

<<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 : ほ乳類-イヌ.  
投与量・期間 : 5 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

Fortschritte der Arzneimittelforschung. Progress in Drug Research. (Birkhauser Boston, Inc., c/o Springer-Verlag New York, 44 Hartz Way, Secaucus, NJ 07094) 17,108,1973

<<試験方法>> 認知されている最低致死量に関する試験  
曝露経路 : 報告なし.  
被験動物 : ほ乳類-イヌ.  
投与量・期間 : 5 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

"Abderalden's Handbuch der Biologischen Arbeitsmethoden." (Leipzig, Ger. Dem. Rep.) 1289,1935  
\*\*\*催腫瘍性に関するデータ\*\*\*

<<試験方法>> 最小毒性量(TDLo).  
曝露経路 : 皮膚への塗布  
被験動物 : げっ歯類-ハムスター.  
投与量・期間 : 2698 mg/kg/65 週間間欠投与  
毒性影響 : [催腫瘍性] RTECS 基準による催腫瘍性.  
[胃腸] 腫瘍.

参照文献

Journal of the National Cancer Institute. (Washington, DC) 53,1259,1974  
\*\*\*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 umol/plate

参照文献

Mutation Research. (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherlands) 360,165,1996  
<<試験方法>> DNA 損傷  
試験系 : ヒトの細胞(種は未特定).  
投与量・期間 : 20 ug/tube

参照文献

Mutation Research. (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherlands) 278,271,1992  
<<試験方法>> DNA 阻害.  
試験系 : ヒトの細胞(種は未特定).  
投与量・期間 : 339 umol/L

参照文献

International Journal of Cancer. (International Union Against Cancer, 3 rue du Conseil- General, 1205 Geneva, Switzerland) 47,396,1991  
<<試験方法>> 小核試験.  
曝露経路 : 腹腔内投与.  
試験系 : げっ歯類-マウス.  
投与量・期間 : 80 mg/kg

参照文献

Carcinogenesis (London). (Oxford Univ. Press, Pinkhill House, Southfield Road, Eynsham, Oxford OX8 1JJ, UK) 5,501,1984  
<<試験方法>> 不定期 DNA 合成.  
曝露経路 : 腹腔内投与.  
試験系 : げっ歯類-マウス.  
投与量・期間 : 20 mg/kg

参照文献

Mutation Research. (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherlands) 158,189,1985  
<<試験方法>> 細胞遺伝学的分析.  
曝露経路 : 腹腔内投与.  
試験系 : げっ歯類-マウス.  
投与量・期間 : 100 mg/kg/10 日間 (連続的)