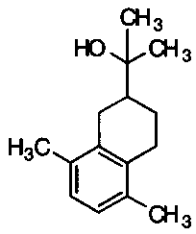
[分子量]236.353
[正確な分子量]236.17763
[基原]*Thuja occidentalis*
[性状]結晶
[融点]Mp 42-44 ℃
[比旋光度]:[α]$_D$ -139
[溶解性]メタノール, クロロホルム, エーテルに可溶; 水に難溶

----------文献----------

Tomita, B. et al., Tet. Lett., 1970, 235

§ Occidol; (*R*)-form

[CAS No.]5986-36-7
[化合物分類]テルペノイド(Emmotin sesquiterpenoid)
[構造式]



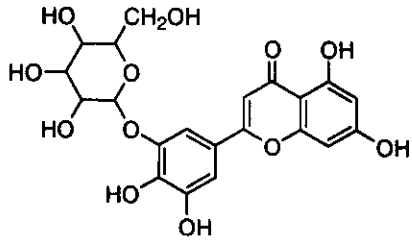
[基原]*Thuja occidentalis*
[性状]結晶
[融点]Mp 69-70 ℃
[比旋光度]:[α]$_D$ +163.7 (c, 1.2 in $CHCl_3$)

----------文献----------

Nakazaki, M. et al., Bull. Chem. Soc. Jpn., 1962, 35, 1387, (絶対構造)
Ho, T.-L., J.C.S. Perkin 1, 1973, 2579
Reddy, P.A. et al., Indian J. Chem., Sect. B, 1980, 19, 753, (合成法)
Sattar, A. et al., Indian J. Chem., Sect. B, 1992, 31, 187, (合成法)
Banerjee, A.K. et al., Tetrahedron, 1993, 49, 4761, (合成法, レビュー)
Weyerstahl, P. et al., Annalen, 1996, 99, (分離, H-NMR, Mas)
Ho, T.-L. et al., J.C.S. Perkin 1, 1999, 1207, (合成法)

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

[CAS No.]22149-72-0
[化合物分類]フラボノイド(Flavones; 5 × O-置換基)
[構造式]



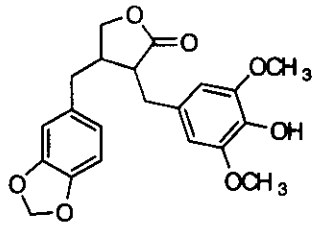
[分子式]$C_{21}H_{20}O_{12}$
[分子量]464.382
[正確な分子量]464.09548
[基原]*Lathyrus pratensis* と *Thuja occidentalis* の葉
[性状]針状結晶(Me_2CO 溶液)
[融点]Mp 284-285 ℃

----------文献----------

Malcher, E. et al., Acta Pol. Pharm., 1967, 24, 339; CA, 68, 93469, (分離, 構造決定)
Lamer, E. et al., Tet. Lett., 1968, 1419, (分離, 構造決定)
D'Arcy, A. et al., Phytochemistry, 1978, 17, 826, (分離)
Reynaud, J. et al., Phytochemistry, 1981, 20, 2052, (3'-glucoside, 7-diglucoside)
Markham, K.R. et al., Phytochemistry, 1984, 23, 1931, (3',5'-diglucoside)
Kraut, L. et al., Phytochemistry, 1993, 34, 211; 1999, 52, 749, (誘導体)

§ 3,3',4,4',5-Pentahydroxylignan-9,9'-olide; (8*R*,8'*R*)-form, 3',4'-Methylene, 3,5-di-Me ether

[化学名・別名]4-Hydroxy-3,5-dimethoxy-3',4'-methylenedioxylignan-9,9'-olide.
4-*O*-Demethylyatein
[化合物分類]リグナン化合物(Saturated dibenzylbutyrolactone lignan)
[構造式]

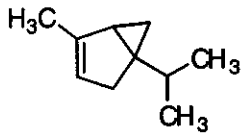


[分子式]$C_{21}H_{22}O_7$
[分子量]386.401
[正確な分子量]386.136555
[基原]*Thuja occidentalis*
[性状]オイル

[比旋光度]:[α]$_D$25 -25 (c, 0.32 in CH_2Cl_2)

----------文献----------

Feliciano, A.S. et al., Phytochemistry, 1991, 30, 3483, (Demethylyatein)
Kawai, S. et al., Phytochemistry, 1994, 37, 1699, (4-Demethylyatein)



§ 3-Thujene; (-)-form

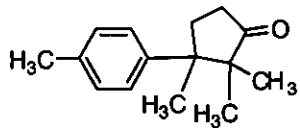
[CAS No.]3917-48-4
[化合物分類]テルペノイド(Thujane monoterpenoid)
[構造式]
[基原]次の植物から分離: *Thuja occidentalis* のオイルとその他の精油
[沸点]Bp 150.5-152.5 ℃
[比旋光度]:[α]$_D$ -14.76
[屈折率]n^{20}_D 1.4559

----------文献----------

Shaw, A.C., Can. J. Chem., 1953, 31, 277, (分離)
Norin, T., Acta Chem. Scand., 1962, 16, 640, (絶対構造)
Acharya, S.P. et al., J.O.C., 1969, 34, 3015, (絶対構造)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 59, (生育)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 1, 77, (レビュー)

§§ ヒノキ科コノテガシワ(*Thuja orientalis* L.)の葉または材。

§ α-Cuparenone; (*S*)-form

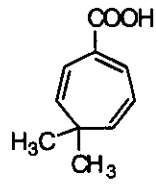


[化合物分類]テルペノイド(Cuparane sesquiterpenoid)
[構造式]
[基原]Mayur pankhi(*Thuja orientalis* もしくは *Thuja compacta*)の木部
[性状]結晶
[融点]Mp 52-53 ℃
[比旋光度]:[α]$_D^{30}$ +177.1

----------文献----------

Chetty, F.-L. et al., Tet. Lett., 1964, 73, (分離)
Irie, T. et al., Tet. Lett., 1967, 3187, (絶対構造)
Tomita, B. et al., Tet. Lett., 1968, 843, (α-Cuparenol)
Benesova, V. et al., Coll. Czech. Chem. Comm., 1976, 41, 3812, (分離)
Greene, A.E. et al., J.O.C., 1983, 48, 4763, (合成法, 成書)
Posner, G.H. et al., Tet. Lett., 1984, 25, 383, (合成法, 成書)
Avila-Zaacuterraga, J.G. et al., Chem. Lett., 2000, 512, (合成法)
Nakashima, H. et al., Tet. Lett., 2000, 41, 2639, (合成法)

§ 5,5-Dimethyl-1,3,6-cycloheptatriene-1-carboxylic acid(CAS 名)



[化学名・別名]Thujic acid. Dehydroperillic acid
[CAS No.]499-89-8
[化合物分類]テルペノイド(Cycloheptane monoterpenoid)
[構造式]
[分子式]$C_{10}H_{12}O_2$
[分子量]164.204
[正確な分子量]164.08373
[基原]*Thuja plicata* の心材. また *Thuja orientalis, Libocedrus formosana*
[性状]結晶(petrol)
[融点]Mp 88-89 ℃
[溶解性]メタノール, エーテルに可溶; 水に難溶
[UV]:[neutral] λ $_{max}$ 220 (ε 18620); 280 (ε 3980) (EtOH)

[その他のデータ]不安定

----------文献----------

Gripenberg, J., Acta Chem. Scand., 1949, 3, 1137,（分離, 構造決定）
Kurth, E.F., J.A.C.S., 1950, 72, 5778,（分離, エステル）
Gripenberg, J., CA, 1952, 46, 5005,（合成法）
Davis, R.E. et al., J.A.C.S., 1966, 88, 4583,（結晶構造）
Hack, V. et al., Can. J. Chem., 1973, 51, 3230,（分離）
Guenther, H. et al., Org. Magn. Reson., 1974, 6, 388,（H-NMR）

§ 1,16-Hexadecanediol（CAS 名）

[CAS No.]7735-42-4
[関連 CAS No.]23079-20-1
[化合物分類]脂肪族化合物(Saturated unbranched alcohol)
[構造式] $HOCH_2(CH_2)_{14}CH_2OH$
[分子式]$C_{16}H_{34}O_2$
[分子量]258.443
[正確な分子量]258.25588
[基原]針葉樹のワックス, 例えば, *Pinus thunbergii*, *Thuja orientalis* から分離, *Cycas revoluta* から分離
[性状]針状結晶(C_6H_6), 板状結晶（EtOH）
[融点]Mp 91.5 ℃

----------文献----------

Aldrich Library of NMR Spectra, 2nd edn., 1983, 1, 129B,（H-NMR）
Aldrich Library of FT-IR Spectra, 1st edn., 1985, 3, 200A,（IR）
Chiut, P., Helv. Chim. Acta, 1926, 9, 264; 274,（合成法）
Kariyone, T. et al., CA, 1952, 46, 5869; 1956, 50, 13748; 1959, 53, 10031,（分離）
Tanaka, A., Yakugaku Zasshi, 1959, 79, 1327,（合成法）
Taits, S.Z. et al., Izv. Akad. Nauk SSSR, Ser. Khim., 1963, 1289; CA, 59, 13990,（合成法）
Saotome, K. et al., Bull. Chem. Soc. Jpn., 1966, 39, 480,（合成法）
Nakamura, N. et al., Acta Cryst. C, 1994, 50, 946,（結晶構造）
Braun, M. et al., Eur. J. Org. Chem., 2000, 1173,（合成法, IR, H-NMR, C13-NMR, Mas）

*********シトラス（Citrus）*********

§§ ミカン科イヨカン(*Citrus iyo* Hort. ex Tanaka)の果実。

§ Bis(1-hydroxydecyl) peroxide

[化学名・別名]1,1'-Dioxybis-1-decanol(CAS 名)
[CAS No.]26536-63-0
[構造式] $H_3C(CH_2)_8CH(OH)$-O-O-$CH(OH)(CH_2)_8CH_3$
[分子式]$C_{20}H_{42}O_4$
[分子量]346.549
[正確な分子量]346.30831
[基原]*Citrus iyo* の皮

----------文献----------

Hiroi, M. et al., CA, 1973, 79, 70085m,（分離）
Kobayashi, A. et al., Agric. Biol. Chem., 1990, 54, 561-562,（分離）
Kobayashi, A. et al., J. Agric. Food Chem., 1993, 41, 1297-1299,（合成法）

§ Bis(1-hydroxydodecyl) peroxide

[化学名・別名]1,1'-Dioxybis-1-dodecanol(CAS 名)
[CAS No.]73321-58-1
[構造式] $H_3C(CH_2)_{10}CH(OH)$-O-O-$CH(OH)(CH_2)_{10}CH_3$
[分子式]$C_{24}H_{50}O_4$

[分子量]402.657
[正確な分子量]402.37091
[基原]*Citrus iyo* の皮

----------文献----------

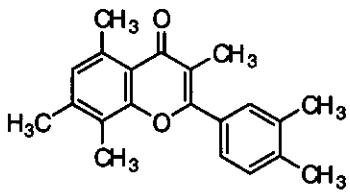
Kobayashi, A. et al., Agric. Biol. Chem., 1990, 54, 561-562,（分離）
Kobayashi, A. et al., J. Agric. Food Chem., 1993, 41, 1297-1299,（合成法）

§ Bis(1-hydroxyundecyl) peroxide
[化学名・別名]1,1'-Dioxybis-1-undecanol（CAS 名）
[CAS No.]66443-78-5
[構造式]$H_3C(CH_2)_9CH(OH)$-O-O-$CH(OH)(CH_2)_9CH_3$
[分子式]$C_{22}H_{46}O_4$
[分子量]374.603
[正確な分子量]374.33961
[基原]*Citrus iyo* の皮

----------文献----------

Kobayashi, A. et al., Agric. Biol. Chem., 1990, 54, 561-562,（分離）
Kobayashi, A. et al., J. Agric. Food Chem., 1993, 41, 1297-1299,（合成法）

§ 3,3',4',5,7,8-Hexamethylflavone
[化学名・別名]2-(3,4-Dimethylphenyl)-3,5,7,8-tetramethyl-4*H*-1-benzopyran-4-one（CAS 名）
[CAS No.]119637-11-5
[化合物分類]フラボノイド(Flavone)
[構造式]

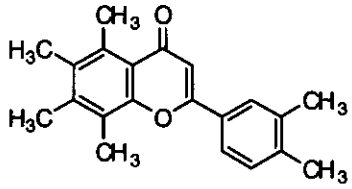


[分子式]$C_{21}H_{22}O_2$
[分子量]306.404
[正確な分子量]306.16198
[基原]*Citrus iyo* の皮

----------文献----------

Machida, K. et al., CA, 1989, 110, 132219c,（分離）

§ 3',4',5,6,7,8-Hexamethylflavone
[化学名・別名]2-(3,4-Dimethylphenyl)-5,6,7,8-tetramethyl-4*H*-1-benzopyran-4-one（CAS 名）
[CAS No.]119610-97-8
[化合物分類]フラボノイド(Flavone)
[構造式]

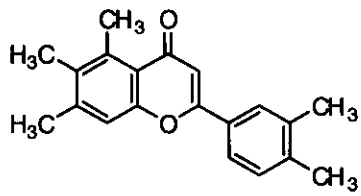


[分子式]$C_{21}H_{22}O_2$
[分子量]306.404
[正確な分子量]306.16198
[基原]*Citrus iyo* の皮

----------文献----------

Machida et al., CA, 1989, 110, 132219c,（分離）

§ 3',4',5,6,7-Pentamethylflavone
[化学名・別名]2-(3,4-Dimethylphenyl)-5,6,7-trimethyl-4*H*-1-benzopyran-4-one（CAS 名）
[CAS No.]119610-96-7
[化合物分類]フラボノイド(Flavone)
[構造式]

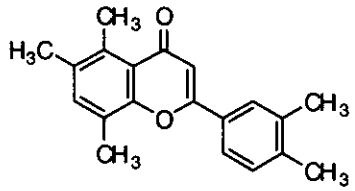


[分子式]$C_{20}H_{20}O_2$
[分子量]292.377
[正確な分子量]292.14633
[基原]*Citrus iyo* の皮

----------文献----------

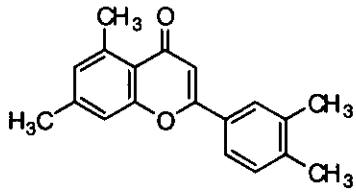
Machida, K. et al., CA, 1989, 110, 132219c,（分離）

§ 3',4',5,6,8-Pentamethylflavone
[化学名・別名]2-(3,4-Dimethylphenyl)-5,6,8-trimethyl-4*H*-1-benzopyran-4-one(CAS 名)
[CAS No.]119637-10-4
[化合物分類]フラボノイド(Flavone)
[構造式]
[分子式]$C_{20}H_{20}O_2$
[分子量]292.377
[正確な分子量]292.14633
[基原]*Citrus iyo* の皮



----------文献----------
Machida, K. et al., CA, 1989, 110, 132219c, (分離)

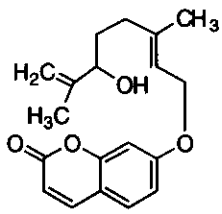
§ 3',4',5,7-Tetramethylflavone
[化学名・別名]2-(3,4-Dimethylphenyl)-5,7-dimethyl-4*H*-1-benzopyran-4-one(CAS 名)
[CAS No.]119610-94-5
[化合物分類]フラボノイド(Flavone), フラボノイド(Flavanones)
[構造式]
[分子式]$C_{19}H_{18}O_2$
[分子量]278.35
[正確な分子量]278.13068
[基原]*Citrus iyo* の皮



----------文献----------
Machida, K. et al., CA, 1989, 110, 132219c, (分離)

§§ ミカン科ハッサク(*Citrus hassaku* Hort. ex Tanaka)の果実。

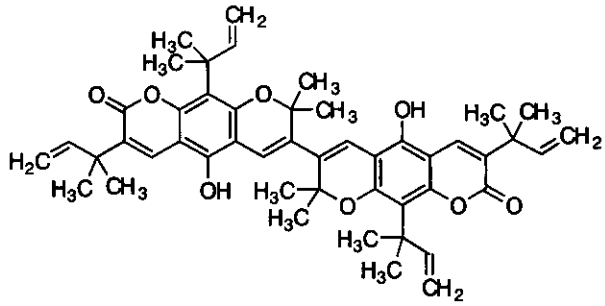
§ Auraptene; Δ $^{7'}$-Isomer, 6'*R*-hydroxy
[化学名・別名]7-[(6-Hydroxy-3,7-dimethyl-2,7-octadienyl) oxy]-2*H*-1-benzopyran-2-one
[CAS No.]118584-19-3
[化合物分類]ベンゾピラノイド(7-Oxygenated coumarins, unsubstituted)
[構造式]
[分子式]$C_{19}H_{22}O_4$
[分子量]314.38
[正確な分子量]314.15181
[基原]次の植物から分離:*Citrus hassaku* の果汁オイル
[性状]結晶
[融点]Mp 75 ℃
[比旋光度]:$[\alpha]_D^{26}$ +10 (c, 1.0 in EtOH)



----------文献----------
Kariyone, T. et al., Chem. Pharm. Bull., 1959, 1, 119, (構造決定, 合成法, 成書)
Bohlmann, F. et al., Chem. Ber., 1970, 103, 3619; 1974, 107, 1780; 1976, 109, 1584, (分離, Diversinin)
Bevalot, F. et al., Phytochemistry, 1988, 27, 1546, (誘導体)
Aziz, M. et al., Tetrahedron, 1988, 44, 101, (Auraptenol, 合成法)
Rashid, M.A. et al., J. Nat. Prod., 1992, 55, 851, (6'-hydroperoxy)
Masuda, T. et al., Phytochemistry, 1992, 31, 1363, (6'-hydroxy)
Chen, I.-S. et al., Phytochemistry, 1995, 39, 1091, (Acetoxyauraptene)
Yamada, Y. et al., Biosci., Biotechnol., Biochem., 1997, 61, 740, (活性)
Chang, C.T. et al., Phytochemistry, 1997, 45, 1419, (分離, 誘導体)

§ Bisclausarin
[CAS No.]137472-62-9
[化合物分類]ベンゾピラノイド(Bis- and tris-coumarin)

[構造式]



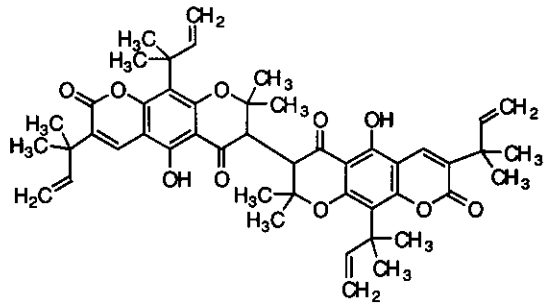
[分子式]$C_{48}H_{54}O_8$
[分子量]758.95
[正確な分子量]758.38187
[基原]*Citrus hassaku* の根
[性状]不安定な黄色オイル

----------文献----------

Ju-ichi, M. et al., Heterocycles, 1991, 32, 1189,（分離, H-NMR, C13-NMR）

§ Bishassinidin

[CAS No.]158402-62-1
[化合物分類]ベンゾピラノイド(5,7-Dioxygenated coumarin), ベンゾピラノイド(Bis- and tris-coumarin), ベンゾピラノイド(Pyranocoumarin)
[構造式]



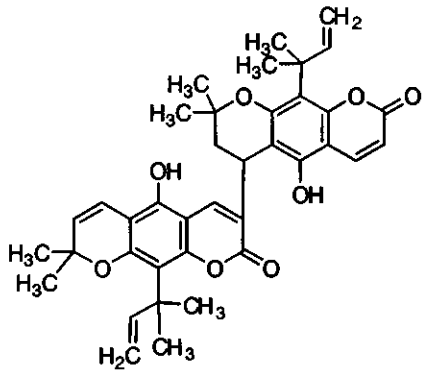
[分子式]$C_{48}H_{54}O_{10}$
[分子量]790.949
[正確な分子量]790.3717
[基原]*Citrus hassaku*（ミカン科）の根
[性状]淡黄色のオイル
[UV]:[neutral] λ max 203 ; 226 (sh); 293 ; 331 (EtOH)
[その他のデータ]ラセミ体

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1994, 42, 1213,（分離, UV, IR, H-NMR, C13-NMR）

§ Bisnorponcitrin

[CAS No.]158443-92-6
[化合物分類]ベンゾピラノイド(Pyranocoumarin), ベンゾピラノイド(Bis- and tris-coumarin), ベンゾピラノイド(5,7-Dioxygenated coumarin)
[構造式]



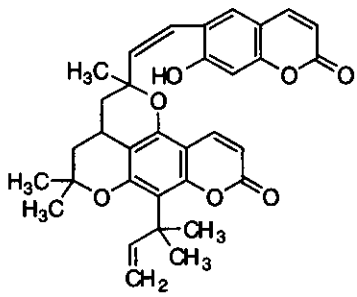
[分子式]$C_{38}H_{40}O_8$
[分子量]624.729
[正確な分子量]624.27232
[基原]*Citrus hassaku*（ミカン科）の根
[性状]淡黄色のプリズム結晶
[融点]Mp 220-225 ℃
[UV]:[neutral] λ max 208 ; 269 ; 288 ; 330 (EtOH)
[その他のデータ]ラセミ体

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1994, 42, 1213,（分離, UV, IR, H-NMR）

§ Citrumarin D

[CAS No.]147920-91-0
[化合物分類]ベンゾピラノイド(Dihydropyranocoumarin), ベンゾピラノイド(5,7-Dioxygenated coumarin), ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted)
[構造式]



[分子式]$C_{33}H_{32}O_7$
[分子量]540.612
[正確な分子量]540.214805
[基原]次の植物の根から分離: *Citrus hassaku*
[性状]オイル

[比旋光度]:[α]$_D$ -15.4 (c, 0.14 in $CHCl_3$)

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1993, 41, 73, (分離, H-NMR, C13-NMR)

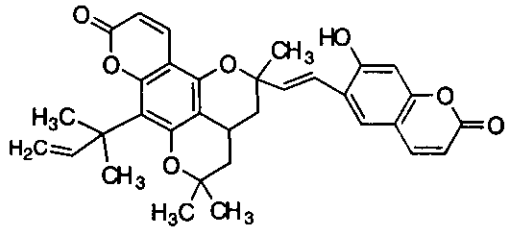
§ Citrumarin D; 9*E*-Isomer

[化学名・別名]Citrumarin C

[CAS No.]147816-72-6

[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(Dihydropyranocoumarin), ベンゾピラノイド(5,7-Dioxygenated coumarin)

[構造式]



[分子式]$C_{33}H_{32}O_7$

[分子量]540.612

[正確な分子量]540.214805

[基原]次の植物の根から分離: *Citrus hassaku*

[性状]オイル

[比旋光度]:[α]$_D$ +7.8 (c, 0.07 in $CHCl_3$)

----------文献----------

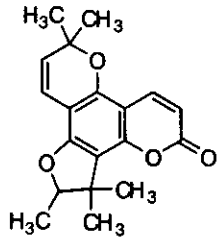
Takemura, Y. et al., Chem. Pharm. Bull., 1993, 41, 73, (分離, H-NMR, C13-NMR)

§ Citrusarin A

[CAS No.]139726-52-6

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

[構造式]



[分子式]$C_{19}H_{20}O_4$

[分子量]312.365

[正確な分子量]312.13616

[基原]*Citrus hassaku*

[性状]青白い黄色のオイル

[比旋光度]:[α]$_D$ +5.2 (c, 0.172 in $CHCl_3$)

----------文献----------

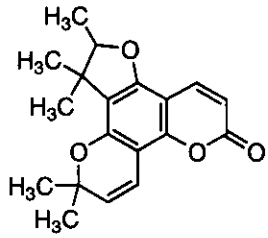
Ito, C. et al., Chem. Pharm. Bull., 1991, 39, 2509

§ Citrusarin B

[CAS No.]139726-53-7

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

[構造式]



[分子式]$C_{19}H_{20}O_4$

[分子量]312.365

[正確な分子量]312.13616

[基原]*Citrus hassaku*

[性状]青白い黄色のオイル

[比旋光度]:[α]$_D$ +3 (c, 0.148 in $CHCl_3$)

----------文献----------

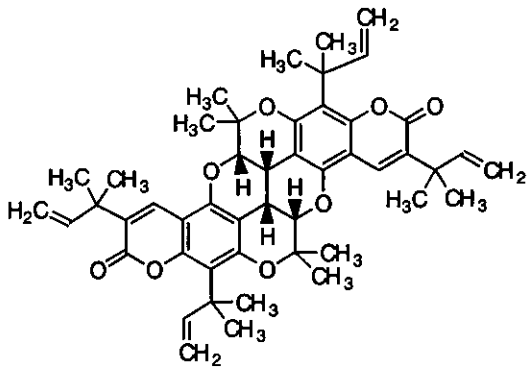
Ito, C. et al., Chem. Pharm. Bull., 1991, 39, 2509

§ Claudimerin A

[CAS No.]155233-22-0

[化合物分類]ベンゾピラノイド(Bis- and tris-coumarin)

[構造式]

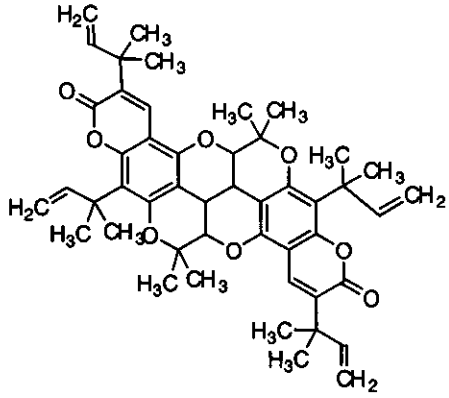


[分子式]$C_{48}H_{54}O_8$
[分子量]758.95
[正確な分子量]758.38187
[基原]*Citrus hassaku*（ミカン科）の根
[性状]立方体状の結晶（$CHCl_3$）
[融点]Mp 318-320 ℃
[その他のデータ]ラセミ体. 非天然物

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1993, 41, 2061,（分離, H-NMR, C13-NMR, 構造決定）
Ju-ichi, H. et al., Chem. Pharm. Bull., 1996, 44, 11,（分離, UV, IR, H-NMR, C13-NMR, Mas）

§ Claudimerin A; Stereoisomer

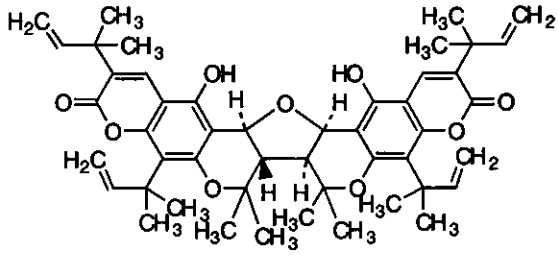


[化学名・別名]Claudimerin B
[化合物分類]ベンゾピラノイド(Bis- and tris-coumarin)
[構造式]
[分子式]$C_{48}H_{54}O_8$
[分子量]758.95
[正確な分子量]758.38187
[基原]*Citrus hassaku*（ミカン科）
[性状]立方体状の結晶（$CHCl_3$）
[融点]Mp 356-358 ℃で分解
[その他のデータ]ラセミ体. 非天然物

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1993, 41, 2061,（分離, H-NMR, C13-NMR, 構造決定）
Ju-ichi, H. et al., Chem. Pharm. Bull., 1996, 44, 11,（分離, UV, IR, H-NMR, C13-NMR, Mas）

§ Furobiclausarin

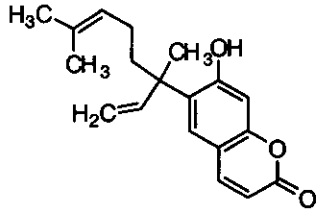


[CAS No.]163047-17-4
[化合物分類]ベンゾピラノイド(5,7-Dioxygenated coumarin), ベンゾピラノイド(Bis- and tris-coumarin), ベンゾピラノイド(Pyranocoumarin)
[構造式]
[分子式]$C_{48}H_{56}O_9$
[分子量]776.965
[正確な分子量]776.392435
[基原]*Citrus hassaku*（ミカン科）の根
[性状]黄色オイル
[UV]:[neutral] λ_{max} 213 ; 268 ; 295 ; 323（EtOH）
[その他のデータ]ラセミ体

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1994, 42, 2436,（分離, UV, IR, H-NMR, C13-NMR, 結晶構造）

§ Hasakol;（±）-form



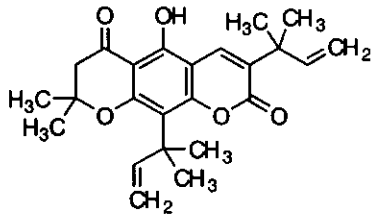
[CAS No.]142628-35-1
[化合物分類]ベンゾピラノイド(7-Oxygenated coumarins, 6-substituted)
[構造式]
[基原]*Citrus hassaku* の果汁オイル
[用途]抗甲状腺作用物質
[性状]結晶(hexane)
[融点]Mp 75-76 ℃（65 ℃）
[比旋光度]:$[\alpha]_D^{26}$ 0 (c, 1.0 in EtOH)

----------文献----------

Masuda, T. et al., Phytochemistry, 1992, 31, 1363
Masuda, T. et al., Biosci., Biotechnol., Biochem., 1996, 60, 506, (合成法, IR, H-NMR)

§ Hassanidin

[化学名・別名]Claucavatin A
[CAS No.]154161-99-6
[化合物分類]ベンゾピラノイド(Pyrano-1-benzopyran), ベンゾピラノイド(5,7-Dioxygenated coumarin), ベンゾピラノイド(Dihydropyranocoumarin)
[構造式]



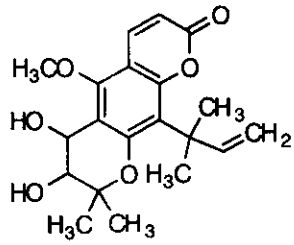
[分子式]$C_{24}H_{28}O_5$
[分子量]396.482
[正確な分子量]396.193675
[基原]*Citrus hassaku*, *Clausena excavata*
[性状]立方体状の結晶
[融点]Mp 109-110 ℃
[UV]:[neutral] λ_{max} 201 ; 219 (sh); 237 ; 287 ; 328 (MeOH)

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1993, 41, 1530, (分離, H-NMR)
Huang, S.-C. et al., Phytochemistry, 1997, 44, 179, (分離, UV, IR, H-NMR, Mas)

§ Hassanin; (3'*R*,4'*R*)-form

[化学名・別名](+)-*cis*-form
[CAS No.]154279-39-7
[化合物分類]ベンゾピラノイド(5,7-Dioxygenated coumarin), ベンゾピラノイド(Dihydropyranocoumarin)
[構造式]



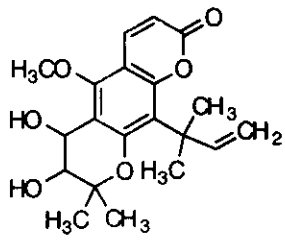
[基原]*Citrus hassaku*
[性状]オイル
[比旋光度]:[α]$_D$ +45.4 (c, 0.0009 in $CHCl_3$)

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1993, 41, 1530, (分離, H-NMR)

§ Hassanin; (3'*S*,4'*R*)-form

[化学名・別名](+)-*trans*-form
[CAS No.]154205-15-9
[化合物分類]ベンゾピラノイド(5,7-Dioxygenated coumarin), ベンゾピラノイド(Dihydropyranocoumarin)
[構造式]



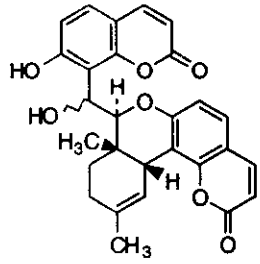
[基原]*Citrus hassaku*
[性状]オイル
[比旋光度]:[α]$_D$ +18.2 (c, 0.002 in $CHCl_3$)

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1993, 41, 1530, (分離, H-NMR)

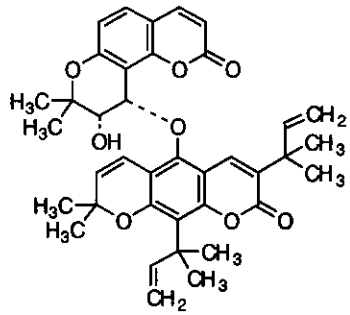
§ Hassmarin

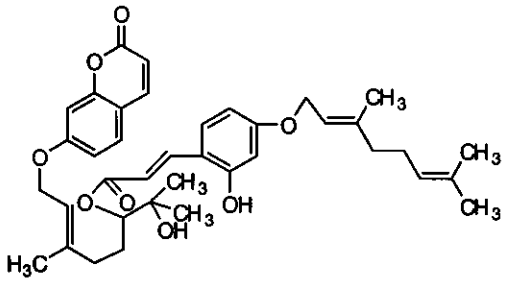
[CAS No.]152551-90-1
[化合物分類]ベンゾピラノイド(Bis- and tris-coumarin), ベンゾピラノイド(7-Oxygenated coumarins, 8-substituted)
[構造式]

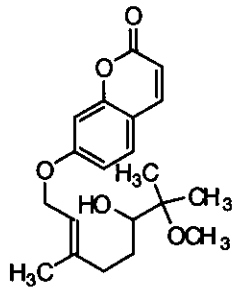


[分子式]$C_{28}H_{24}O_7$
[分子量]472.493
[正確な分子量]472.152205
[基原]*Citrus hassaku* の乾燥根
[性状]プリズム結晶

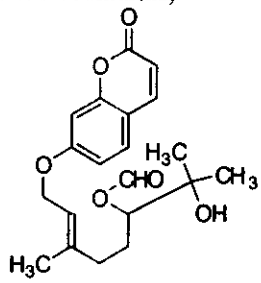
[融点]Mp 235-238 ℃
[比旋光度]:[α]$_D$ -3.9 (c, 0.43 in $CHCl_3$)
----------文献----------
Ito, C. et al., Chem. Pharm. Bull., 1993, 41, 1302, (分離, H-NMR, C13-NMR)

§ Khelmarin C
[CAS No.]158443-93-7
[化合物分類]ベンゾピラノイド(Pyranocoumarin), ベンゾピラノイド(Dihydropyranocoumarin), ベンゾピラノイド(Bis- and tris-coumarin)
[構造式]

[分子式]$C_{38}H_{40}O_8$
[分子量]624.729
[正確な分子量]624.27232
[基原]*Citrus hassaku* (ミカン科)の根
[性状]淡黄色のオイル
[比旋光度]:[α]$_D$ -32.5 (c, 0.21 in $CHCl_3$)
[UV]:[neutral] λ $_{max}$ 219 (sh); 265 (sh); 277 ; 328 (MeOH)
----------文献----------
Takemura, Y. et al., Chem. Pharm. Bull., 1994, 42, 1213, (分離, UV, IR, H-NMR)

§ Marmin; (*R*)-form, 6'-*O*-(4-Geranyloxy-2-hydroxycinnamoyl)
[化合物分類]テルペノイド(Acyclic monoterpenoid)ベンゾピラノイド(7-Oxygenated coumarins, unsubstituted)
[構造式]

[分子式]$C_{38}H_{46}O_8$
[分子量]630.777
[正確な分子量]630.31927
[基原]*Citrus hassaku* の果汁オイル
[性状]粘調性のオイル
[比旋光度]:[α]$_D^{26}$ +72 (c, 1.0 in EtOH)
----------文献----------
Chatterjea, A. et al., J.C.S., 1959, 1922, (分離, UV)
Chatterjea, A. et al., Tet. Lett., 1967, 471, (構造決定, UV, IR, H-NMR, Mas)
Dreyer, D.L. et al., Phytochemistry, 1972, 11, 763, (分離)
Kamilov, K.M. et al., Khim. Prir. Soedin., 1974, 10, 781; Chem. Nat. Compd. (Engl. Transl.), 1974, 10, 800, (分離)
Yamada, Y. et al., Agric. Biol. Chem., 1987, 51, 1105, (活性)
Aziz, M. et al., Tetrahedron, 1988, 44, 101, (合成法)
Masuda, T. et al., Biosci., Biotechnol., Biochem., 1992, 56, 1257, (O-Methylmarmin)
Halim, A.F. et al., Phytochemistry, 1995, 40, 927, (Pituranthoside)

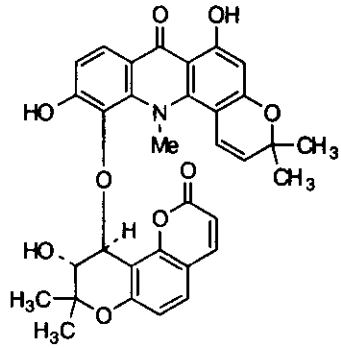
§ Marmin; (*R*)-form, 7'-Me ether
[化学名・別名]7'-*O*-Methylmarmin
[CAS No.]144424-82-8
[化合物分類]ベンゾピラノイド(7-Oxygenated coumarins, unsubstituted)テルペノイド(Acyclic monoterpenoid)
[構造式]

[分子式]$C_{20}H_{26}O_5$
[分子量]346.422
[正確な分子量]346.178025
[基原]*Citrus hassaku*
[性状]針状結晶(hexane)
[融点]Mp 65 ℃
[比旋光度]:[α]$_D^{14}$ +23 (c, 1 in EtOH)
----------文献----------

Masuda, T. et al., Biosci., Biotechnol., Biochem., 1992, 56, 1257, (*O*-Methylmarmin)

§ Marmin; (*R*)-form, 6'-*O*-Formyl
[化学名・別名]6'-*O*-Formylmarmin
[CAS No.]144398-51-6
[化合物分類]テルペノイド(Acyclic monoterpenoid)ベンゾピラノイド(7-Oxygenated coumarins, unsubstituted)
[構造式]

[分子式]$C_{20}H_{24}O_6$
[分子量]360.406
[正確な分子量]360.15729
[基原]*Citrus hassaku*
[性状]粘調性のオイル
[比旋光度]:$[\alpha]_D^{14}$ +8.9 (c, 1 in EtOH)

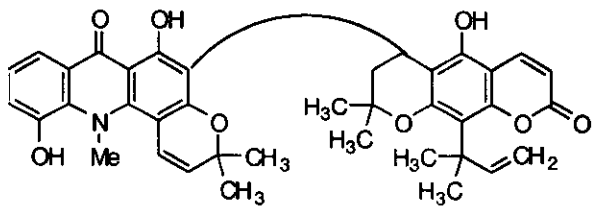
----------文献----------

Chatterjea, A. et al., J.C.S., 1959, 1922, (分離, UV)
Chatterjea, A. et al., Tet. Lett., 1967, 471, (構造決定, UV, IR, H-NMR, Mas)
Dreyer, D.L. et al., Phytochemistry, 1972, 11, 763, (分離)
Kamilov, K.M. et al., Khim. Prir. Soedin., 1974, 10, 781; Chem. Nat. Compd. (Engl. Transl.), 1974, 10, 800, (分離)
Yamada, Y. et al., Agric. Biol. Chem., 1987, 51, 1105, (活性)
Bevalot, F. et al., Phytochemistry, 1988, 27, 1547, (2',3'-dihydro)
Masuda, T. et al., Biosci., Biotechnol., Biochem., 1992, 56, 1257, (*O*-Methylmarmin)
Ohashi, K. et al., Chem. Lett., 1995, 881, (Aeglin, Chloromarmin)
Halim, A.F. et al., Phytochemistry, 1995, 40, 927, (Pituranthoside)

§ Neoacrimarine C
[CAS No.]155519-79-2
[化合物分類]アルカロイド化合物(Acridone-coumarin alkaloid dimer)
[構造式]

[分子式]$C_{33}H_{29}NO_9$
[分子量]583.593
[正確な分子量]583.184234
[基原]次の植物の根から得られるアルカロイド: *Citrus hassaku* (ミカン科)
[性状]黄色の立方体状結晶
[融点]Mp 111-113 ℃
[比旋光度]:$[\alpha]_D$ +42.3 (c, 0.026 in $CHCl_3$)

----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1993, 41, 1757; 1998, 46, 1518, (分離, UV, IR, H-NMR, C13-NMR, Mass, 構造決定)

§ Neoacrimarine D
[CAS No.]155519-80-5
[化合物分類]アルカロイド化合物(Acridone-coumarin alkaloid dimer)
[構造式]

[分子式]$C_{38}H_{37}NO_8$
[分子量]635.712
[正確な分子量]635.251919
[基原]次の植物の根から得られるアルカロイド: *Citrus hassaku* (ミカン科)
[性状]黄色オイル
[その他のデータ]光学不活性

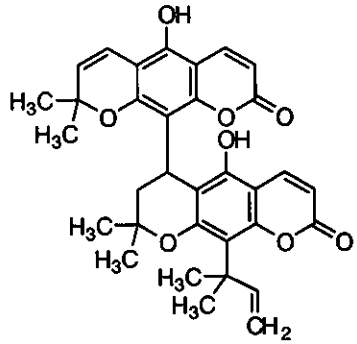
----------文献----------

Takemura, Y. et al., Chem. Pharm. Bull., 1993, 41, 1757, (分離, UV, IR, H-NMR, C13-NMR, Mass, 構造決

定)

§ Nordenletin

[化合物分類]ベンゾピラノイド(Dihydropyranocoumarin), ベンゾピラノイド(5,7-Dioxygenated coumarin), ベンゾピラノイド(Bis- and tris-coumarin), ベンゾピラノイド(Pyranocoumarin)



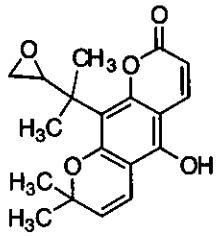
[構造式]
[分子式]$C_{33}H_{32}O_8$
[分子量]556.611
[正確な分子量]556.20972
[基原]*Citrus hassaku* の根
[性状]淡黄色のプリズム結晶
[融点]Mp 265-270 ℃
[比旋光度]:[α]$_D$ -61.8 (c, 0.076 in Py)

----------文献----------

Ju-ichi, M. et al., Chem. Pharm. Bull., 1991, 39, 2252

§ Nordentatin; 2'',3''-Epoxide

[化学名・別名]Oxanordentatin
[化合物分類]ベンゾピラノイド(Pyranocoumarin), ベンゾピラノイド(5,7-Dioxygenated coumarin)



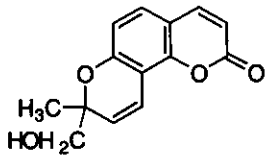
[構造式]
[分子式]$C_{19}H_{20}O_5$
[分子量]328.364
[正確な分子量]328.131075
[基原]次の植物の根から分離: *Citrus hassaku*
[性状]オイル
[比旋光度]:[α]$_D$ -59 (c, 0.078 in EtOH)

----------文献----------

Tomimatsu, T. et al., Tetrahedron, 1972, 28, 2003, (分離, UV, H-NMR)
Ju-ichi, M. et al., Chem. Pharm. Bull., 1991, 39, 2252, (Oxanordentatin)
Yenjai, C. et al., Planta Med., 2000, 66, 277, (活性, Poncitrin)

§ Seselinol

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



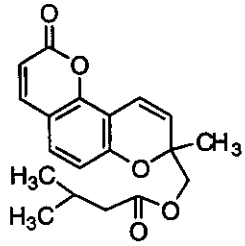
[構造式]
[分子式]$C_{14}H_{12}O_4$
[分子量]244.246
[正確な分子量]244.07356
[基原]*Citrus hassaku* の根
[性状]淡黄色のオイル
[比旋光度]:[α]$_D$ -111.6 (c, 0.108 in $CHCl_3$)

----------文献----------

Ju-ichi, M. et al., Chem. Pharm. Bull., 1991, 29, 2252
Elgamel, M.H.A. et al., Phytochemistry, 1993, 34, 819, (Ammirol)

§ Seselinol; *O*-(3-Methylbutanoyl)

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



[構造式]
[分子式]$C_{19}H_{20}O_5$
[分子量]328.364
[正確な分子量]328.131075
[基原]*Citrus hassaku* の根
[性状]淡黄色のオイル

[比旋光度]:[α]$_D$ +50.84 (c, 0.118 in $CHCl_3$)

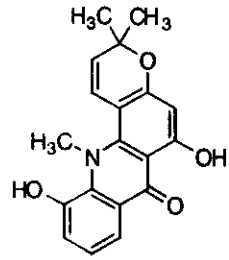
----------文献----------

Ju-ichi, M. et al., Chem. Pharm. Bull., 1991, 29, 2252
Elgamel, M.H.A. et al., Phytochemistry, 1993, 34, 819, (Ammirol)

§§ ミカン科シークワーシャー(*Citrus depressa* Hayata)の果実。

§ Atalaphyllidine; *N*-Me

[化学名・別名]12-Methylatalaphyllidine. 11-Hydroxynoracronycine
[CAS No.]27067-70-5
[化合物分類]アルカロイド化合物(Acridone alkaloid)
[構造式]
[分子式]$C_{19}H_{17}NO_4$
[分子量]323.348
[正確な分子量]323.115759
[基原]次の植物から得られるアルカロイド: *Atalantia ceylanica*, *Citrus depressa* ; metab. of Acronycine in the guinea pig (ミカン科)
[性状]赤色の針状結晶 (Et_2O/petrol)
[融点]Mp 252-254 ℃

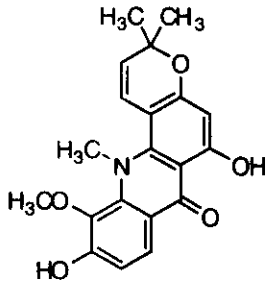


----------文献----------

Sullivan, H.R. et al., J. Med. Chem., 1970, 13, 904, (分離, 誘導体)
Fraser, A.W. et al., J.C.S. Perkin 1, 1973, 1173, (分離, UV, IR, NMR, Mass, 構造決定, 誘導体)
Basa, S.C., Experientia, 1975, 31, 1387, (分離, UV, IR, H-NMR, Mass, 構造決定)
Adams, J.H. et al., J. Nat. Prod., 1976, 39, 399, (合成法, 誘導体)
Wu, T.-S. et al., Heterocycles, 1982, 19, 273, (分離, 誘導体)
Wu, T.S., Phytochemistry, 1987, 26, 871, (Baiyumine A)

§ Citracridone III; 5-Me ether

[化学名・別名]Citracridone I
[CAS No.]81525-61-3
[化合物分類]アルカロイド化合物(Acridone alkaloid)
[構造式]
[分子式]$C_{20}H_{19}NO_5$
[分子量]353.374
[正確な分子量]353.126324
[基原]次の植物から得られるアルカロイド: *Citrus depressa* の根皮, *Citrus sinensis* var. *brasiliensis*, *Citrus grandis* f. *hakunikuyu* (ミカン科)
[性状]橙色の板状結晶(Me_2CO)
[融点]Mp 275-278 ℃

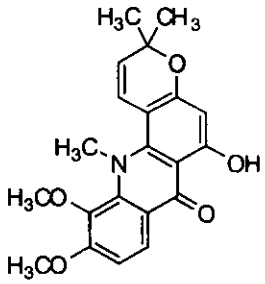


----------文献----------

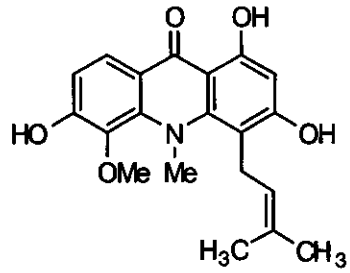
Wu, T.-S. et al., Chem. Pharm. Bull., 1983, 31, 895; 901, (分離, 構造決定)
Wu, T.-S. et al., Phytochemistry, 1983, 22, 1493, (分離)
Ju-ichi, M. et al., Heterocycles, 1991, 32, 1781, (分離, H-NMR, C13-NMR, 構造決定)
Takemura, Y. et al., Heterocycles, 1995, 41, 187, (Dihydroxycitracridone I)
Ono, T. et al., J. Nat. Prod., 1995, 58, 1629, (Acrifoline)

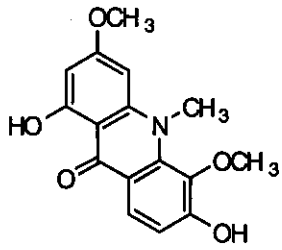
§ Citracridone III; 5,6-Di-Me ether

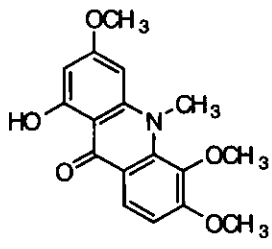
[化学名・別名]Citracridone II
[CAS No.]81525-62-4
[化合物分類]アルカロイド化合物(Acridone alkaloid)
[構造式]
[分子式]$C_{21}H_{21}NO_5$
[分子量]367.401
[正確な分子量]367.141974
[基原]*Citrus depressa*, *Citrus grandis* f. *hakunikuyu* (ミカン科)



[性状]黄色の針状結晶(Et_2O)
[融点]Mp 161-163 ℃
----------文献----------
Wu, T.-S. et al., Chem. Pharm. Bull., 1983, 31, 895; 901, (分離, 構造決定)
Wu, T.-S. et al., Phytochemistry, 1983, 22, 1493, (分離)
Ju-ichi, M. et al., Heterocycles, 1991, 32, 1781, (分離, H-NMR, C13-NMR, 構造決定)
Takemura, Y. et al., Heterocycles, 1995, 41, 187, (Dihydroxycitracridone I)
Ono, T. et al., J. Nat. Prod., 1995, 58, 1629, (Acrifoline)

§ Prenylcitpressine
[化学名・別名]1,3,6-Trihydroxy-5-methoxy-10-methyl-4-(3-methyl-2-butenyl)-9(10*H*)-acridinone(CAS名). 1,3,6-Trihydroxy-5-methoxy-10-methyl-4-*C*-prenylacridone

[CAS No.]81525-60-2
[化合物分類]アルカロイド化合物(Acridone alkaloid)
[構造式]
[分子式]$C_{20}H_{21}NO_5$
[分子量]355.39
[正確な分子量]355.141974
[基原]次の植物から得られるアルカロイド: *Citrus depressa* と *Citrus grandis* f. *hakunikuyu* の根皮(ミカン科)
[性状]黄色の板状結晶 + 1/2·H_2O (Et_2O)
[融点]Mp 160-162 ℃
----------文献----------
Wu, T.-S., Chem. Pharm. Bull., 1983, 31, 895, (分離, UV, IR, H-NMR, Mass, 構造決定)
Wu, T.-S. et al., Phytochemistry, 1983, 22, 1493; 1987, 26, 871, (分離, UV, IR, H-NMR, C13-NMR, Mass, 構造決定, 誘導体)

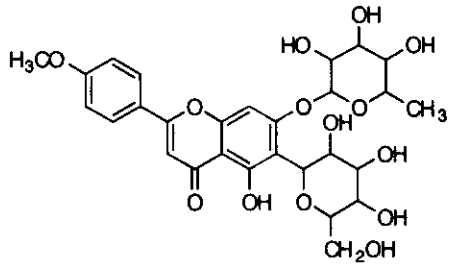
§ 1,3,5,6-Tetrahydroxyacridone; 3,5,10-*O*, *O*, *N*-Tri-Me
[化学名・別名]1,6-Dihydroxy-3,5-dimethoxy-10-methylacridone. Citpressine I

[CAS No.]81525-58-8
[化合物分類]アルカロイド化合物(Acridone alkaloid)
[構造式]
[分子式]$C_{16}H_{15}NO_5$
[分子量]301.298
[正確な分子量]301.095024
[基原]次の植物から得られるアルカロイド: *Citrus depressa* と *Citrus grandis*, f. *hakunikuyu* の根皮(ミカン科)
[性状]黄色の針状結晶+ 1/2·H_2O(Me_2CO)
[融点]Mp 183-185 ℃
----------文献----------
Wu, T.-S. et al., Chem. Pharm. Bull., 1983, 31, 895, (分離, 構造決定, Citpressine)

§ 1,3,5,6-Tetrahydroxyacridone; 3,5,6,10-*O*, *O*, *O*, *N*-Tetra-Me
[化学名・別名]1-Hydroxy-3,5,6-trimethoxy-10-methylacridone. Citpressine II

[CAS No.]81525-59-9
[化合物分類]アルカロイド化合物(Acridone alkaloid)
[構造式]
[分子式]$C_{17}H_{17}NO_5$
[分子量]315.325
[正確な分子量]315.110674
[基原]次の植物から得られるアルカロイド: *Citrus depressa* と *Citrus grandis* f. *hakunikuyu* の根皮(ミカン科)
[性状]黄色の針状結晶(Et_2O)
[融点]Mp 168-170 ℃

----------文献----------
Wu, T.-S. et al., Chem. Pharm. Bull., 1983, 31, 895, (分離, UV, IR, H-NMR, Mass, 構造決定, Citpressine)

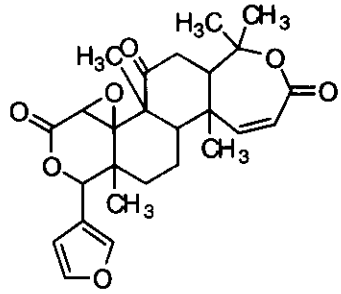
§ § キンカン属のナガミキンカン(*Fortunella margarita* Swingle)の果実。

§ **Isocytisoside; 2''-*O*-α-L-Rhamnopyranoside**



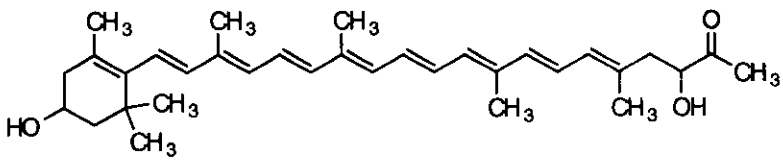
[化学名・別名]Isomargaritene. Semiaquilinoside
[CAS No.]64271-11-0
[化合物分類]フラボノイド(Flavones; 3 × O-置換基)
[構造式]
[分子式]$C_{28}H_{32}O_{14}$
[分子量]592.552
[正確な分子量]592.17921
[基原]次の植物から分離:*Fortunella margarita*, *Fortunella japonica*, *Semiaquilegia adoxoides*
[性状]黄色の針状結晶
[融点]Mp 218-220 ℃
----------文献----------
Chopin, J. et al., C. R. Hebd. Seances Acad. Sci. Ser. C, 1977, 284, 1007, (Isomargaritene)
Kumamoto, H. et al., Agric. Biol. Chem., 1985, 49, 2613, (Isomargaritene)
Liu, Y. et al., Zhongcaoyao, 1999, 30, 5, (Semiaquilinoside)

§ **Obacunol; 7-Ketone**



[化学名・別名]Obacunone. Casimirolide. Tricoccin S_3
[CAS No.]751-03-1
[化合物分類]テルペノイド(Ring cleaved tetranortriterpenoid)
[構造式]
[分子式]$C_{26}H_{30}O_7$
[分子量]454.519
[正確な分子量]454.199155
[基原]*Citrus* spp., *Poncirus trifoliata*, *Fortunella margarita*, *Casimiroa edulis*, *Phellodendron* spp., その他のミカン科の植物
[性状]結晶(MeOH)
[融点]Mp 229-230 ℃
[比旋光度]:[α]$_D$ -50 ($CHCl_3$)
[UV]:[neutral] λ_{max} 288 (ε 1360) (MeOH)
----------文献----------
Barton, D.H.R. et al., J.C.S., 1961, 255, (Obacunone, 構造決定)
Dreyer, D.L., Tetrahedron, 1965, 21, 75, (Obacunone, H-NMR)
Taylor, D.R., Rev. Latinoam. Quim., 1971, 2, 87, (分離)
Adesida, G.A. et al., Phytochemistry, 1972, 11, 2641, (分離)
Taylor, D.A.H. et al., J. Chem. Res., Synop., 1977, 2, (Obacunone, C13-NMR)

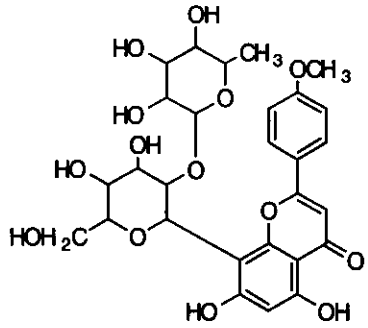
§ **Reticulataxanthin; 7',8'-Dihydro, 8'-hydroxy**



[化学名・別名]7',8'-Dihydro-8'-hydroxyreticulataxanthin
[化合物分類]テルペノイド(Apocarotenoid)
[構造式]
[分子式]$C_{33}H_{46}O_3$
[分子量]490.725
[正確な分子量]490.344695
[基原]次の植物から分離:Sinton citrangequat (hybrid of *Citrus sinensis*, *Poncirus trifoliata*, *Fortunella margarita*)
[その他のデータ]λ_{max} 401,422, 448 nm (hexane)
----------文献----------

Yokoyama, H. et al., Phytochemistry, 1966, 5, 1159,（8'-hydroxy-7',8'-dihydroreticulataxanthin）

§ Vitexin; 2''-*O*-α-L-Rhamnopyranosyl, 4'-Me ether



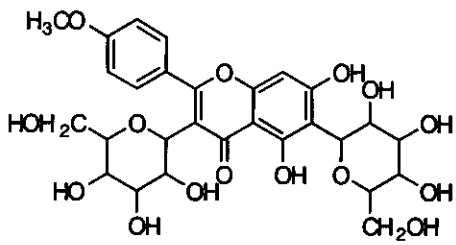
[化学名・別名]Margaritene
[CAS No.]64271-10-9
[化合物分類]フラボノイド(Flavones; 3 × O-置換基)
[構造式]
[分子式]$C_{28}H_{32}O_{14}$
[分子量]592.552
[正確な分子量]592.17921
[基原]次の植物から分離:*Fortunella margarita, Fortunella japonica*
[性状]黄色の針状結晶
[融点]Mp 192-193 ℃

----------文献----------

Chopin, J. et al., C. R. Hebd. Seances Acad. Sci. Ser. C, 1977, 284, 1007,（Margaritene）
Tillequin, F. et al., Planta Med., 1978, 33, 46,（Marginatoside）

§§ キンカン属のマルキンカン(*Fortunella japonica* (Thunberg) Swingle)の果実。

§ 3,6-Diglucopyranosyl-4',5,7-trihydroxyflavone; 4'-Me ether

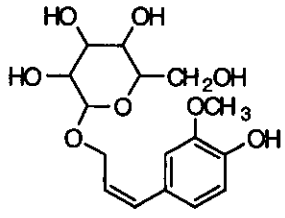


[化学名・別名]3,6-Diglucopyranosyl-5,7-dihydroxy-4'-methoxyflavone. 3,6-Diglucopyranosylacacetin. 3,6-Diglucosylacacetin
[CAS No.]98891-91-9
[化合物分類]フラボノイド(Flavones; 3 × O-置換基)
[構造式]
[分子式]$C_{28}H_{32}O_{15}$
[分子量]608.552
[正確な分子量]608.174125
[基原]次の植物から分離:*Fortunella japonica*
[性状]黄色の針状結晶
[融点]Mp 210 ℃で分解

----------文献----------

Matsubara, Y. et al., Agric. Biol. Chem., 1985, 49, 909,（分離）
Kumamoto, H. et al., Agric. Biol. Chem., 1985, 49, 2613,（誘導体）

§ 3-(3,4-Dihydroxyphenyl)-2-propen-1-ol; (*E*)-form, 3'-Me ether, 1-*O*-β-D-glucopyranoside



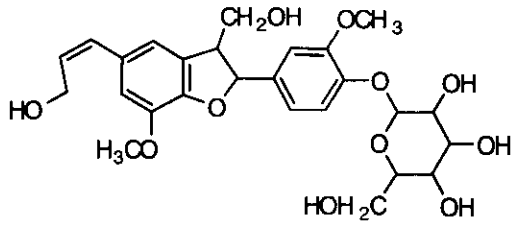
[化学名・別名]Citrusin D. Isoconiferin
[CAS No.]65995-51-9
[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]
[分子式]$C_{16}H_{22}O_8$
[分子量]342.345
[正確な分子量]342.13147
[基原]次の植物から分離:*Citrus limon, Citrus unshiu, Fortunella japonica, Pinus sylvestris*
[用途]抗高血圧作用を示す
[比旋光度]:$[\alpha]_D^{20}$ -16.9 (c, 4.1 in MeOH)
[UV]:[neutral] λ_{max} 275 nm (ε 5000) (MeOH)

----------文献----------

Sawabe, A. et al., Nippon Kagaku Kaishi, 1988, 62, 1067,（Citrusin D）
Sugiyama, M. et al., Phytochemistry, 1993, 33, 1215,（Isoconiferinoside）
Greca, M.D. et al., Phytochemistry, 1998, 49, 1299,（Coniferyl alcohol, Citrusin D）

§ 4,7'-Epoxy-3,8'-bilign-7-ene-3',4',5,9,9'-pentol; (7'*S*,8'*S*)-form, 3',5-Di-Me ether, 4'-*O*-β-D-glucopyranoside

[CAS No.]96738-84-0
[化合物分類]リグナン化合物(Neolignan)
[構造式]

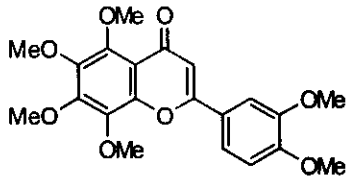


[分子式]$C_{26}H_{32}O_{11}$
[分子量]520.532
[正確な分子量]520.194465
[基原]*Chamaecyparis obtusa*, *Citrus* spp., *Fortunella japonica*, *Plagiorhegma dubium*
[融点]Mp 125 ℃

----------文献----------

Freudenberg, K. et al., Chem. Ber., 1960, 93, 1354; 1963, 96, 1265
Weinges, K. et al., Annalen, 1970, 736, 170, (分離)
Arens, H. et al., Planta Med., 1985, 52, (glucoside)
Binns, A.N. et al., Proc. Natl. Acad. Sci. U.S.A., 1987, 84, 980, (glucoside)
Yoshizawa, F. et al., Chem. Pharm. Bull., 1990, 38, 1927, (glucoside)
Hirai, N. et al., Biosci., Biotechnol., Biochem., 1994, 58, 1679, (絶対構造, 分割)
Hashimoto, Y. et al., CA, 1994, 121, 251213h

§ 3',4',5,6,7,8-Hexamethoxyflavone
[化学名・別名]2-(3,4-Dimethoxyphenyl)-5,6,7,8-tetramethoxy-4*H*-1-benzopyran-4-one(CAS 名). Nobiletin
[CAS No.]478-01-3
[化合物分類]フラボノイド(Flavones; 6 × O-置換基), 脂肪族化合物(Simple heteroalicyclics (2 × O))
[構造式]



[分子式]$C_{21}H_{22}O_8$
[分子量]402.4
[正確な分子量]402.13147
[基原]次の植物から分離: king orange (*Citrus nobili*)の皮, セビリアオレンジ(*Citrus aurantium*)とその他の *Citrus* spp., and the round kumquat (*Fortunella japonica*), *Eupatorium coelestinum*, *Eupatorium leucolepis*
[性状]青白い黄色の結晶 (MeOH)
[融点]Mp 134 ℃

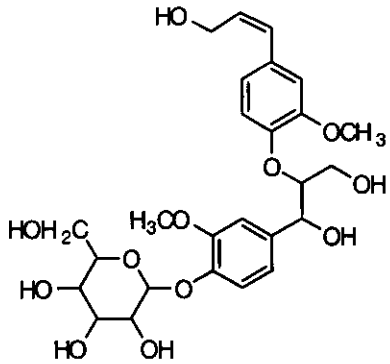
----------文献----------

Robinson, R. et al., J.C.S., 1938, 1004, (分離, 構造決定)
Schneider, G. et al., Arch. Pharm. (Weinheim, Ger.), 1968, 301, 785, (分離)
Talapatra, S.K. et al., Phytochemistry, 1975, 14, 309, (分離)
Yinon, J. et al., Org. Mass Spectrom., 1978, 13, 167, (Mas)
Tatum, J.H. et al., Phytochemistry, 1978, 17, 447, (分離)
Ngo, Le-Van et al., Phytochemistry, 1979, 18, 1859, (分離)
Iinuma, M. et al., Chem. Pharm. Bull., 1980, 28, 708, (C13-NMR)
Herz, W. et al., Phytochemistry, 1982, 21, 2363, (分離)

§ 1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxy-1-propenyl)-2-methoxyphenoxy]-1,3-propanediol;

4-*O*-β-D-Glucopyranoside

[化学名・別名]Citrusin A
[CAS No.]105279-09-2
[化合物分類]WI3500, , リグナン化合物(Neolignan)
[構造式]
[分子式]$C_{26}H_{34}O_{12}$
[分子量]538.547
[正確な分子量]538.20503
[基原]次の植物から分離:レモン(*Citrus limon*), round kumquat (*Fortunella japonica*) の皮
[融点]Mp 108-109 ℃
[比旋光度]:$[\alpha]_D^{20}$ -17.2 (c, 0.3 in MeOH)

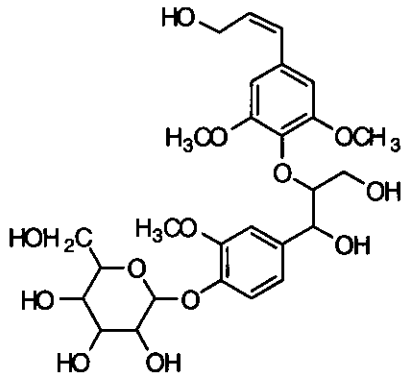


----------文献----------

Sawabe, A. et al., Nippon Kagaku Kaishi, 1986, 60, 593, (Citrusin)
Matsubara, Y. et al., Agric. Biol. Chem., 1991, 55, 647, (Citrusin A)
Li, S. et al., Phytochemistry, 1998, 49, 2125, (合成法, H-NMR, C13-NMR)

§ 1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxy-1-propenyl)-2-methoxyphenoxy]-1,3-propanediol; 5'-Methoxy, 4-*O*-β-D-glucopyranoside

[化学名・別名]Citrusin B
[CAS No.]105279-10-5
[化合物分類]リグナン化合物(Neolignan)
[構造式]
[分子式]$C_{27}H_{36}O_{13}$
[分子量]568.574
[正確な分子量]568.215595
[基原]次の植物から分離: レモン(*Citrus limon*), round kumquat (*Fortunella japonica*), *Eucommia ulmoides* の樹皮
[融点]Mp 105-106 ℃
[比旋光度]:$[\alpha]_D^{20}$ -11.3 (c, 0.3 in MeOH)

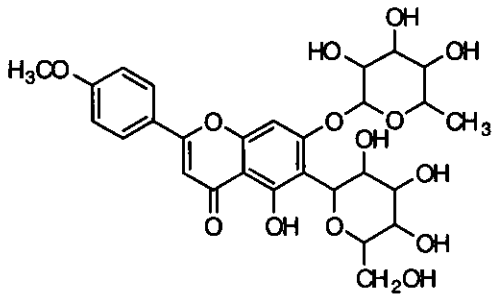


----------文献----------

Sawabe, A. et al., Nippon Kagaku Kaishi, 1986, 60, 593, (Citrusin)
Deyama, T. et al., Chem. Pharm. Bull., 1987, 35, 1803, (Citrusin B)

§ Isocytisoside; 2''-*O*-α-L-Rhamnopyranoside

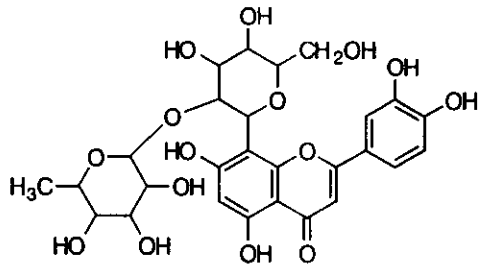
[化学名・別名]Isomargaritene. Semiaquilinoside
[CAS No.]64271-11-0
[化合物分類]フラボノイド(Flavones; 3 × O-置換基)
[構造式]
[分子式]$C_{28}H_{32}O_{14}$
[分子量]592.552
[正確な分子量]592.17921
[基原]次の植物から分離:*Fortunella margarita*, *Fortunella japonica*, *Semiaquilegia adoxoides*
[性状]黄色の針状結晶
[融点]Mp 218-220 ℃



----------文献----------

Chopin, J. et al., C. R. Hebd. Seances Acad. Sci. Ser. C, 1977, 284, 1007, (Isomargaritene)
Kumamoto, H. et al., Agric. Biol. Chem., 1985, 49, 2613, (Isomargaritene)
Liu, Y. et al., Zhongcaoyao, 1999, 30, 5, (Semiaquilinoside)

§ Orientin; 2''-*O*-α-L-Rhamnopyranosyl

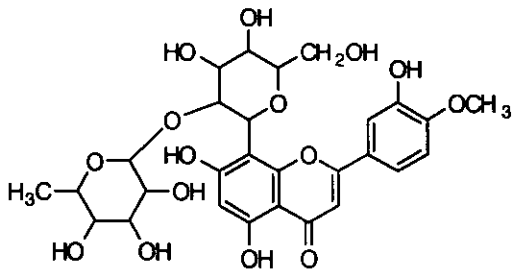


[CAS No.]81398-30-3
[化合物分類]フラボノイド(Flavones; 4 × O-置換基)
[構造式]
[分子式]$C_{27}H_{30}O_{15}$
[分子量]594.525
[正確な分子量]594.158475
[基原]次の植物から分離:*Fortunella japonica*, *Crataegus* spp., その他の植物属
[性状]黄色の針状結晶
[融点]Mp 225-227 ℃ (218-220 ℃)

----------文献----------

Siekel, W. et al., J.O.C., 1959, 24, 1995, (分離)
Chernobai, V.T. et al., Khim. Prir. Soedin., 1968, 4, 51; Chem. Nat. Compd. (Engl. Transl.), 1968, 4, 43, (6''-xylosyl)
Kitanov, G. et al., Khim. Prir. Soedin., 1979, 15, 154; Chem. Nat. Compd. (Engl. Transl.), 1979, 15, 129, (2''-Ac)
Nikolov, N. et al., Planta Med., 1982, 44, 50, (2''-rhamnoside)
Kumamoto, H. et al., Agric. Biol. Chem., 1985, 49, 2613, (2''-rhamnoside)

§ Orientin; 4'-Me ether, 2''-*O*-α-L-rhamnopyranosyl

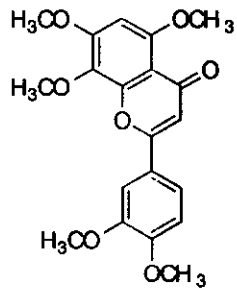


[CAS No.]98891-92-0
[化合物分類]フラボノイド(Flavones; 4 × O-置換基)
[構造式]
[分子式]$C_{28}H_{32}O_{15}$
[分子量]608.552
[正確な分子量]608.174125
[基原]次の植物から分離:*Fortunella japonica*
[性状]黄色の針状結晶
[融点]Mp 214-216 ℃

----------文献----------

Siekel, W. et al., J.O.C., 1959, 24, 1995, (分離)
Koeppen, H. et al., Biochem. J., 1962, 83, 507; 1965, 97, 444, (分離, 合成法)
Horowitz, S. et al., Chem. Ind. (London), 1964, 499, (分離)
Zemtsova, G.N. et al., Khim. Prir. Soedin., 1975, 11, 516; Chem. Nat. Compd. (Engl. Transl.), 1975, 11, 538, (分離)
Nikolov, N. et al., Planta Med., 1982, 44, 50, (2''-rhamnoside)
Kumamoto, H. et al., Agric. Biol. Chem., 1985, 49, 2613, (2''-rhamnoside)

§ 3',4',5,7,8-Pentahydroxyflavone; Penta-Me ether

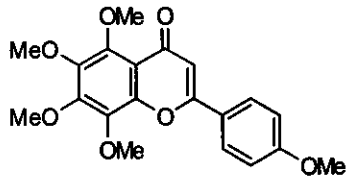


[化学名・別名]3',4',5,7,8-Pentamethoxyflavone. Isosinensetin
[CAS No.]17290-70-9
[化合物分類]フラボノイド(Flavones; 5 × O-置換基)
[構造式]
[分子式]$C_{20}H_{20}O_7$
[分子量]372.374
[正確な分子量]372.120905
[基原]次の植物から分離:*Citrus* spp., *Fortunella japonica*
[性状]結晶(EtOH)
[融点]Mp 206-207 ℃

----------文献----------

Iinuma, M. et al., Yakugaku Zasshi, 1980, 100, 657, (Isosinensetin)
Rizzi, G.P. et al., J. Agric. Food Chem., 1984, 32, 551, (Isosinensetin, Mas)

§ 4',5,6,7,8-Pentamethoxyflavone

[化学名・別名]5,6,7,8-Tetramethoxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one(CAS 名). Tangeritin. Ponkanetin. Tangeretin
[CAS No.]481-53-8
[化合物分類]フラボノイド(Flavones; 5 × O-置換基)
[構造式]

[分子式]$C_{20}H_{20}O_7$
[分子量]372.374
[正確な分子量]372.120905
[基原]タンジェリンの皮, *Deuterophoma traceiphila*, *Fortunella japonica*
[性状]棒状の結晶もしくは針状結晶(EtOAc)
[融点]Mp 154 ℃
[その他のデータ]以前は 3,4',5,6,7-pentamethoxy 構造は確立していた
[化学物質毒性データ総覧(RTECS)登録番号]DJ3102725

----------文献----------

Sehgal, J.M. et al., Proc. - Indian Acad. Sci., Sect. A, 1955, 42, 252, (合成法)
Goldsworthy, L.J. et al., Chem. Ind. (London), 1957, 47, (構造決定)
Okigawa, M. et al., J.C.S. Perkin 1, 1975, 1563, (H-NMR)
Talapatra, S.K. et al., Phytochemistry, 1975, 14, 309, (分離)
Matsuura, S. et al., Chem. Pharm. Bull., 1978, 26, 305, (合成法)
Tatum, J.H. et al., Phytochemistry, 1978, 17, 447, (分離)
Iinuma, M. et al., Chem. Pharm. Bull., 1980, 28, 708, (C13-NMR)
Elgamal, M.H.A. et al., J. Prakt. Chem., 1986, 328, 893, (Mas)

***RTECS (化学物質毒性データ) ***

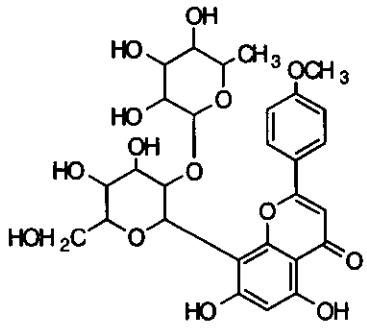
生体影響物質　　: 医薬品.

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　　: 腹腔内投与
被験動物　　: げっ歯類-ラット.
投与量・期間 : >1 gm/kg
毒性影響　　: 致死量以外に毒性影響に関する報告はない.
参照文献

ADTEAS Advances in Teratology. (New York, NY) V.1-5, 1966-72. Discontinued. [Vol.,頁,年(19-)]3,181,1968

§ Vitexin; 2''-*O*-α-L-Rhamnopyranosyl, 4'-Me ether
[化学名・別名]Margaritene
[CAS No.]64271-10-9
[化合物分類]フラボノイド(Flavones; 3 × O-置換基)
[構造式]

[分子式]$C_{28}H_{32}O_{14}$
[分子量]592.552
[正確な分子量]592.17921
[基原]次の植物から分離:*Fortunella margarita*, *Fortunella japonica*
[性状]黄色の針状結晶
[融点]Mp 192-193 ℃

----------文献----------

Evans, W.H. et al., J.C.S., 1957, 3510, (分離)
Chopin, J. et al., C. R. Hebd. Seances Acad. Sci. Ser. C, 1977, 284, 1007, (Margaritene)
Tillequin, F. et al., Planta Med., 1978, 33, 46, (Marginatoside)

*********シトロネラ (Citronella) *********

§ §イネ科コウスイガヤ(*Cymbopogon nardus* Rendle)の葉または全草。