

[性状] 針状結晶
[融点] Mp 293-294 °C で分解
[比旋光度]: $[\alpha]_D^{20}$ -69.4 (c, 0.36 in Py)

----- 文献 -----

Atkinson, J.E. et al., Tetrahedron, 1969, 25, 1507, (分離, 合成法)
Stout, G.H. et al., Tetrahedron, 1969, 25, 1961, (分離, 合成法)
Hostettmann, K. et al., Helv. Chim. Acta, 1974, 57, 1155, (分離)
Peres, V. et al., Phytochemistry, 1997, 44, 191, (レビュー, 生育)

§ 1,3,7-Trihydroxyxanthone; 7-Me ether

[化学名・別名] 1,3-Dihydroxy-7-methoxyxanthone. Isogentisin
[CAS No.] 491-64-5

[化合物分類] 単環芳香族 (Xanthenes; 3 × O-置換基)

[構造式]

[分子式] $C_{14}H_{10}O_5$

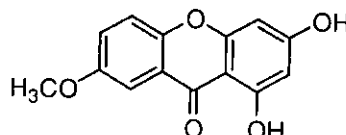
[分子量] 258.23

[基原] 次の植物から分離: *Gentiana lutea* の根, *Swertia japonica*

[性状] 黄色の板状結晶 (EtOH)

[融点] Mp 241 °C

[化学物質毒性データ総覧 (RTECS) 登録番号] ZD6034500



----- 文献 -----

Atkinson, J.E. et al., Tetrahedron, 1969, 25, 1507, (分離, 合成法)
Stout, G.H. et al., Tetrahedron, 1969, 25, 1961, (分離, 合成法)
Hostettmann, K. et al., Helv. Chim. Acta, 1974, 57, 1155, (分離)
Peres, V. et al., Phytochemistry, 1997, 44, 191, (レビュー, 生育)
***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>> 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 : 5 ug/plate

参照文献

Mutation Research.116,103,1983

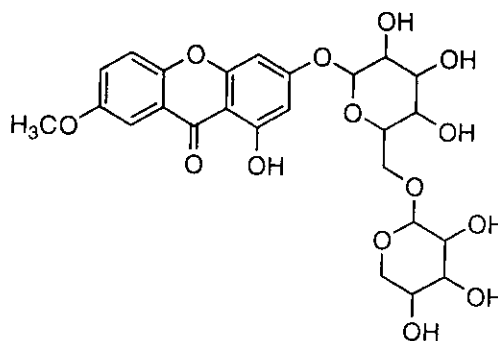
§ 1,3,7-Trihydroxyxanthone; 7-Me ether, 3-O-[β-D-xylopyranosyl-(1 → 6)-β-D-glucopyranoside]

[化学名・別名] Gentioside †. Gentiin

[CAS No.] 529-48-6

[化合物分類] 単環芳香族 (Xanthenes; 3 × O-置換基)

[構造式]



[分子式] $C_{25}H_{32}O_{14}$

[分子量] 552.488

[基原] *Gentiana lutea* の根

[性状] 針状結晶

[融点] Mp 278-279 °C で分解

[比旋光度]: $[\alpha]_D^{25}$ -107 (60% EtOH 溶液). $[\alpha]_D^{20}$ -50 (c, 0.3 in Py)

----- 文献 -----

Atkinson, J.E. et al., Tetrahedron, 1969, 25, 1507, (分離, 合成法)
Stout, G.H. et al., Tetrahedron, 1969, 25, 1961, (分離, 合成法)
Hostettmann, K. et al., Helv. Chim. Acta, 1974, 57, 1155, (分離)
Peres, V. et al., Phytochemistry, 1997, 44, 191, (レビュー, 生育)

§ 1,3,7-Trihydroxyxanthone; 3,7-Di-Me ether

[化学名・別名] 1-Hydroxy-3,7-dimethoxyxanthone

[化合物分類] 単環芳香族 (Xanthenes; 3 × O-置換基)

[構造式]

[分子式] C₁₅H₁₂O₅

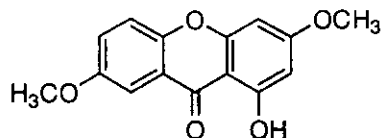
[分子量] 272.257

[基原] 次の植物から分離: *Gentiana lutea*, *Frasera albicaulis*

[性状] 結晶 (MeOH), 黄色の針状結晶 (CH₂Cl₂/hexane)

[融点] Mp 169-170 °C

[化学物質毒性データ総覧 (RTECS) 登録番号] ZD6035500



-----文献-----

Atkinson, J.E. et al., Tetrahedron, 1969, 25, 1507, (分離, 合成法)

Stout, G.H. et al., Tetrahedron, 1969, 25, 1961, (分離, 合成法)

Hostettmann, K. et al., Helv. Chim. Acta, 1974, 57, 1155, (分離)

Peres, V. et al., Phytochemistry, 1997, 44, 191, (レビュー, 生育)

***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>> 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 : 10 ug/plate

参考文献

Mutation Research.150,141,1985

§ Venoterpine

[化学名・別名] Gentialutine. Alkaloid RW47

[CAS No.] 17948-42-4

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

[構造式]

[分子式] C₉H₁₁NO

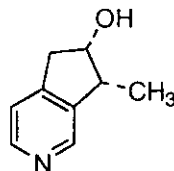
[分子量] 149.192

[一般的性質] Config. revised in 1985

[基原] 次の植物から得られるアルカロイド: *Alstonia venenata*, *Rauwolfia verticillata*, *Melodinus aeneus*, *Gentiana lutea*, *Camptotheca acuminata* (キョウチクトウ科, リンドウ科, ヌママズキ科)

[融点] Mp 130-132 °C

[比旋光度]: [α]_D +27 (CHCl₃)



-----文献-----

Arthur, H.R. et al., Aust. J. Chem., 1967, 20, 2505, (UV, IR, H-NMR, Mass, 構造決定)

Ray, A.B. et al., Tet. Lett., 1968, 2763, (UV, IR, H-NMR, 構造決定)

Mitscher, L.A. et al., Experientia, 1971, 27, 16

Ravao, T. et al., Tet. Lett., 1985, 26, 837, (構造, C13-NMR)

§ § リンドウ科チャボリンドウ (*Gentiana acaulis* L.) の根または全草。

§ 3,3',4',5',7-Hexahydroxyflavylum (1+); Glycoside

[化学名・別名] Gentianin †

[化合物分類] フラボノイド (Anthocyanidins and anthocyanins; 6 × 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] C₃₀H₂₇O₁₄⁽⁺⁾

[分子量] 611.535

[基原] 次の植物から分離: *Gentiana acaulis* の青い花

[性状] 紫色の粉末 (as chloride)

[その他のデータ] Hydrol. gave Delphinidin, Glc + 4-hydroxycinnamic acid

-----文献-----

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972. nos. 1727; 1730; 1734; 1735; 1737; 1739. (Delphinidin, Myrtillin B, Hibiscin, Nasunin A. Gentianin,

Basel, 1972, nos. 1727; 1730; 1734; 1735; 1737; 1739, (Delphinidin, Myrtillin B, Hibiscin, Nasunin A, Gentianin, Delphinin)
 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

§ 1,2,6,8-Tetrahydroxyxanthone; 1,6-Di-Me ether

[化学名・別名] 2,8-Dihydroxy-1,6-dimethoxyxanthone. Gentiacaulein

[CAS No.] 15402-27-4

[化合物分類] 単環芳香族 (Xanthenes; 4 × O-置換基)

[構造式]

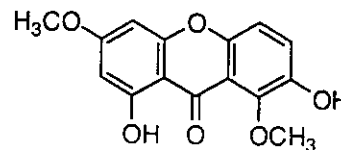
[分子式] C₁₅H₁₂O₆

[分子量] 288.256

[基原] 次の植物を含む *Gentiana* spp.; *Gentiana bavarica*, *Gentiana acaulis*

[性状] 結晶 (MeOH)

[融点] Mp 194 °C



-----文献-----

Rivaille, P. et al., Phytochemistry, 1969, 8, 1533, (Gentiacauloside, Gentiakochianoside)

Chaudhuri, R.K. et al., Phytochemistry, 1971, 10, 2425, (分離)

Hostettmann, K. et al., Helv. Chim. Acta, 1974, 57, 294; 1155; 1976, 59, 1584; 1977, 60, 262; 1978, 61, 1549, (分離, H-NMR, UV, 構造決定, 成書)

Hostettmann, K. et al., Helv. Chim. Acta, 1976, 59, 2592-2595, (Gentiabavarutinoside)

Versluys, C. et al., Experientia, 1982, 38, 771, (分離)

Prakash, A. et al., Planta Med., 1982, 45, 61, (分離, 誘導體)

Peres, V. et al., Phytochemistry, 2000, 55, 683-710, (レビュー, 生育)

§ 1,2,6,8-Tetrahydroxyxanthone; 1,6-Di-Me ether, 2-O-[β-D-xylopyranosyl-(1 → 6)-β-D-glucopyranoside]

[化学名・別名] Gentiacauloside. Gentiacaulin

[CAS No.] 20398-10-1

[化合物分類] 単環芳香族 (Xanthenes; 4 × O-置換基)

[構造式]

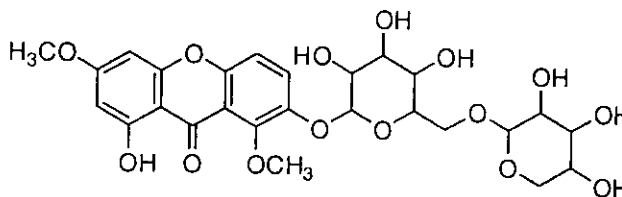
[分子式] C₂₆H₃₀O₁₅

[分子量] 582.514

[基原] *Gentiana acaulis*, *Gentiana kochiana*

[性状] 黄色の針状結晶 (EtOH)

[融点] Mp 223 °C



-----文献-----

Rivaille, P. et al., Phytochemistry, 1969, 8, 1533, (Gentiacauloside, Gentiakochianoside)

Hostettmann, K. et al., Helv. Chim. Acta, 1974, 57, 294; 1155; 1976, 59, 1584; 1977, 60, 262; 1978, 61, 1549, (分離, H-NMR, UV, 構造決定, 成書)

Hostettmann, K. et al., Helv. Chim. Acta, 1976, 59, 2592-2595, (Gentiabavarutinoside)

Peres, V. et al., Phytochemistry, 2000, 55, 683-710, (レビュー, 生育)

*****ルー (Rue) *****

§ § ミカン科ヘンルーダ (*Ruta graveolens* L.) の全草。

§ Angustifolin; Me ether

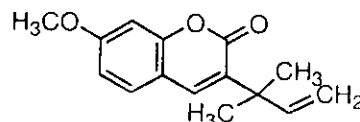
[化学名・別名] 3-(1,1-Dimethyl-2-propenyl)-7-methoxy-2H-1-benzopyran-2-one. 3-(1,1-Dimethylallyl)-7-methoxycoumarin. 3-(1,1-Dimethylallyl) herniarin

[CAS No.] 20958-63-8

[化合物分類] ベンゾピラノイド (7-Oxygenated coumarins with miscellaneous 置換基)

[構造式]

[分子式] C₁₅H₁₆O₃



[性状] 結晶 (MeOH or hexane)

[融点] Mp 126-128 °C

-----文献-----

Reisch, J. et al., Tet. Lett., 1968, 4395, (分離, 誘導体)

Raj, K. et al., Indian J. Chem., 1975, 13, 404, (合成法)

Del Castillo, J.B. et al., Phytochemistry, 1984, 23, 2095, (分離)

Macías, F.A. et al., Acta Cryst. C, 1990, 46, 2482, (結晶構造)

§ 2-Benzyl-1-methyl-4(1H)-quinazolinone

[化学名・別名] 1-Methyl-2-(phenylmethyl)-4(1H)-quinazolinone (CAS 名). Arborine. Glycosine

[CAS No.] 6873-15-0

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

[構造式]

[分子式] C₁₆H₁₃N₂O

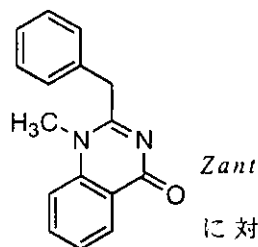
[分子量] 250.299

[基原] *Glycosmis arborea* の葉から得られる主アルカロイド。また *Ruta graveolens*, *hoxylum budrunga* の果実に存在する (ミカン科)

[用途] アセチルコリン抑制因子, 主要な血圧降下薬。 *G. arborea* は熱病, 貧血症, 黄疸して民間医学で用いられる

[性状] 結晶 (MeOH/CHCl₃)

[融点] Mp 161-162 °C (155-156 °C)



-----文献-----

Chakraborty, D.P. et al., Synthesis, 1981, 977, (合成法)

Johne, S., Alkaloids (N.Y.), 1986, 29, 129, (レビュー, 薬理)

Muthukrishnan, J. et al., Phytochemistry, 1999, 50, 249-254, (分離, H-NMR, C13-NMR)

§ 2,3-Butanediol; (2R,3R)-form

[CAS No.] 24347-58-8

[化合物分類] 脂肪族化合物 (Saturated unbranched alcohols)

[構造式]

[分子式] C₄H₁₀O₂

[分子量] 90.122

[基原] 色々な微生物によって生産される。次の植物から分離: ココアバター, *Ruta graveolens* の根

[用途] Used in the resolution of carbonyl compds. by gc

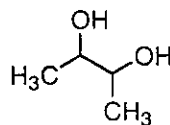
[性状] 吸湿性の結晶

[融点] Mp 19.7 °C

[沸点] Bp₁₀ 77.5-77.6 °C

[比旋光度]: [α]_D²⁵ -13 (neat)

[販売元] Aldrich:23763-9; Fluka:18965; Sigma:B6262



-----文献-----

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, 1, 81; 1992, 16, 52; 1986, 12, 80; 1984, 11, 84; 1979, 7, 242, (用途)

Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1643-1646, (分離, 配糖体)

§ Byakangelicin; (S)-form

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

[構造式]

[分子式] C₁₇H₁₈O₇

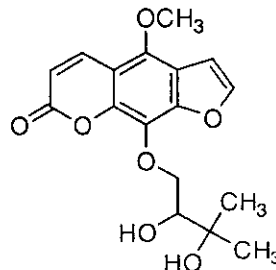
[分子量] 334.325

[基原] *Ruta graveolens*

[性状] 結晶

[融点] Mp 124-126 °C

[比旋光度]: [α]_D²⁵ -19 (MeOH)



-----文献-----

-----文献-----

Noguchi, T. et al., Ber., 1938, 71, 344; 1428, (分離, 構造決定, 合成法)
 Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 580, (生育)

§ Chalepensin; 5,8-Dimethoxy

[化学名・別名] 5,8-Dimethoxychalepensin
 [CAS No.] 42438-50-6
 [化合物分類] ベンゾピラノイド (Furanocoumarins), ベンゾピラノイド (5,7,8-Trioxxygenated coumarins)
 [構造式]

[分子式] C₁₈H₁₈O₅

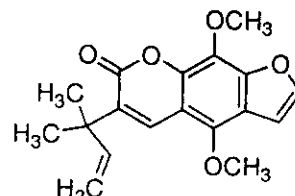
[分子量] 314.337

[基原] *Dorstenia gigas*, *Ruta graveolens*

[性状] 黄色の針状結晶 (hexane/EtOAc)

[融点] Mp 132-134 °C

UV: [neutral] λ_{max} 222 (log ε 4.44); 241 (log ε 4.15); 249 (log ε 4.15); 271 (log ε 4.32); 313 (log ε 4.15) (MeOH)



-----文献-----

Delle Monache, F. et al., Gazz. Chim. Ital., 1976, 106, 681, (分離)
 Franke, K. et al., Phytochemistry, 2001, 56, 611-621, (5,8-Dimethoxychalepensin)

§ Chalepin; (S)-form, Ac

[化学名・別名] Rutamarin. Chalepin acetate
 [CAS No.] 14882-94-1
 [化合物分類] ベンゾピラノイド (Dihydrofuranocoumarins), ベンゾピラノイド (7-Oxygenated coumarins with miscellaneous 置換基)
 [構造式]

[分子式] C₂₁H₂₄O₅

[分子量] 356.418

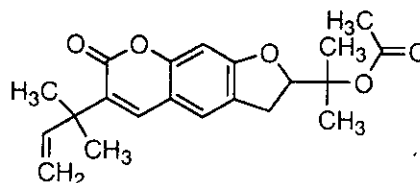
[基原] *Ruta chalepensis*, *Ruta graveolens*

[性状] 結晶

[融点] Mp 107-108 °C

[比旋光度]: [α]_D²² +14 (c, 2.3 in CHCl₃)

[化学物質毒性データ総覧 (RTECS) 登録番号] LV1045200



-----文献-----

Reisch, J. et al., Acta Pharm. Suec., 1967, 4, 179, (分離)
 Brooker, R.M. et al., J. Nat. Prod., 1967, 30, 73, (分離)
 Pozzi, H. et al., Tetrahedron, 1967, 23, 1129, (分離)
 Burke, B.A. et al., Heterocycles, 1981, 16, 897, (絶対構造)
 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>> DNA 阻害.

試験系 : げっ歯類-マウス腹水性腫瘍..

投与量・期間 : 5 mg/L

参照文献

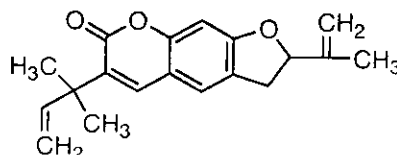
Planta Medica.31.351,1977

§ Chalepin; (S)-form, Deoxy, 1',2'-didehydro

[化学名・別名] *exo*-Dehydrochalepin
 [化合物分類] ベンゾピラノイド (Dihydrofuranocoumarins), ベンゾピラノイド (7-Oxygenated coumarins with miscellaneous 置換基)
 [構造式]

[分子式] C₁₇H₂₀O₄

[分子量] 296.365



[性状] 結晶

[融点] Mp 100 °C

[比旋光度]: $[\alpha]_D^{25} +7.4$ (CHCl₃)

-----文献-----

Reisch, J. et al., Acta Pharm. Suec., 1967, 4, 179, (分離)

Brooker, R.M. et al., J. Nat. Prod., 1967, 30, 73, (分離)

Pozzi, H. et al., Tetrahedron, 1967, 23, 1129, (分離)

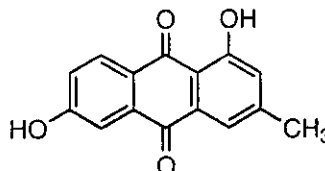
§ 1,6-Dihydroxy-3-methylantraquinone (旧 CAS 名)

[化学名・別名] 1,6-Dihydroxy-3-methyl-9,10-anthracenedione (CAS 名). Phomarin. Digoemodin

[CAS No.] 6866-87-1

[化合物分類] 多環芳香族 (9,10-Anthraquinones; 2 × O-置換基)

[構造式]



[分子式] C₁₅H₁₀O₄

[分子量] 254.242

[基原] *Digitalis orientalis* の根, *Digitalis schischkinii*, *Digitalis viridiflora* の葉; また *Ruta graveolens* の根からも得られる。また *Phoma foveata* (*Phoma exigua*)

[性状] 橙-赤色の針状結晶 (EtOH)

[融点] Mp 258-260 °C (200 °C (分解))

UV: [neutral] λ_{max} 220 (ϵ 28200); 245 (ϵ 10960); 271 (ϵ 28840); 337 (ϵ 1480) (EtOH) (Berdy)

-----文献-----

Brew, E.J.C. et al., J.C.S. (C), 1971, 2007, (分離)

Imre, S. et al., Phytochemistry, 1976, 15, 317, (分離)

Rozsa, Z. et al., Planta Med., 1977, 32, 57, (分離)

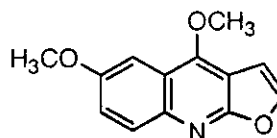
§ 4,6-Dimethoxyfuro [2,3-b]quinoline (CAS 名)

[化学名・別名] Pteleine. 6-Methoxydictamnine

[CAS No.] 2221-41-2

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

[構造式]



[分子式] C₁₃H₁₁NO₃

[分子量] 229.235

[基原] 次の植物から得られるアルカロイド: *Platydesma campanulata*, *Ptelea trifoliata*; tentatively identified in cells of *Ruta graveolens* grown in continuous light in liq. medium (ミカン科)

[性状] 立方結晶 (C₆H₆/petrol)

[融点] Mp 134-135 °C

[化学物質毒性データ総覧 (RTECS) 登録番号] LV2708180

-----文献-----

Werny, F. et al., Tetrahedron, 1963, 19, 1293, (分離, UV, IR, 構造決定)

Frolova, V.I. et al., Zh. Obshch. Khim., 1964, 34, 3499; CA, 62, 2800f, (分離, 構造決定)

Steck, W. et al., Phytochemistry, 1971, 10, 191, (分離, UV, H-NMR)

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>> 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 : 1360 ng/plate

参照文献

Mutagenesis. 2,271,1987

§ 3-(1,1-Dimethyl-2-propenyl)-6,7-dihydroxy-2H-1-benzopyran-2-one; 6-Me ether

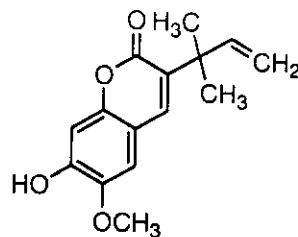
[化学名・別名] 3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-6-methoxy-2H-1-benzopyran-2-one. 3-(1,1-Dimethylallyl)

scopoletin

[CAS No.] 19723-23-0

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

[分子式] $C_{15}H_{16}O_4$
[分子量] 260.289
[基原] *Ruta graveolens*
[性状] 黄色の針状結晶 (petrol)
[融点] Mp 132-135 °C



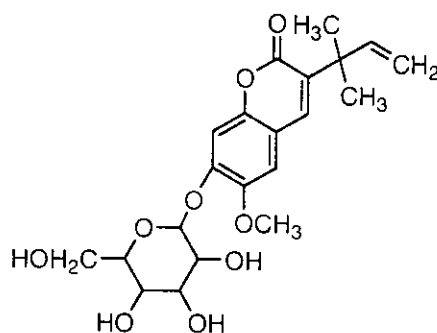
-----文献-----

Steck, W. et al., *Phytochemistry*, 1971, 10, 191, (分離)
von Brocke, W. et al., *Z. Naturforsch., B*, 1971, 26, 1252, (分離)
Borges del Castillo, J. et al., *An. Quim., Ser. C*, 1987, 83, 15, (Dimethylallylisoscapoletin)
Srivastava, S.D. et al., *Fitoterapia*, 1998, 69, 80-81, (3-(1,1-Dimethylallyl)scopolatin 7-glucoside)

§ 3-(1,1-Dimethyl-2-propenyl)-6,7-dihydroxy-2H-1-benzopyran-2-one; 6-Me ether, 7-O-β

-D-glucopyranoside
[CAS No.] 208333-72-6
[化合物分類] ベンゾピラノイド (6,7-Dioxygenated coumarins)
[構造式]

[分子式] $C_{21}H_{26}O_6$
[分子量] 422.431
[基原] *Ruta graveolens*
[性状] 結晶
[融点] Mp 112-114 °C



-----文献-----

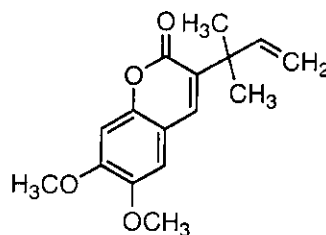
Steck, W. et al., *Phytochemistry*, 1971, 10, 191, (分離)
von Brocke, W. et al., *Z. Naturforsch., B*, 1971, 26, 1252, (分離)
Borges del Castillo, J. et al., *An. Quim., Ser. C*, 1987, 83, 15, (Dimethylallylisoscapoletin)
Srivastava, S.D. et al., *Fitoterapia*, 1998, 69, 80-81, (3-(1,1-Dimethylallyl)scopolatin 7-glucoside)

§ 3-(1,1-Dimethyl-2-propenyl)-6,7-dihydroxy-2H-1-benzopyran-2-one; Di-Me ether

[化学名・別名] 3-(1,1-Dimethyl-2-propenyl)-6,7-dimethoxy-2H-1-benzopyran-2-one (CAS 名), 3-(1,1-Dimethylallyl)-6,7-dimethoxycoumarin. Rutacultin
[CAS No.] 31526-60-0

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

[分子式] $C_{18}H_{18}O_4$
[分子量] 274.316
[基原] *Ruta graveolens*
[性状] 青白い黄色の針状結晶 (petrol)
[融点] Mp 103-104 °C



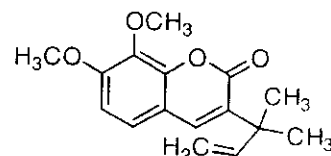
-----文献-----

Steck, W. et al., *Phytochemistry*, 1971, 10, 191, (分離)
von Brocke, W. et al., *Z. Naturforsch., B*, 1971, 26, 1252, (分離)
Bergenthal, D. et al., *Arch. Pharm. (Weinheim, Ger.)*, 1978, 311, 1026, (C13-NMR)
Borges del Castillo, J. et al., *An. Quim., Ser. C*, 1987, 83, 15, (Dimethylallylisoscapoletin)
Srivastava, S.D. et al., *Fitoterapia*, 1998, 69, 80-81, (3-(1,1-Dimethylallyl)scopolatin 7-glucoside)

§ 3-(1,1-Dimethyl-2-propenyl)-7,8-dihydroxy-2H-1-benzopyran-2-one; Di-Me ether

[化学名・別名] 3-(1,1-Dimethyl-2-propenyl)-7,8-dimethoxy-2H-1-benzopyran-2-one (CAS 名), 3-(1,1-Dimethylallyl)-7,8-dimethoxycoumarin

[CAS No.] 30310-54-4
[化合物分類] ベンゾピラノイド (7,8-Dioxygenated coumarins)
[構造式]



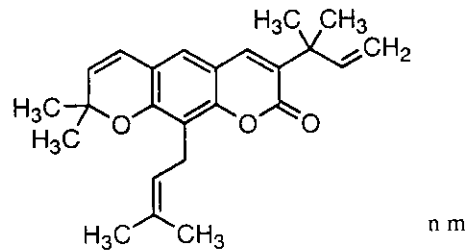
[分子式] $C_{16}H_{16}O_3$
 [分子量] 274.316
 [基原] 次の植物から分離: *Ruta graveolens* の根
 [性状] 結晶 (hexane)
 [融点] Mp 85-86 °C

-----文献-----

Reisch, J. et al., Tet. Lett., 1970, 4305, (分離)
 González, A.G. et al., An. Quim., 1976, 72, 191, (分離, 合成法, 誘導体)

§ 3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl) xanthyletin

[化学名・別名] 3-(1,1-Dimethylallyl)-8-(3,3-dimethylallyl) xanthyletin
 [CAS No.] 30310-55-5
 [化合物分類] ベンゾピラノイド (Pyranocoumarins), ベンゾピラノイド (7-Oxygenated coumarins with miscellaneous 置換基)
 [構造式]



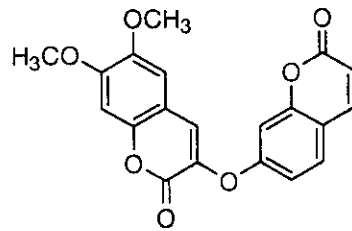
[分子式] $C_{23}H_{28}O_3$
 [分子量] 364.483
 [基原] 次の植物から分離: *Ruta graveolens* の根
 [その他のデータ] λ_{max} 226 infl (log ϵ 4.39), 265 (4.24) and 335 (4.11) (MeOH)

-----文献-----

Reisch, J. et al., Tet. Lett., 1970, 4305, (分離)
 Sharma, R.B. et al., Indian J. Chem., Sect. B, 1983, 22, 538, (合成法)

§ Edgeworthin; Di-Me ether

[化学名・別名] Daphnoretin methyl ether. Isodaphnoretin (incorr.)
 [CAS No.] 3749-38-0
 [化合物分類] ベンゾピラノイド (Bis- and tris-coumarins)
 [構造式]



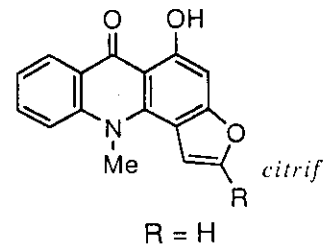
[分子式] $C_{20}H_{14}O_7$
 [分子量] 366.326
 [基原] *Ruta graveolens*, *Ruta montana*
 [性状] 黄色の針状結晶 (EtOH)
 [融点] Mp 240 °C
 UV: [neutral] λ_{max} 224 ; 264 ; 322 ; 338 (MeOH)

-----文献-----

Chakrabarti, R. et al., Phytochemistry, 1986, 25, 557, (分離)
 Liu, G.F. et al., J. Chin. Pharm. Sci., 1997, 6, 125-128, (Isodaphnoretin)

§ Furofoline

[化学名・別名] 5-Hydroxy-11-methylfuro[2,3-c]acridin-6(11H)-one (CAS 名). Furofoline I. Furacridone
 [CAS No.] 62541-22-4
 [化合物分類] アルカロイド化合物 (Acridone alkaloids)
 [構造式]



[分子式] $C_{16}H_{11}NO_3$
 [分子量] 265.268
 [基原] 次の植物から得られるアルカロイド: *Ruta graveolens* の根 *Glycosmis* の根と茎皮 (ミカン科)
 [性状] 黄色の板状結晶 (Me₂CO)
 [融点] Mp 245-246 °C

-----文献-----

Reisch, J. et al., Phytochemistry, 1977, 16, 151, (分離)
 Reisch, J. et al., Annalen, 1981, 85, (合成法)
 Wu, T.-S. et al., J.C.S. Perkin 1, 1983, 1681, (分離, UV, IR, H-NMR, Mass, 構造決定)

§ Gravelliferone

[化学名・別名] 3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-6-(3-methyl-2-butenyl)-2H-1-benzopyran-2-one (CAS名), 3-(1,1-Dimethylallyl)-7-hydroxy-6-(3-methyl-2-butenyl) coumarin (旧CAS名)

[CAS No.] 21316-80-3

[化合物分類] ベンゾピラノイド (7-Oxygenated coumarins with miscellaneous 置換基)

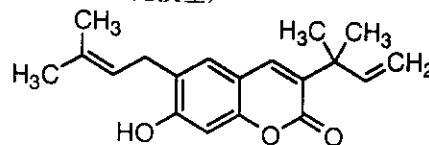
[構造式]

[分子式] $C_{19}H_{22}O_3$

[分子量] 298.381

[基原] 次の植物から分離: *Ruta graveolens*

[融点] Mp 166-168 °C



----- 文献 -----

Reisch, J. et al., *Experientia*, 1968, 24, 992, (分離, IR, UV)

Gonzalez, A.G. et al., *An. Quim.*, 1972, 68, 415; 1977, 73, 1015, (分離, UV, IR)

§ Gravelliferone; 8-Methoxy

[CAS No.] 30430-91-2

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

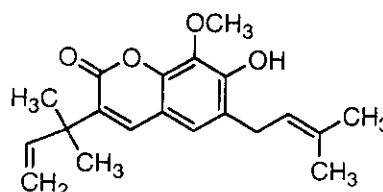
[構造式]

[分子式] $C_{20}H_{22}O_4$

[分子量] 328.407

[基原] *Ruta graveolens*

[融点] Mp 131-133 degree



----- 文献 -----

Reisch, J. et al., *Experientia*, 1968, 24, 992, (分離, IR, UV)

Reisch, J. et al., *Tet. Lett.*, 1968, 4395; 1970, 4305, (誘導體)

Gonzalez, A.G. et al., *An. Quim.*, 1972, 68, 415; 1977, 73, 1015, (分離, UV, IR)

Bergenthal, D. et al., *Arch. Pharm. (Weinheim, Ger.)*, 1978, 311, 1026, (C13-NMR)

§ Graveoline

[化学名・別名] 2-(1,3-Benzodioxol-5-yl)-1-methyl-4(1H)-quinolinone (CAS名), 1-Methyl-2-(3,4-methylenedioxyphenyl)-4(1H)-quinolinone. Rutamine. Foliosine

[CAS No.] 485-61-0

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

[構造式]

[分子式] $C_{17}H_{13}NO_3$

[分子量] 279.295

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens*, *Ruta bracteosa*, *Haplophyllum* spp. (ミカン科)

[性状] 針状結晶 (EtOH)

[融点] Mp 186-187 °C. Mp 205-205.5 °C (dimorph.)

[その他のデータ] Rutamine was the metastable lower-melting modification

----- 文献 -----

Schneider, G. et al., *Arch. Pharm. (Weinheim, Ger.)*, 1967, 300, 953-954, (Rutamine)

§ Gravolenic acid

[CAS No.] 13781-46-9

[化合物分類] ベンゾフラノイド (Benzofurans)

[構造式]

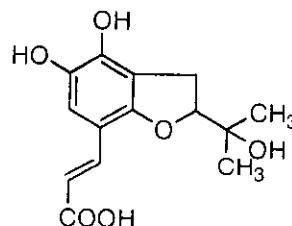
[分子式] $C_{17}H_{16}O_6$

[分子量] 280.277

[基原] 次の植物から分離: *Ruta graveolens* の地上部

[性状] 淡黄色の結晶 (EtOAc or Me₂CO 溶液)

[融点] Mp 194 °C



----- 文献 -----

Reisch, J. et al., *Acta Pharm. Suec.*, 1966, 3, 423, (H-NMR, ORD)

Novák, I. et al., *Planta Med.*, 1966, 14, 151, (分離, UV, IR, 構造決定)

§ Hallacridone

[化学名・別名] 2-Acetyl-5-hydroxy-11-methylfuro[2,3-c]acridin-6(11H)one (CAS 名)

[CAS No.] 109897-77-0

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

[構造式]

[分子式] $C_{18}H_{13}NO_4$

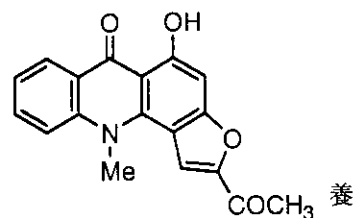
[分子量] 307.305

[一般的性質] Struct. revised in 1989

[基原] 次の植物から得られる微量アルカロイド: *Ruta graveolens* の組織培 (ミカン科)

[性状] 黄色の針状結晶 ($CHCl_3$)

[融点] Mp 295-298 °C



-----文献-----

Baumert, A. et al., Pharmazie, 1987, 42, 67; CA, 107, 93537w

Baumert, A. et al., Fitoterapia, 1988, 59, 83; CA, 109, 226730u

Reisch, J. et al., J.C.S. Perkin 1, 1989, 1047, (合成法, IR, 構造決定)

§ 2,4-Heptadecanedione (CAS 名)

[化学名・別名] Tetradecanoylacetone, Myristoylacetone

[CAS No.] 64042-18-8

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

[構造式] $H_3C(CH_2)_{12}COCH_2COCH_3$

[分子式] $C_{17}H_{32}O_2$

[分子量] 268.439

[一般的性質] Acetogenin

[基原] *Ruta graveolens* and the brown alga *Caulocystis cephalornithos*. Also found in various mammalian tissues

[性状] オイル

[融点] Mp 42.5 °C (39 °C)

-----文献-----

Morgan, G.T. et al., J.C.S., 1925, 127, 2891, (合成法)

Douglas, D.E. et al., Lipids, 1977, 12, 635, (合成法)

Douglas, D.E. et al., Can. J. Biochem., 1978, 56, 691, (生育)

Tattje, D.H.E. et al., Pharm. Weekbl., 1978, 113, 1169, (分離)

Amico, V. et al., J. Nat. Prod., 1990, 53, 1379, (分離)

§ 1-Hydroxyacridone; N-Me

[化学名・別名] 1-Hydroxy-10-methylacridone

[CAS No.] 16584-54-6

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

[構造式]

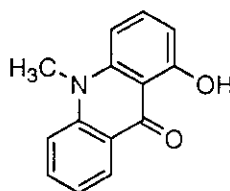
[分子式] $C_{17}H_{17}NO_2$

[分子量] 225.246

[基原] 次の植物の根から得られるアルカロイド: *Boenninghausenia albiflora*, *Ruta graveolens*. Also isol. from the callus cultures obt. from the meristematic cells of *Ruta graveolens* (ミカン科)

[性状] 黄色の針状結晶 (Me:CO)

[融点] Mp 192-194 °C



-----文献-----

Hughes, G.K., Aust. J. Sci. Res., Ser. A, 1952, 5, 206, (合成法)

Reisch, J. et al., Experientia, 1971, 27, 1005, (誘導體, 分離, H-NMR, 構造決定)

Scharlemann, W., Z. Naturforsch., B, 1972, 27, 806, (誘導體, 分離, UV)

Rózsa, Zs. et al., Pharmazie, 1975, 30, 753, (分離, 誘導體)

Adams, J.H. et al., J.C.S. Perkin 1, 1977, 2173, (誘導體, 合成法, UV, IR, H-NMR)

Rózsa, Zs. et al., Phytochemistry, 1978, 17, 169, (UV, IR, H-NMR, Mass, 誘導體, 分離, 合成法)

Gibbons, S. et al., Phytochemistry, 1997, 44, 1109, (1-Methoxy-10-methylacridone)

Coppola, G.M., Org. Prep. Proced. Int., 1999, 31, 225-227, (合成法, IR, H-NMR)

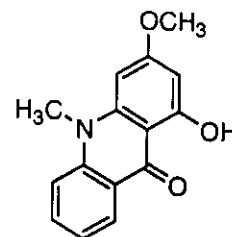
§ 1-Hydroxy-3-methoxy-10-methylacridone

[化学名・別名] 1-Hydroxy-3-methoxy-10-methyl-9(10H)-acridinone (CAS 名)

[CAS No.] 13161-83-6

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

[構造式]



[分子式] $C_{15}H_{15}NO_3$

[分子量] 255.273

[基原] 次の植物から得られるアルカロイド: *Esenbeckia littoralis* の樹皮, *Glycosmis mauritiana* と *Ruta graveolens* の根, *Fagara leprieurii* と *Fagara rubescens* の根と茎皮 (ミカン科)

[性状] 黄色の結晶 (EtOAc/petrol or EtOAc/ C_6H_6)

[融点] Mp 164-165 °C. Mp 174-176 °C

----- 文献 -----

Bowie, J.H. et al., Aust. J. Chem., 1967, 20, 1179, (Mass)

Fish, F. et al., Phytochemistry, 1971, 10, 3322, (分離, UV, IR)

Scharlemann, W., Z. Naturforsch., B, 1972, 27, 806, (分離, UV)

Reisch, J. et al., Phytochemistry, 1977, 16, 151, (分離)

Bergenthal, D. et al., Phytochemistry, 1979, 18, 161, (C13-NMR)

Mester, I. et al., Z. Naturforsch., B, 1979, 34, 516, (C13-NMR)

Dreyer, D.L., Phytochemistry, 1980, 19, 941, (分離, UV, H-NMR, Mass, 合成法)

Rastogi, K. et al., Phytochemistry, 1980, 19, 945, (分離, UV, H-NMR)

Bahar, M.H. et al., Indian J. Chem., Sect. B, 1987, 26, 782, (合成法, UV, IR, H-NMR, Mass)

§ 4-Methoxy-2-(3,4-methylenedioxyphenyl)quinoline

[化学名・別名] 2-(1,3-Benzodioxol-5-yl)-4-methoxyquinoline (CAS 名). Graveolinine

[CAS No.] 4179-37-7

[化合物分類] アルカロイド化合物 (Simple quinoline alkaloids), 薬物: 鎮痙薬 (Antispasmodics)

[構造式]

[分子式] $C_{17}H_{17}NO_3$

[分子量] 279.295

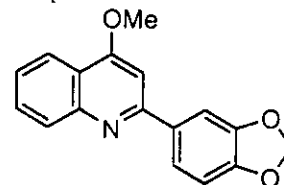
[基原] 次の植物のアルカロイド: *Ruta graveolens*, *Lunasia amara* (ミカン科)

[用途] 鎮痙作用

[性状] プリズム結晶 (pentane/EtOAc)

[融点] Mp 116-117 °C

[Log P 計算値] Log P 3.97 (計算値)



----- 文献 -----

Goodwin, S. et al., J.A.C.S., 1959, 81, 6209, (分離, IR, UV, 構造決定)

Chatterjee, A. et al., Chem. Ind. (London), 1962, 1982, (分離, IR, UV, 合成法)

Reisch, J. et al., Naturwissenschaften, 1967, 54, 200, (合成法)

§ 3-Methyldecane

[CAS No.] 13151-34-3

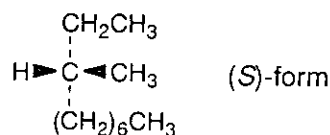
[化合物分類] 脂肪族化合物 (Branched aliphatic hydrocarbons)

[構造式]

[分子式] $C_{11}H_{24}$

[分子量] 156.311

[基原] 次の植物から分離: *Cicer arietinum*, *Lycium halimifolium*, *Pinus* spp., *Ruta graveolens*, ココナッツ. Also obt. from the glandular secretions of various ant spp.



----- 文献 -----

Francis, A.W., Ind. Eng. Chem., 1943, 35, 442, (性質)

Christen, P. et al., Pharm. Acta Helv., 1987, 62, 158, (分離)

Bagnères, A.G. et al., Biochem. Syst. Ecol., 1991, 19, 25, (分離)

§ 2-[4-(3,4-Methylenedioxyphenyl)butyl]-4-(1H)-quinolinone

[CAS No.] 17889-77-9

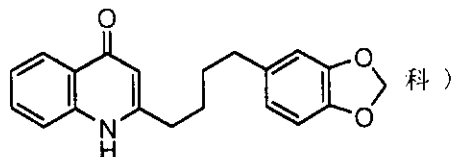
[分子式] $C_{20}H_{19}NO_3$

[分子量] 321.375

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* (ミカン

[性状] 結晶 (MeOH)

[融点] Mp 224 °C



-----文献-----

Novák, I. et al., *Pharmazie*, 1965, 20, 654, (分離, IR, H-NMR, Mass, 構造決定)

Reisch, J. et al., *Naturwissenschaften*, 1967, 54, 517, (合成法)

§ 6-[(3,4-Methylenedioxy) phenyl]-3,3-dimethyl-1-hexene (旧 CAS 名)

[化学名・別名] 5-(4,4-Dimethyl-5-hexenyl)-1,3-benzodioxole (CAS 名)

[CAS No.] 30310-56-6

[化合物分類] 単環芳香族 (Simple phenols)

[構造式]

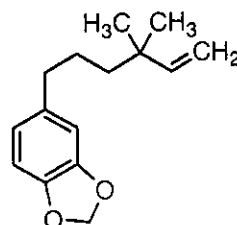
[分子式] $C_{15}H_{20}O_2$

[分子量] 232.322

[基原] *Ruta graveolens* の根

[性状] オイル

[屈折率] n_D^{20} 1.5135



-----文献-----

Reisch, J. et al., *Tet. Lett.*, 1970, 4305, (分離, IR, UV, H-NMR)

§ 6-Methylheptadecane

[CAS No.] 26741-13-9

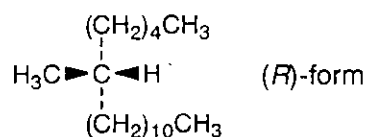
[化合物分類] 脂肪族化合物 (Branched aliphatic hydrocarbons)

[構造式]

[分子式] $C_{18}H_{38}$

[分子量] 254.498

[基原] 次の植物から分離: 藍藻植物 *Nostoc muscorum*, *Ruta graveolens* のオイル



-----文献-----

Calvin, M. et al., *Chem. Comm.*, 1970, 1490, (分離)

Schlenk, W. et al., *Annalen*, 1973, 1179, (合成法)

Tattje, D.H.E. et al., *Pharm. Weekbl.*, 1978, 113, 1169, (分離)

§ 3-Methyltetradecane

[CAS No.] 18435-22-8

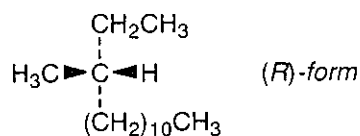
[化合物分類] 脂肪族化合物 (Branched aliphatic hydrocarbons)

[構造式]

[分子式] $C_{15}H_{32}$

[分子量] 212.418

[基原] *Hierochloe odorata*, *Ruta graveolens*, *Zea mays*. Also found in the Dufour glands of various ants



-----文献-----

Thompson, A.C. et al., *Phytochemistry*, 1974, 13, 2029, (分離)

Feldhues, M. et al., *Tetrahedron*, 1985, 41, 4195, (合成法, H-NMR, Mass)

Brown, C.A. et al., *J.O.C.*, 1986, 51, 162, (合成法, C13-NMR)

Ueyama, Y. et al., *Flavour Fragrance J.*, 1991, 6, 63, (分離)

Nascimento, R.R. et al., *J. Chem. Ecol.*, 1993, 19, 1993, (生育)

§ Naphthoherniarin 6

[化学名・別名] 2-Methoxy-8-(7-methoxy-2-oxo-2H-1-benzopyran-6-yl)-6-methyl-1,4-naphthalenedione (CAS 名)

[CAS No.] 114032-22-3

[化合物分類] 多環芳香族 (Naphthoquinones; 1 × O-置換基),
ベンゾピラノイド (7-Oxygenated coumarins, 6-substituted)

[構造式]

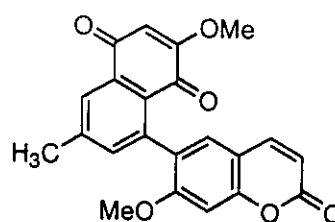
[分子式] $C_{22}H_{16}O_6$

[分子量] 376.365

[基原] *Ruta graveolens*

[性状] 結晶 (toluene)

[融点] Mp 242-244 °C. Mp 285 °C (278-283 °C)



----- 文献 -----

Reisch, J. et al., *Annalen*, 1988, 543, (IR, H-NMR, UV, 合成法)

Rózsa, Z. et al., *Planta Med.*, 1989, 55, 68, (分離, UV, H-NMR, C13-NMR)

§ 2-Nonyl-4(1H)-quinolinone; N-Me

[化学名・別名] 1-Methyl-2-nonyl-4(1H)-quinolinone

[CAS No.] 68353-24-2

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

[構造式]

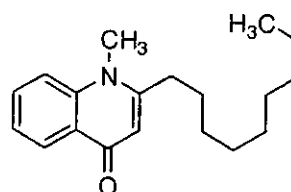
[分子式] $C_{19}H_{27}NO$

[分子量] 285.428

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens*, *Evodia rutaecarpa* の熟した実 (ミカン科)

[性状] 板状結晶 (C_6H_6 /cyclohexane)

[融点] Mp 71-75 °C



----- 文献 -----

Hays, E.E. et al., *J. Biol. Chem.*, 1945, 159, 725, (分離, UV)

Wells, I.C., *J. Biol. Chem.*, 1952, 196, 331, (分離, 構造決定, 合成法)

Kamikado, T. et al., *Agric. Biol. Chem.*, 1978, 42, 1515, (誘導体)

Budzikiewicz, H. et al., *Monatsh. Chem.*, 1979, 110, 947, (分離, UV)

Grundon, M.F. et al., *Phytochemistry*, 1979, 18, 1768, (誘導体)

Somanathan, R. et al., *J. Het. Chem.*, 1981, 18, 1077, (合成法, UV, IR, H-NMR)

Touati, D. et al., *Phytochemistry*, 2000, 53, 277-279, (8-oxononyl derivs)

§ Oleanolic acid 3-glycosides; Triglycosides, 3-O-[α -L-Rhamnopyranosyl-(1 → 4)- β -D-glucopyranosyl-(1 → 6)- β -D-glucopyranoside]

[CAS No.] 160845-07-8

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

[構造式]

[分子式] $C_{48}H_{78}O_{17}$

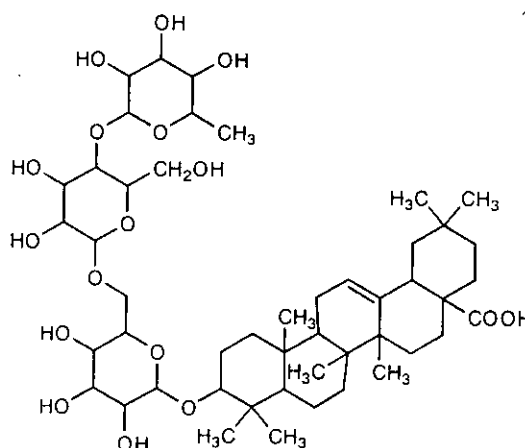
[分子量] 927.134

[基原] *Ruta graveolens*

[性状] 結晶

[融点] Mp 223-224 °C

[比旋光度]: $[\alpha]_D^{25} +16.5$ (MeOH)



----- 文献 -----

Srivastava, S.K. et al., *Fitoterapia*, 1994, 65, 301. (*Ruta graveolens* saponin)

§ Pabulenol; (R)-form

[CAS No.] 33783-80-1

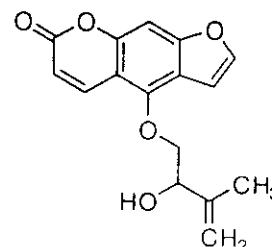
[化合物分類] ベンゾピラノイド (5,7-Dioxygenated coumarins).

ベンゾピラノイド (Furanocoumarins)

[構造式]

[分子式] $C_{16}H_{14}O_5$

[分子量] 286.284



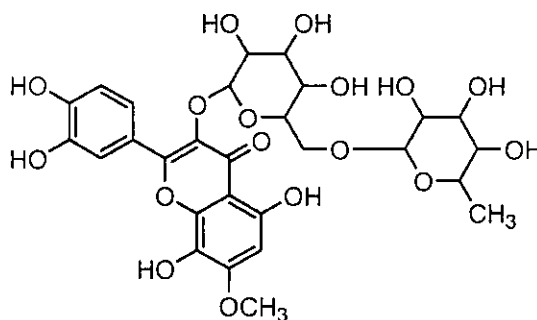
[基原] *Angelica panceicii*, *Heracleum sosnowskyi*, *Hippomarathrum caspicum*, *Ruta graveolens*, *Ruta pinnata*
 [性状] 結晶
 [融点] Mp 136.5-138.5 °C. Mp 123-125 °C
 [比旋光度]: $[\alpha]_D^{18} +8.6$ (c, 0.46 in EtOH)

-----文献-----

Neilsen, B.E. et al., *Acta Chem. Scand.*, 1965, 19, 1810, (分離)
 Abyshev, A.Z. et al., *Khim. Prir. Soedin.*, 1965, 5, 3; 1971, 7, 522; 1972, 8, 49; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, 5, 3; 1971, 7, 498; 1972, 8, 43, (分離, 合成法)
 Ognyanov, I. et al., *Dokl. Bolg. Akad. Nauk*, 1971, 24, 315, (分離)
 Basa, S.C. et al., *Tet. Lett.*, 1971, 1977, (分離)
 Chatterjea, A. et al., *Tetrahedron*, 1972, 28, 5175, (分離)
 Reisch, J. et al., *Phytochemistry*, 1975, 14, 1889, (分離)
 Babu, K. et al., *Chem. Pharm. Bull.*, 1981, 29, 2565, (分離)
 Meacutendez, J. et al., *Phytochemistry*, 1983, 22, 2599, (分離)
 Grande, M. et al., *Phytochemistry*, 1986, 25, 505, (分離)
 Adebajo, A.C. et al., *Fitoterapia*, 2000, 71, 334-337, (H-NMR)

§ 3,3',4',5,8-Pentahydroxy-7-methoxyflavone; 3-O-[α -L-Rhamnopyranosyl-(1 → 6)- β -D-glucopyranoside]

[化学名・別名] Ranupenin 3-rutinoside
 [CAS No.] 85122-22-1
 [化合物分類] フラボノイド (Flavonols; 6 × O-置換基)
 [構造式]



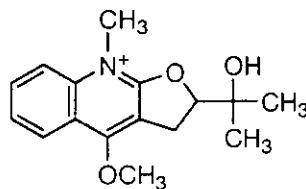
[分子式] $C_{28}H_{32}O_{17}$
 [分子量] 640.551
 [基原] 次の植物から分離: *Ruta graveolens*

-----文献-----

Harborne, J.B. et al., *Phytochemistry*, 1965, 4, 647; 1969, 8, 177; 1978, 17, 589, (配糖体)
 Chumbalov, T.K. et al., *Khim. Prir. Soedin.*, 1976, 12, 658; 660; *Chem. Nat. Compd. (Engl. Transl.)*, 591; 593, (Purifolin, Purifolinin)
 Wagner, H. et al., *Chem. Ber.*, 1977, 110, 737, (合成法, 構造決定)
 Harborne, J.B. et al., *Z. Naturforsch., C*, 1983, 38, 148, (3-rutinoside)
 Sultana, N. et al., *Phytochemistry*, 1999, 52, 895-900, (3-glucoside, 3-coumaroylglucoside)

§ Platydesmine; (R)-form, N-Me

[化学名・別名] Platydesminium
 [化合物分類] アルカロイド化合物 (Furanoquinoline alkaloids)
 [構造式]



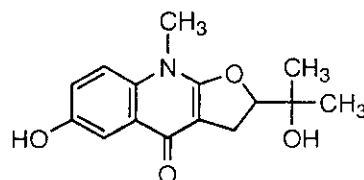
[分子式] $C_{16}H_{20}NO_3^{(+)}$
 [分子量] 274.339
 [基原] 次の植物から得られるアルカロイド: *Ruta graveolens*, その他多くのミカン科の種
 [融点] Mp 192-196 °C (as chloride)

-----文献-----

Wernhey, F. et al., *Tetrahedron*, 1963, 19, 1293, (分離, 構造決定, IR, UV, Mass)
 Johns, S.R. et al., *Aust. J. Chem.*, 1966, 19, 1991, (分離, H-NMR)
 Murphy, S.T. et al., *Aust. J. Chem.*, 1974, 27, 187, (分離)
 Rideau, M. et al., *Phytochemistry*, 1979, 18, 155, (分離, Mass)
 Ramesh, M. et al., *Heterocycles*, 1984, 22, 125, (合成法, IR, H-NMR)

§ Ribaline; (±)-form

[CAS No.] 41234-32-6
 [化合物分類] アルカロイド化合物 (Furanoquinoline alkaloids)
 [構造式]
 [分子式] $C_{15}H_{17}NO_4$



[分子式] $C_{15}H_{17}NO_4$

[分子量] 275.304

[基原] 次の植物から得られる微量アルカロイド: *Balfourodendron riedelianum*, *Ruta graveolens* (ミカン科)

[性状] 針状結晶 (MeOH)

[融点] Mp 268-269 °C (259-260 °C (分解))

-----文献-----

Szendrei, K. et al., *Herba Hung.*, 1971, 10, 131-139, (分離)

Corral, R.A. et al., *Tetrahedron*, 1973, 29, 205, (分離, UV, IR, 構造決定, 合成法)

Hammerum, S. et al., *Acta Chem. Scand., Ser. B*, 1977, 31, 31, (Mass)

Jurd, L. et al., *Aust. J. Chem.*, 1983, 36, 1615, (分離, IR, H-NMR, C13-NMR, Mass)

Corral, R.A. et al., *Tet. Lett.*, 1983, 24, 2359, (合成法)

§ Ribalinium

[化学名・別名] 2,3-Dihydro-6-hydroxy-2-(1-hydroxy-1-methylethyl)-4-methoxy-9-methylfuro[2,3-b]quinolinium (CAS名)

[CAS No.] 6883-22-3

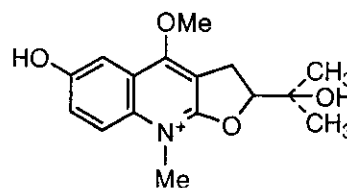
[化合物分類] アルカロイド化合物 (Furanoquinoline alkaloids)

[構造式]

[分子式] $C_{16}H_{20}NO_4$

[分子量] 290.338

[基原] 次の植物から得られるアルカロイド: *Balfourodendron riedelianum* の幹樹皮, *Ruta graveolens* の葉 (ミカン科)



-----文献-----

Corral, R.A. et al., *Tetrahedron*, 1965, 21, 909, (分離, UV, IR, H-NMR, 構造決定)

Rideau, M. et al., *Phytochemistry*, 1979, 18, 155, (分離, H-NMR, Mass, 構造決定)

§ Rutacridone

[化学名・別名] 1,11-Dihydro-5-hydroxy-11-methyl-2-(1-methylethenyl)furo[2,3-c]acridin-6(2H)-one

[CAS No.] 17948-33-3

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

[構造式]

[分子式] $C_{19}H_{17}NO_3$

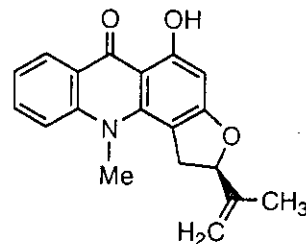
[分子量] 307.348

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens*, *Ruta chalepensis* (ミカン科)

[融点] Mp 161-162 °C

[比旋光度]: $[\alpha]_D^{21} - 43$

[化学物質毒性データ総覧 (RTECS) 登録番号] VM2050000



-----文献-----

Reisch, J. et al., *Acta Pharm. Suec.*, 1967, 4, 265; *CA*, 68, 39861, (分離, IR, H-NMR)

Reisch, J. et al., *Z. Naturforsch., B*, 1978, 33, 957, (レビュー, H-NMR, 構造決定)

Nahrstedt, A. et al., *Z. Naturforsch., C*, 1981, 36, 200, (Rutacridone epoxide)

Zschunke, A. et al., *Chem. Comm.*, 1982, 1263, (生合成)

Eilert, U. et al., *Z. Naturforsch., C*, 1982, 37, 132, (20-Hydroxyrutacridone epoxide)

Nahrstedt, A. et al., *Planta Med.*, 1985, 517, (1-Hydroxyrutacridone epoxide)

Reisch, J. et al., *Monatsh. Chem.*, 1990, 121, 829, (合成法)

Reisch, J. et al., *Annalen*, 1991, 299, (Gravacridonol)

Baumert, A. et al., *Plant Cell. Tissue Organ Cult.*, 1992, 28, 159; *CA*, 117, 66678t, (Alkaloid A6)

Baumert, A. et al., *Planta Med.*, 1994, 60, 143, (Gravacridonol monoglucoside)

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>> 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 : 5 ug/plate

§ Rutacridone; 1',2'-Epoxide

[化学名・別名] Rutacridone epoxide

[CAS No.] 77996-03-3

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

[構造式]

[分子式] $C_{19}H_{17}NO_4$

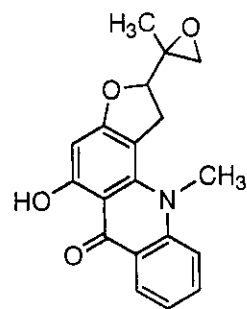
[分子量] 323.348

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* の根とカルス組織培 (ミカン科)

[溶解性] BERDY SOL: メタノール, クロロホルムに可溶; 水, ヘキサンに難溶

UV: [neutral] λ_{max} 226 (ϵ 3710); 263 (ϵ 6760); 300 (ϵ 3710); 390 (ϵ 1200) (MeOH) (Berdy)

[化学物質毒性データ総覧 (RTECS) 登録番号] LV0850000



養

-----文献-----

Nahrstedt, A. et al., Z. Naturforsch., C, 1981, 36, 200, (Rutacridone epoxide)

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>> 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: 1 ng/plate

参照文献

Mutagenesis, 4, 45, 1989

§ Rutacridone; 3'-Hydroxy

[化学名・別名] Gravacridonol

[CAS No.] 81545-69-9

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

[構造式]

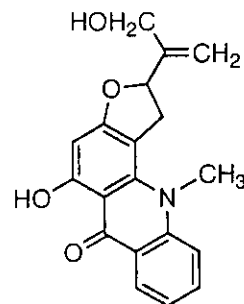
[分子式] $C_{19}H_{17}NO_4$

[分子量] 323.348

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* (ミカン科)

[融点] Mp 155-156 °C (153 °C)

[その他のデータ] C-2 config. not detd.



-----文献-----

Reisch, J. et al., Annalen, 1991, 299, (Gravacridonol)

Baumert, A. et al., Planta Med., 1994, 60, 143, (Gravacridonol monoglucoside)

§ Rutacridone; 1',2'-Epoxide, 1-hydroxy

[化学名・別名] 1-Hydroxyrutacridone epoxide

[CAS No.] 101330-59-0

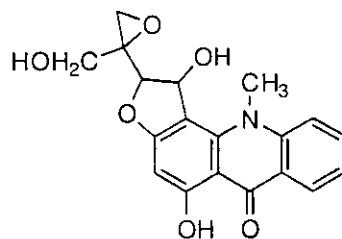
[化合物分類] アルカロイド化合物 (Acridone alkaloids)

[構造式]

[分子式] $C_{19}H_{17}NO_5$

[分子量] 339.347

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* のカルス組 (ミカン科)



織

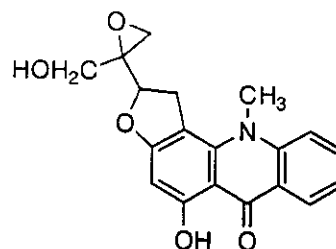
-----文献-----

Nahrstedt, A. et al., Planta Med., 1985, 517, (1-Hydroxyrutacridone epoxide)

§ Rutacridone; 3'-Hydroxy, 1',2'-epoxide

[化学名・別名] 20-Hydroxyrutacridone epoxide

[CAS No.] 80565-10-2
[化合物分類] アルカロイド化合物 (Acridone alkaloids)
[構造式]



[分子式] $C_{19}H_{17}NO_3$

[分子量] 339.347

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* の根とカルス組織培養 (ミカン科)

[溶解性] BERDY SOL: メタノール, クロロホルムに可溶; 水, ヘキサンに難溶

UV: [neutral] λ_{max} 227 (ϵ 8910); 250 (ϵ 9770); 264 (ϵ 10470); 274 (ϵ 13800); 301 (ϵ 5370); 330 (ϵ 2450); 392 (ϵ 1740) (MeOH) (Berdy)

[その他のデータ] 20-Posn. in the authors' numbering scheme called here 3'

----- 文献 -----

Eilert, U. et al., Z. Naturforsch., C, 1982, 37, 132, (20-Hydroxyrutacridone epoxide)

§ Rutacridone; 1',2'-Dihydro, 1'-chloro, 2'-hydroxy

[化学名・別名] 2-(1-Chloro-2-hydroxy-1-methylethyl)-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-c]acridin-6(2H)-one. Gravacridonechlorine

[CAS No.] 38494-84-7

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

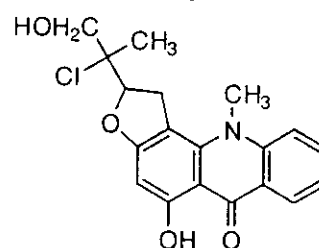
[構造式]

[分子式] $C_{19}H_{18}ClNO_4$

[分子量] 359.808

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* (ミカン科)

[融点] Mp 254-257 °C



----- 文献 -----

Reisch, J. et al., Acta Pharm. Suec., 1967, 4, 265; CA, 68, 39861, (分離, IR, H-NMR)

Rózsa, Zs., Fitoterapia, 1976, 47, 147, (Gravacridonediol, 分離)

Reisch, J. et al., Z. Naturforsch., B, 1978, 33, 957, (レビュー, H-NMR, 構造)

Zschunke, A. et al., Chem. Comm., 1982, 1263, (合成)

Reisch, J. et al., Annalen, 1991, 299, (Gravacridonol)

Paulini, H. et al., Planta Med., 1991, 57, 59; 82, (Isogravacridonechlorine, Gravacridonediolacetate)

Baumert, A. et al., Planta Med., 1994, 60, 143, (Gravacridonol monoglucoside)

§ Rutacridone; 1',2'-Dihydro, 2'-chloro, 1'-hydroxy

[化学名・別名] 2-(2-Chloro-1-hydroxy-1-methylethyl)-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-c]acridin-6(2H)-one. Isogravacridonechlorine

[CAS No.] 62512-94-1

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

[構造式]

[分子式] $C_{19}H_{18}ClNO_4$

[分子量] 359.808

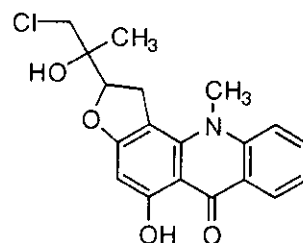
[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* (ミカン科)

[性状] 黄色の粉末 (Me₂CO)

[融点] Mp 224-226 °C で分解. Mp 247-250 °C

[比旋光度]: $[\alpha]_D^{25}$ -9.2 (c, 0.08 in CHCl₃)

[傷害・毒性] 変異原物質



----- 文献 -----

Paulini, H. et al., Planta Med., 1991, 57, 59; 82, (Isogravacridonechlorine, Gravacridonediolacetate)

§ Rutacridone; 1',2'-Dihydro, 1',2'-dihydroxy

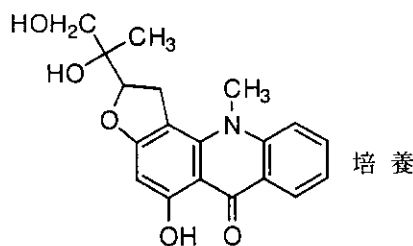
[化学名・別名] 2-(1,2-Dihydroxy-1-methylethyl)-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-c]acridin-6(2H)-one. Gravacridonediol

[CAS No.] 37551-75-0

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

[構造式]

[分子式] $C_{19}H_{19}NO_5$
 [分子量] 341.363
 [基原] 次の植物から得られるアルカロイド: *Ruta graveolens* の根の組織 (ミカン科)
 [性状] 結晶 (Me_2CO or Me_2CO/C_6H_6)
 [融点] Mp 224-227 °C (分解), 246-250 °C



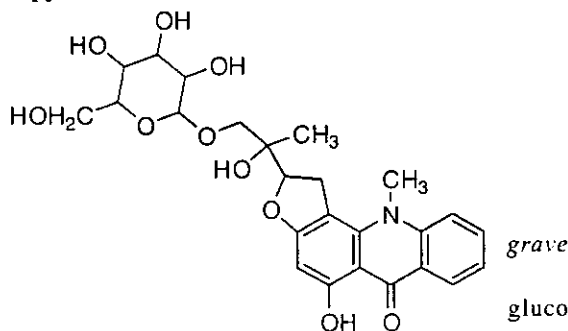
培養

-----文献-----

Rózsa, Zs., Fitoterapia, 1976, 47, 147, (Gravacridonediol, 分離)

§ Rutacridone; 1',2'-Dihydro, 1',2'-dihydroxy, 2'-O-β-D-glucopyranoside

[化学名・別名] Gravacridonediol glucoside
 [CAS No.] 59086-97-4
 [化合物分類] アルカロイド化合物 (Acridone alkaloids)
 [構造式]



grave
gluco

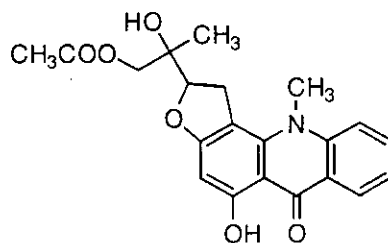
[分子式] $C_{25}H_{29}NO_{11}$
 [分子量] 503.505
 [基原] 次の植物から得られるアルカロイド: *Ruta olens* (ミカン科)
 [その他のデータ] Isol. as a mixt. with Gravacridonetriol side

-----文献-----

Rózsa, Zs., Fitoterapia, 1976, 47, 147, (Gravacridonediol, 分離)
 Baumert, A. et al., Planta Med., 1994, 60, 143, (Gravacridonol monoglucoside)

§ Rutacridone; 1',2'-Dihydro, 1',2'-dihydroxy, 2'-Ac

[化学名・別名] Gravacridonediolacetate
 [CAS No.] 136591-55-4
 [化合物分類] アルカロイド化合物 (Acridone alkaloids)
 [構造式]



ン

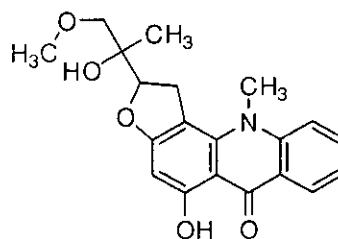
[分子式] $C_{21}H_{21}NO_6$
 [分子量] 383.4
 [基原] 次の植物から得られるアルカロイド: *Ruta graveolens* (ミカン科)
 [性状] 黄色の針状結晶 ($CHCl_3$)
 [融点] Mp 221-223 °C
 [比旋光度]: $[\alpha]_D^{21} +59.8$ (c, 0.4 in $CHCl_3$)

-----文献-----

Paulini, H. et al., Planta Med., 1991, 57, 59; 82, (Isogravacridonechlorine, Gravacridonediolacetate)

§ Rutacridone; 1',2'-Dihydro, 1'-hydroxy, 2'-methoxy

[化学名・別名] Gravacridonediol methyl ether
 [CAS No.] 37551-76-1
 [化合物分類] アルカロイド化合物 (Acridone alkaloids)
 [構造式]



ン

[分子式] $C_{20}H_{21}NO_5$
 [分子量] 355.39
 [基原] 次の植物から得られるアルカロイド: *Ruta graveolens* の根 (ミカン科)
 [性状] 結晶 ($EtOAc$)
 [融点] Mp 219-221 °C

-----文献-----

Rózsa, Zs., Fitoterapia, 1976, 47, 147, (Gravacridonediol, 分離)
 Reisch, J. et al., Z. Naturforsch., B, 1978, 33, 957, (レビュー, H-NMR, 構造)

Paulini, H. et al., *Planta Med.*, 1991, 57, 59; 82, (Isogravacridonechlorine, Gravacridonediolacetate)

§ **Rutacridone; 1',2'-Dihydro, 1',3'-dihydroxy, 2'-chloro**

[化学名・別名] 2-[1-Chloro-2-hydroxy-1-(hydroxymethyl) ethyl] -1,11-dihydro-5-hydroxy-11-methylfuro [2,3-c] acridin-6 (2H) -one. Gravacridonolchlorine

[CAS No.] 38494-85-8

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

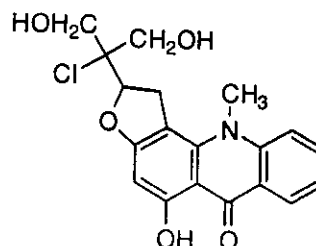
[構造式]

[分子式] $C_{19}H_{18}ClNO_5$

[分子量] 375.808

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* (ミカン科)

[融点] Mp 223-227 °C



-----文献-----

Reisch, J. et al., *Acta Pharm. Suec.*, 1967, 4, 265; *CA*, 68, 39861, (分離, IR, H-NMR)

Rózsa, Zs., *Fitoterapia*, 1976, 47, 147, (Gravacridonediol, 分離)

Reisch, J. et al., *Z. Naturforsch., B*, 1978, 33, 957, (レビュー, H-NMR, 構造)

§ **Rutacridone; 1',2'-Dihydro, 1',2',3'-trihydroxy**

[化学名・別名] 2-[1,2-Dihydroxy-1-(hydroxymethyl) ethyl] -1,11-dihydro-5-hydroxy-11-methylfuro [2,3-c] acridin-6 (2H) -one. Gravacridonediol

[CAS No.] 59086-94-1

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

[構造式]

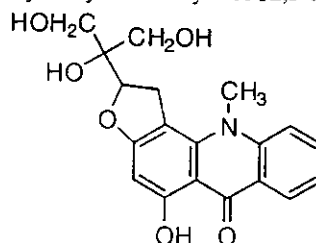
[分子式] $C_{19}H_{19}NO_6$

[分子量] 357.362

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* (ミカン科)

[性状] 結晶 (MeOH)

[融点] Mp 230-232 °C



-----文献-----

Reisch, J. et al., *Acta Pharm. Suec.*, 1967, 4, 265; *CA*, 68, 39861, (分離, IR, H-NMR)

Rózsa, Zs., *Fitoterapia*, 1976, 47, 147, (Gravacridonediol, 分離)

Reisch, J. et al., *Z. Naturforsch., B*, 1978, 33, 957, (レビュー, H-NMR, 構造)

§ **Rutacridone; 1',2'-Dihydro, 1',2',3'-trihydroxy, 2'-O-β-D-glucopyranoside**

[化学名・別名] Gravacridonediol glucoside

[CAS No.] 59086-96-3

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

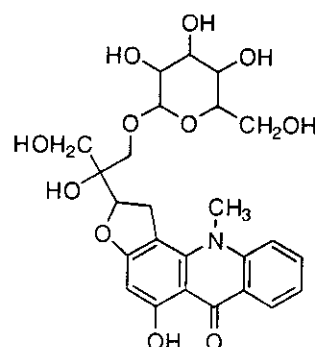
[構造式]

[分子式] $C_{25}H_{29}NO_{11}$

[分子量] 519.504

[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* (ミカン科)

[その他のデータ] Isol. as a mixt. with Gravacridonediol glucoside



-----文献-----

Reisch, J. et al., *Acta Pharm. Suec.*, 1967, 4, 265; *CA*, 68, 39861, (分離, IR, H-NMR)

Reisch, J. et al., *Phytochemistry*, 1972, 11, 2121; 2359; 1976, 15, 240; 1977, 16, 151

Rózsa, Zs., *Fitoterapia*, 1976, 47, 147, (Gravacridonediol, 分離)

Reisch, J. et al., *Z. Naturforsch., B*, 1978, 33, 957, (レビュー, H-NMR, 構造)

§ **Rutaevin; 6 β-Alcohol, 7-Ac**

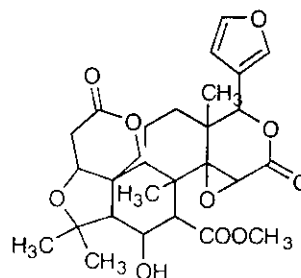
[化学名・別名] 7-Acetoxy-6-hydroxylimonin

[CAS No.] 208333-73-7

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoids)

[構造式]

[分子式] $C_{25}H_{36}O_{10}$



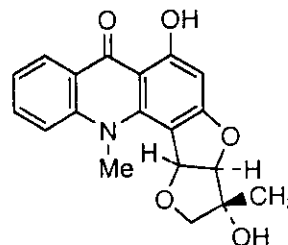
[分子量] 530.571
[基原] *Ruta graveolens*
[性状] 結晶
[融点] Mp 278-280 °C

-----文献-----

Dreyer, D.L. et al., *Tetrahedron*, 1976, 32, 2367
Zheng, S. et al., *Planta Med.*, 1997, 63, 379-380, (*Microula sikkimensis* esters)
Srivastava, S.D. et al., *Fitoterapia*, 1998, 69, 80-81, (7-Acetoxy-6-hydroxylimonin)
Wang, D. et al., *Indian J. Chem., Sect. B*, 1999, 38, 240-242, (acyl derivs)

§ **Rutagravine**

[CAS No.] 101330-60-3
[化合物分類] アルカロイド化合物 (Acridone alkaloids)
[構造式]



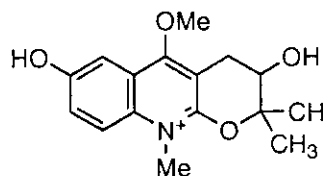
[分子式] $C_{19}H_{17}NO_3$
[分子量] 339.347
[基原] 次の植物から得られるアルカロイド: *Ruta graveolens* のカルス組織 (ミカン科)
UV: [neutral] λ_{max} 252 ; 265 ; 275 ; 299 ; 330 ; 394 (CH₂CL₂) (Berdy)

-----文献-----

Nahrstedt, A. et al., *Planta Med.*, 1985, 517, (分離, H-NMR, C13-NMR, 構造決定)

§ **Rutalinium**

[CAS No.] 27539-40-8
[化合物分類] アルカロイド化合物 (Pyranoquinoline alkaloids)
[構造式]



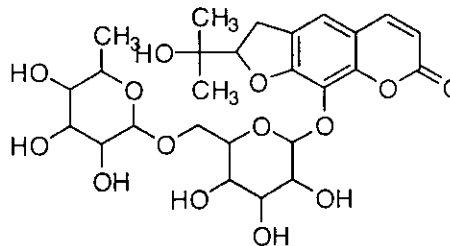
[分子式] $C_{16}H_{20}NO_4^{+}$
[分子量] 290.338
[基原] 次の植物から得られるアルカロイド: *Ruta graveolens*, *Ruta graveolens* subsp. *hortensis*, *Balfourodendron riedelianum* (ミカン科)

-----文献-----

Szendrei, K. et al., *Herba Hung.*, 1971, 10, 131; CA, 79, 15853k, (分離, H-NMR, 構造決定)
Varga, E. et al., *Acta Pharm. Hung.*, 1978, 48, 193; CA, 89, 176400g, (分離)

§ **Rutaretin; 9-O-[α -L-Rhamnopyranosyl-(1 \rightarrow 6)- β -D-glucopyranoside]**

[化学名・別名] Rutaretin 9-rutinoside
[CAS No.] 160845-05-6
[化合物分類] ベンゾピラノイド (Dihydrofuranocoumarins), ベンゾピラノイド (7,8-Dioxygenated coumarins)
[構造式]



[分子式] $C_{26}H_{34}O_{14}$
[分子量] 570.546
[基原] *Ruta graveolens*
[性状] 淡黄色の結晶
[融点] Mp 150-152 °C
[比旋光度]: $[\alpha]_D^{25} +45$ (EtOH)
UV: [neutral] λ_{max} 230 ; 260 ; 310 (溶媒の報告はない)

-----文献-----

Schneider, G. et al., *Arch. Pharm. (Weinheim, Ger.)*, 1967, 300, 73; 913, (分離, IR, UV, H-NMR, Mass)
Shagova, L.I. et al., *Khim. Prir. Soedin.*, 1973, 9, 665; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, 9, 631, (分離)
Varga, E. et al., *Acta Pharm. Hung., Suppl. No. 36*, 1974, 44 ; CA, 82, 13996, (分離)
Srivastava, S.K. et al., *Fitoterapia*, 1994, 65, 301-303, (rutinoside)

§ **Rutaretin; (R)-form, 1'-O- β -D-Glucopyranoside**

[化学名・別名] Isorutarin. Leptophylloside
[CAS No.] 53846-51-8
[その他の CAS No.] 68692-60-4