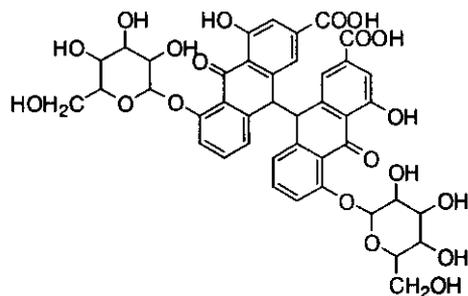


[分子式] $C_{42}H_{36}O_{20}$
[分子量] 862.75
[正確な分子量] 862.19565
[基原] 次の植物から分離: *Cassia angustifolia*
[性状] 黄色の板状結晶
[融点] Mp 162-176 °Cで分解
[比旋光度]: $[\alpha]_D^{25} -110$ (c, 0.1 in 70% dioxan 溶液)



-----文献-----

Stoll, A. et al., *Helv. Chim. Acta*, 1949, 32, 1892; 1950, 33, 313, (構造決定, 分離)
Lemmens, L., *Pharm. Weekbl.*, 1979, 1, 178, (代謝)
Tanaka, H. et al., *Chem. Pharm. Bull.*, 1982, 30, 1550, (分離)
Pharmacology, Suppl. 1, 1988, 36, (薬理, 代謝, 用途, レビュー)
Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, 1993, 903
Pharmacology, Suppl. 1, 1993, 47, (薬理, 代謝, 用途, レビュー)
Negwer, M., *Organic-Chemical Drug and their Synonyms*, 7th edn., Akademie-Verlag, 1994, 11693, (シノニム)

§ 1,3,8,9-Tetrahydroxy-6-methylanthracene; O-Glucoside

[CAS No.] 57077-53-9
[化合物分類] 多環芳香族 (Anthracene)
[構造式] 有効な構造式はない
[分子式] $C_{41}H_{32}O_9$
[分子量] 418.399
[正確な分子量] 418.126385
[基原] *Cassia angustifolia*

-----文献-----

Perkin, A.G., *J.C.S.*, 1894, 65, 937, (分離)
Krassowski, N., *Chem. Zentralbl.*, 1909, 772; 774, (Shesterin)
Tutin, F. et al., *J.C.S.*, 1912, 101, 290, (分離, 構造決定)
Brockmann, H. et al., *Naturwissenschaften*, 1953, 40, 509, (分離)
Ritchie, E. et al., *Tet. Lett.*, 1964, 1431, (Madagascinanthrone)
Grove, J.F., *J.C.S. Perkin 1*, 1972, 2406, (1-Me)
Lemli, J. et al., *Phytochemistry*, 1975, 14, 1397, (配糖体)
Amonkar, A. et al., *Experientia*, 1981, 37, 1138, (Geranyloxydihydroxymethylanthrone)
Abegaz, B. et al., *Bull. Chem. Soc. Ethiop.*, 1988, 2, 15; *CA*, 110, 92025c, (Prinoidin)
Abegaz, B.M. et al., *Phytochemistry*, 1995, 39, 1411, (Prinoidin)

§ 1,3,8,9-Tetrahydroxy-6-methylanthracene; O-Diglucoside

[化合物分類] 多環芳香族 (Anthracene)
[構造式] 有効な構造式はない
[分子式] $C_{47}H_{32}O_{14}$
[分子量] 580.541
[正確な分子量] 580.17921
[基原] *Cassia angustifolia*

-----文献-----

Perkin, A.G., *J.C.S.*, 1894, 65, 937, (分離)
Tutin, F. et al., *J.C.S.*, 1912, 101, 290, (分離, 構造決定)
Jacobson, R.A. et al., *J.A.C.S.*, 1924, 46, 1312, (合成法)
Brockmann, H. et al., *Naturwissenschaften*, 1953, 40, 509, (分離)
Ritchie, E. et al., *Tet. Lett.*, 1964, 1431, (Madagascinanthrone)
Grove, J.F., *J.C.S. Perkin 1*, 1972, 2406, (1-Me)
Lemli, J. et al., *Phytochemistry*, 1975, 14, 1397, (配糖体)

Amonkar, A. et al., *Experientia*, 1981, 37, 1138, (Geranyloxydihydroxymethylantrone)
Abegaz, B. et al., *Bull. Chem. Soc. Ethiop.*, 1988, 2, 15; CA, 110, 92025c, (Prinoidin)
Abegaz, B.M. et al., *Phytochemistry*, 1995, 39, 1411, (Prinoidin)

§ 1,3,8,9-Tetrahydroxy-6-methylantracene; 3-Me ether, O-diglucoside

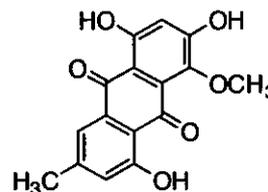
[CAS No.] 57077-56-2
[化合物分類] 多環芳香族 (Anthracene)
[構造式] 有効な構造式はない
[分子式] $C_{28}H_{34}O_{14}$
[分子量] 594.568
[正確な分子量] 594.19486
[基原] *Cassia angustifolia*

-----文献-----

Perkin, A.G., *J.C.S.*, 1894, 65, 937, (分離)
Tutin, F. et al., *J.C.S.*, 1912, 101, 290, (分離, 構造決定)
Brockmann, H. et al., *Naturwissenschaften*, 1953, 40, 509, (分離)
v. Mühlemann, H., *Pharm. Acta Helv.*, 1955, 30, 350
Ritchie, E. et al., *Tet. Lett.*, 1964, 1431, (Madagascinantrone)
Lemli, J. et al., *Phytochemistry*, 1975, 14, 1397, (配糖体)
Amonkar, A. et al., *Experientia*, 1981, 37, 1138, (Geranyloxydihydroxymethylantrone)
Abegaz, B. et al., *Bull. Chem. Soc. Ethiop.*, 1988, 2, 15; CA, 110, 92025c, (Prinoidin)
Abegaz, B.M. et al., *Phytochemistry*, 1995, 39, 1411, (Prinoidin)

§ 1,2,4,8-Tetrahydroxy-6-methylantraquinone; 1-Me ether

[化学名・別名] 2,4,8-Trihydroxy-1-methoxy-6-methylantraquinone
[CAS No.] 214038-63-8
[化合物分類] 多環芳香族 (9,10-Anthraquinone; 4 × O-置換基)
[構造式]
[分子式] $C_{16}H_{12}O_6$
[分子量] 300.267
[正確な分子量] 300.06339
[基原] *Cassia angustifolia* の種子
[融点] Mp 231 °C
[UV]: [neutral] λ_{max} 258 (sh) (); 267 (); 288 (); 436 () (MeOH)

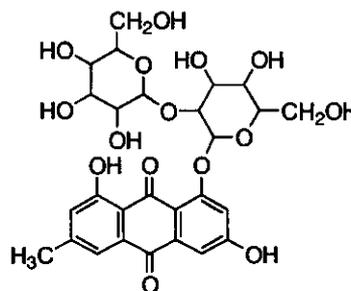


-----文献-----

Yagi, A. et al., *Chem. Pharm. Bull.*, 1977, 25, 1764; 1771, (Isoxanthorin)
Gupta, A. et al., *Indian J. Chem., Sect. B*, 1998, 37, 615, (1-Me ether)

§ 1,3,8-Trihydroxy-6-methylantraquinone; 1-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]

[化学名・別名] Emodin 8-sophoroside
[CAS No.] 162110-87-4
[化合物分類] 多環芳香族 (9,10-Anthraquinone; 3 × 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] *Cassia angustifolia*
[性状] 無定形の粉末
[比旋光度]: $[\alpha]_D -65$ (c, 0.1 in MeOH)



-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhauser Verlag, Basel, 1972, nos. 1265; 1274, (生育)
Kinjo, J. et al., *Phytochemistry*, 1994, 37, 1685, (8-sophoroside)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MQF250

*****ソース (Sauces) *****

§ § ウスターソース, チリソースなどの各種料理用ソース類。

*****ダイオウ (Rhubarb) *****

§ § タデ科ダイオウ (*Rheum officinale* Baillon) の根, 茎または葉。

§ 3,4,5-Trihydroxybenzoic acid; β -D-Glucopyranosyl ester

[化学名・別名] Glucogallin. 1-O-Galloyl- β -D-glucopyranose. β -Glucogallin

[CAS No.] 554-37-0

[化合物分類] タンニン化合物 (Simple gallate ester tannin), 単環芳香族 (Simple benzoic acid and ester)

[構造式]

[分子式] $C_{13}H_{16}O_{10}$

[分子量] 332.263

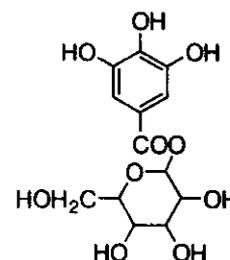
[正確な分子量] 332.07435

[基原] 色々な植物から分離, 例えば, *Rheum officinale*, *Eucalyptus* spp., *Mallotus japonicus*

[性状] 結晶粉末 (H_2O)

[融点] Mp 205-206 °C

[比旋光度]: $[\alpha]_D^{18} -18.6$ (c, 1 in MeOH)



-----文献-----

Schmidt, O.T. et al., *Annalen*, 1961, 649, 149, (Glucogallin)

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhauser Verlag, Basel, 1972, nos. 903; 904; 909; 910, (生育, 誘導体)

Rodd's Chem. Carbon Compd. (2nd edn.), 1976, 3D, 193, (成書)

Kirk-Othmer *Encycl. Chem. Technol.*, 3rd edn., Wiley, 1978, 18, 677, (レビュー)

Kashiwada, Y. et al., *Chem. Pharm. Bull.*, 1986, 34, 3237, (glucogallic acid)

Saijo, R. et al., *Phytochemistry*, 1990, 29, 267, (Glucogallin)

Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. et al), American Pharmaceutical Association/Pharmaceutical Press, 1994, 402

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DXX200; GBE000; MKI100; PNM750

*****ダイズ (Soybeans) *****

§ § マメ科ダイズ (*Glycine max* Merrill) の種子。

「コウジ」参照

*****タイム (Thyme) *****

§ § シソ科タイム (*Thymus vulgaris* L.) の花, 茎葉。

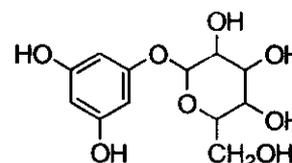
§ 1,3,5-Benzenetriol; O- β -D-Glucopyranoside

[化学名・別名] Phlorin

[CAS No.] 28217-60-9

[化合物分類] 単環芳香族 (Simple phenol)

[構造式]



[分子式] $C_{12}H_{16}O_8$

[分子量] 288.254

[正確な分子量] 288.08452

[基原] 次の植物から分離: thyme (*Thymus vulgaris*), オレンジの果実. Proposed marker for adulteration of orange juice with peel

[性状] 結晶

[融点] Mp 231-233 °C

[比旋光度]: $[\alpha]_D^{22} -74.58$

-----文献-----

Laurence, M.-M. et al., J. Agric. Food Chem., 1998, 46, 4193, (Phlorin)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, PGR000; TKY250

§ 4,4'-Dihydroxy-5,5'-diisopropyl-2,2'-dimethyl-3,6-biphenyldione

[CAS No.] 120866-14-0

[化合物分類] テルペノイド (p-Menthane monoterpeneoid), 単環芳香族 (Benzoquinone; 1 × O-置換基)

[構造式]

[分子式] $C_{20}H_{24}O_4$

[分子量] 328.407

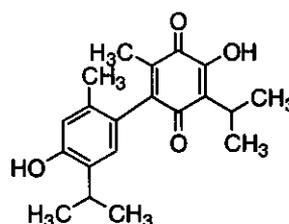
[正確な分子量] 328.16746

[基原] *Thymus vulgaris* の葉

[性状] 赤色の半個体

[融点] Mp 67 °C

[比旋光度]: $[\alpha]_D^{25} -7.9$ (c, 0.42 in $CHCl_3$)



-----文献-----

Nakatani, N. et al., Agric. Biol. Chem., 1989, 53, 1375, (分離, H-NMR, C13-NMR)

§ 5,5-Diisopropyl-2,2'-dimethylbiphenyl-3,3',4,4'-tetrone

[CAS No.] 122548-31-6

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

[構造式]

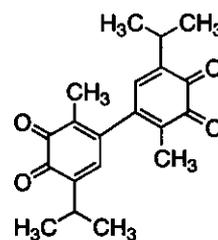
[分子式] $C_{20}H_{22}O_4$

[分子量] 326.391

[正確な分子量] 326.15181

[基原] *Thymus vulgaris* の葉

[性状] 茶色のオイル



-----文献-----

Nakatani, N. et al., Agric. Biol. Chem., 1989, 53, 1375, (分離, H-NMR, C13-NMR)

§ 4'-Hydroxyacetophenone; O-[4-Hydroxybenzoyl-(→ 5)-β-D-apiofuranosyl-(1 → 2)-β-D-glucopyranoside]

[CAS No.] 228405-07-0

[化合物分類] 炭水化物 (Disaccharide), 単環芳香族 (Simple aryl ketone)

[構造式]

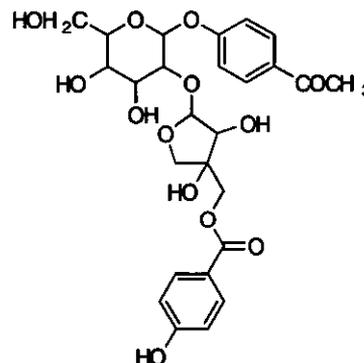
[分子式] $C_{26}H_{30}O_{13}$

[分子量] 550.515

[正確な分子量] 550.168645

[基原] *Thymus vulgaris*

[性状] 粉末



-----文献-----

Edwards, O.E. et al., Can. J. Chem., 1962, 40, 256, (分離)

Tsuzuki, Y. et al., Bull. Chem. Soc. Jpn., 1971, 44, 526, (配糖体)

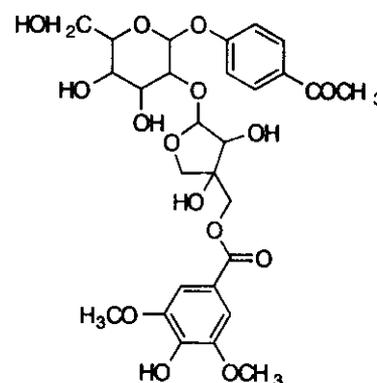
Opdyke, D.L.J., Food Cosmet. Toxicol., Suppl., 1974, 927, (レビュー, 誘導体)
 Maurin, J.K., Acta Cryst. C, 1994, 50, 1354, (結晶構造, oxime)
 Shao, Y. et al., Phytochemistry, 1996, 41, 1593, (Asterbatanocide A)
 Wang, M. et al., J. Agric. Food Chem., 1999, 47, 1911-1914; 2000, 48, 235-238, (benzoylapiosylglucoside)
 Miyase, T. et al., J. Nat. Prod., 1999, 62, 993-996, (Sibiricaphenone)
 Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, HIO000; MDW750

§ 4'-Hydroxyacetophenone; O-[4-Hydroxy-3,5-dimethoxybenzoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]

[CAS No.] 228405-06-9

[化合物分類] 炭水化物 (Disaccharide), 単環芳香族 (Simple aryl ketone)

[構造式]



[分子式] C₂₈H₃₄O₁₅

[分子量] 610.568

[正確な分子量] 610.189775

[基原] *Salvia officinalis*, *Thymus vulgaris*

[性状] 粉末

-----文献

Edwards, O.E. et al., Can. J. Chem., 1962, 40, 256, (分離)
 Opdyke, D.L.J., Food Cosmet. Toxicol., Suppl., 1974, 927, (レビュー, 誘導体)
 Shao, Y. et al., Phytochemistry, 1996, 41, 1593, (Asterbatanocide A)
 Wang, M. et al., J. Agric. Food Chem., 1999, 47, 1911-1914; 2000, 48, 235-238, (benzoylapiosylglucoside)
 Miyase, T. et al., J. Nat. Prod., 1999, 62, 993-996, (Sibiricaphenone)
 Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, HIO000; MDW750

§ 4'-Hydroxy-5,5'-diisopropyl-2,2'-dimethyl-3,4-biphenylquinone

[化学名・別名] 4-(4-Hydroxy-5-isopropyl-2-methylphenyl)

-6-isopropyl-3-methyl-3,5-cyclohexadiene-1,2-dione

[CAS No.] 120866-13-9

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

[構造式]

[分子式] C₂₀H₂₄O₃

[分子量] 312.408

[正確な分子量] 312.172545

[基原] *Thymus vulgaris* の葉

[用途] Exhibits antioxidant and deodorant activities

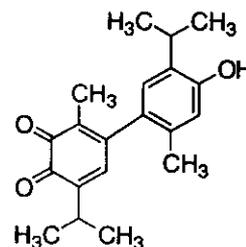
[性状] 暗赤色の結晶 (EtOAc/hexane)

[融点] Mp 174-175 °C (170 °C)

[比旋光度]: [α]_D²⁵ -11.6 (c, 0.14 in CHCl₃)

-----文献

Nakatani, N. et al., Agric. Biol. Chem., 1989, 53, 1375, (分離, H-NMR, C13-NMR)
 Miura, Y. et al., Bull. Chem. Soc. Jpn., 1992, 65, 1159, (合成法, IR, H-NMR)



§ 2-Hydroxy-9,12,15-octadecatrienoic acid; (R)-(all-Z)-form

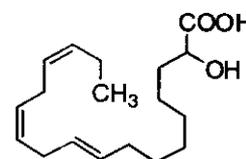
[化学名・別名] 2-Hydroxylinolenic acid

[化合物分類] 脂肪族化合物 (Unbranched alkenic carboxylic acid and lactone)

[構造式]

[基原] *Salvia nilotica*, *Thymus vulgaris* の種子オイル

[比旋光度]: [α]_D⁴⁰⁰ -24.3 (c, 0.16 in CHCl₃)



-----文献-----

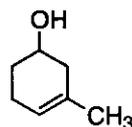
Smith, C.R. et al., *Lipids*, 1969, 4, 9, (分離, 構造決定, ORD)
 Bohannon, M.B. et al., *Lipids*, 1975, 10, 703, (分離, ms. IR, NMR)

§ 3-Methyl-3-cyclohexen-1-ol; (ξ)-form

[化合物分類] 脂肪族化合物 (Monocarbocyclic alcohol)

[構造式]

[基原] *Thymus vulgaris* のオイル



-----文献-----

Reddy, M.V.B. et al., *Phytochemistry*, 1988, 47, 1515, (生育)
 Harris, N.J. et al., *J.A.C.S.*, 1994, 116, 6121, (合成法, H-NMR, C13-NMR)
 Kocovsky, P. et al., *J.O.C.*, 1999, 64, 2765, (H-NMR)

§ 2-Methyl-6-methylene-2,7-octadien-1-ol; (Z)-form

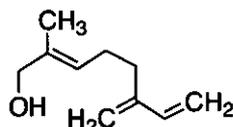
[CAS No.] 38228-40-9

[化合物分類] テルペノイド (Acyclic monoterpene)

[構造式]

[基原] *Thymus vulgaris* の精油

[その他のデータ] ガスクロマトで分離する



-----文献-----

Granger, R. et al., *Phytochemistry*, 1972, 11, 2301, (分離)
 Vig, O.P. et al., *J. Indian Chem. Soc.*, 1975, 52, 161, (合成法)
 Zdero, C. et al., *Phytochemistry*, 1991, 30, 3669, (3-Phenylpropanoyl)

§ 3,3',4,4'-Tetrahydroxy-5,5'-diisopropyl-2,2'-dimethylbiphenyl

[CAS No.] 120901-51-1

[化合物分類] 単環芳香族 (Biphenyl), テルペノイド (p-Menthane monoterpene)

[構造式]

[分子式] C₂₀H₂₆O₄

[分子量] 330.423

[正確な分子量] 330.18311

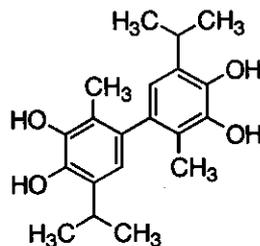
[基原] *Thymus vulgaris*

[用途] 抗酸化剤

[性状] 淡褐色の粉末

[融点] Mp 104 °C

[比旋光度]: [α]_D -9.2 (c, 0.8 in CHCl₃)



-----文献-----

Miura, K. et al., *Chem. Pharm. Bull.*, 1989, 37, 1816, (分離, H-NMR, C13-NMR)
 Miura, K. et al., *Bull. Chem. Soc. Jpn.*, 1992, 65, 1159, (合成法)
 Haraguchi, H. et al., *Planta Med.*, 1996, 62, 217, (分離, C13-NMR, 性質)

§ 3,3',4,4'-Tetrahydroxy-5,5'-diisopropyl-2,2'-dimethylbiphenyl; 3-Deoxy

[化学名・別名] 3,4,4'-Trihydroxy-5,5'-diisopropyl-2,2'-dimethylbiphenyl

[CAS No.] 123132-69-4

[化合物分類] テルペノイド (p-Menthane monoterpene), 単環芳香族 (Biphenyl)

[構造式]

[分子式] C₂₀H₂₆O₃

[分子量] 314.424

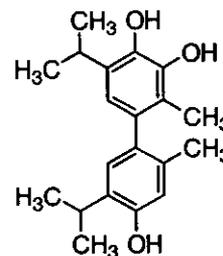
[正確な分子量] 314.188195

[基原] *Thymus vulgaris*

[性状] 淡褐色の粉末 (C₆H₆)

[融点] Mp 75 °C

[比旋光度]: [α]_D²⁵ -48 (c, 0.21 in CHCl₃)



-----文献-----

Miura, K. et al., *Chem. Pharm. Bull.*, 1989, 37, 1816, (分離, H-NMR, C13-NMR)

Miura, K. et al., Bull. Chem. Soc. Jpn., 1992, 65, 1159, (合成法)
Haraguchi, H. et al., Planta Med., 1996, 62, 217, (分離, C13-NMR, 性質)

§ 3,5,6-Trihydroxy-7-megastigmen-9-one; (3*S*,5*R*,6*R*,7*E*)-form

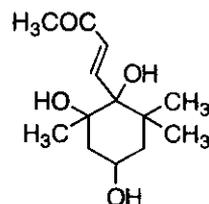
[化合物分類]テルペノイド (Megastigmane norterpeneoid)

[構造式]

[基原] New Zealand thyme honey (*Thymus vulgaris*)

[性状] 結晶 (toluene)

[融点] Mp 68-69 °C



-----文献-----

Tan, S.T. et al., Aust. J. Chem., 1989, 42, 1799, (分離, H-NMR, C13-NMR, 結晶構造)

Tan, S.T. et al., J. Agric. Food Chem., 1990, 38, 1833, (分離, Mass, gc)

Broom, S.J. et al., Tet. Lett., 1992, 33, 3197, (合成法)

§ 4',5,6-Trihydroxy-3',7,8-trimethoxyflavone

[化学名・別名] 5,6-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-7,8-dimethoxy-4*H*-1-benzopyran-4-one.

Majoranin. Thymonin

[CAS No.] 76844-67-2

[化合物分類] フラボノイド (Flavone; 6 × O-置換基)

[構造式]

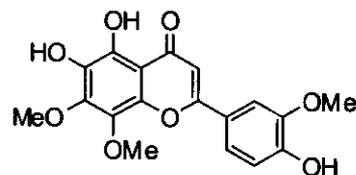
[分子式] C₁₈H₁₆O₈

[分子量] 360.32

[正確な分子量] 360.08452

[基原] 次の植物から分離: *Majorana hortensis*, *Thymus satuireioides*, *Thymus vulgaris*

[融点] Mp 225-226 °C



-----文献-----

Van den Brouke, C.O. et al., Phytochemistry, 1982, 21, 2581, (分離)

Voirin, B., Phytochemistry, 1983, 22, 2107; 1984, 23, 2973, (分離, UV)

Voirin, B. et al., Planta Med., 1985, 523, (分離)

Bosabalidis, A.M. et al., Phytochemistry, 1998, 49, 1549, (分離, UV, H-NMR, Mas)

*****タケノコ (Bamboo shoot) *****

§ § イネ科モウソウチク (*Phyllostachys heterocycla* Freeman-Mitford) の幼茎。

§ 2,6-Dihydroxy-1,4-benzoquinone; Di-Me ether

[化学名・別名] 2,6-Dimethoxy-1,4-benzoquinone

[CAS No.] 530-55-2

[化合物分類] 単環芳香族 (Benzoquinone; 2 × O-置換基)

[構造式]

[分子式] C₆H₆O₄

[分子量] 168.149

[正確な分子量] 168.04226

[基原] Widespread in wood and woody tissues, prob. as degradn. prod. of lignin. 特にニガキ科から分離, 例えば, *Picrasma*, *Ailanthus* spp. Also prod. by the marine fungus *Dendryphiella salina* grown on waste sulfite liquor. *Phyllostachys heterocycla* var. *pubescens* の樹皮成分

[用途] 抗菌性を示す

[性状] 黄色の結晶 (AcOH)

[融点] Mp 252 °C

[UV]: [neutral] λ_{max} 288 (ε 12600) (MeOH)

[傷害・毒性] 皮膚炎を起こす. 変異原性作用を有する.

[化学物質毒性データ総覧 (RTEC) 登録番号] DK4750000

-----文献-----

Polonsky, J. et al., Bull. Soc. Chim. Fr., 1959, 1157; 1962, 1715, (分離, 誘導体)
Bolker, H.I. et al., Can. J. Chem., 1969, 47, 2109, (誘導体)
Schmalle, H. et al., Naturwissenschaften, 1977, 64, 534, (結晶構造, 誘導体)
Org. Synth., 1977, 57, 78, (合成法)
Nishina, A. et al., J. Agric. Food Chem., 1991, 39, 266, (分離, 誘導体)
Frick, E. et al., Nat. Prod. Lett., 1996, 9, 153, (合成法)

RTECS (化学物質毒性データ)

生体影響物質 : 変異原物質

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 損傷.
曝露経路 : 経口投与.
試験系 : げっ歯類-ラット.
投与量・期間 : 33 mg/kg

参考文献

JPETAB Journal of Pharmacology and Experimental Therapeutics. (Williams & Wilkins Co., 428 E. Preston St., Baltimore, MD 21202) V.1- 1909/10- [Vol.,頁,年(19-)]244,1011,1988

<<試験方法>> DNA 損傷.
試験系 : げっ歯類-ラット肝臓
投与量・期間 : 10 umol/L

参考文献

JPETAB Journal of Pharmacology and Experimental Therapeutics. (Williams & Wilkins Co., 428 E. Preston St., Baltimore, MD 21202) V.1- 1909/10- [Vol.,頁,年(19-)]244,1011,1988

<<試験方法>> 不定期 DNA 合成試験.
試験系 : げっ歯類-ラット肝臓
投与量・期間 : 20 umol/L

参考文献

JPETAB Journal of Pharmacology and Experimental Therapeutics. (Williams & Wilkins Co., 428 E. Preston St., Baltimore, MD 21202) V.1- 1909/10- [Vol.,頁,年(19-)]244,1011,1988

<<試験方法>> DNA 損傷.
試験系 : げっ歯類-マウス白血球.
投与量・期間 : 50 umol/L

参考文献

PAACA3 Proceedings of the American Association for Cancer Research. (Waverly Press, 428 E. Preston St., Baltimore, MD 21202) V.1- 1954- [Vol.,頁,年(19-)]27,105,1986

<<試験方法>> DNA 損傷.
試験系 : げっ歯類-ハムスター肺
投与量・期間 : 10 umol/L

参考文献

JPETAB Journal of Pharmacology and Experimental Therapeutics. (Williams & Wilkins Co., 428 E. Preston St., Baltimore, MD 21202) V.1- 1909/10- [Vol.,頁,年(19-)]244,1011,1988

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

参考文献

JPETAB Journal of Pharmacology and Experimental Therapeutics. (Williams & Wilkins Co., 428 E. Preston St., Baltimore, MD 21202) V.1- 1909/10- [Vol.,頁,年(19-)]244,1011,1988

*****タコ (Octopus) *****

§ § マダコ科マダコ (*Octopus vulgaris* Cuvier) の可食部。

§ Adenochrome

[関連 CAS No.] 63026-38-0, 63026-40-4, 64925-68-4
 [化合物分類] アミノ酸とペプチド (Peptide 構造は未知), アミノ酸とペプチド (Oligopeptides (4-10 residue))
 [構造式] 不明
 [基原] Pigment from the branchial heart of *Octopus vulgaris*

-----文献-----

Ito, S. et al., J.C.S. Perkin 1, 1979, 2617, (分離, 構造決定)

§ Adrenochrome

[化合物分類] アミノ酸とペプチド (Peptide 構造は未知)
 [構造式] 不明
 [一般的性質] 構造は完全に知られていない
 [基原] 次の動物から分離: *Octopus vulgaris* の心臓
 [用途] Fe³⁺-binding pigment found in both Fe-chelated and Fe-free forms
 [性状] 赤紫色

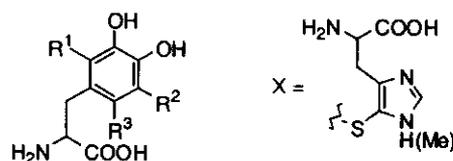
-----文献-----

Ito, S. et al., J.C.S. Perkin 1, 1979, 2617

Michael, J.P. et al., Angew. Chem., Int. Ed., 1993, 32, 1

§ Adrenochromines

[化合物分類] アルカロイド化合物 (Imidazole alkaloid), アルカロイド化合物 (Nitrogenous marine toxin)
 [構造式]
 [基原] Constits. of *Adrenochrome*, the unique iron (III)-containing pigment from the branchial heart of the common octopus *Octopus vulgaris*



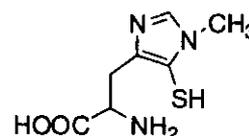
Adrenochrome A: R¹ = R² = X, R³ = H
 Adrenochrome B: R² = R³ = X, R¹ = H
 Adrenochrome C: R¹ = R³ = X, R² = H

-----文献-----

Ito, S. et al., J.C.S. Perkin 1, 1979, 2617, (構造決定)

§ 5-Mercaptohistidine; (L)-form, 1-Me

[化学名・別名] 5-Mercapto-1-methylhistidine
 [CAS No.] 62982-24-5
 [化合物分類] アミノ酸とペプチド (Non-protein α-aminoacid)
 [構造式]
 [分子式] C₇H₁₁N₃O₂S
 [分子量] 201.249
 [正確な分子量] 201.057197



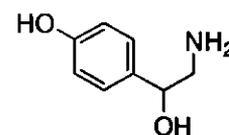
[基原] the unfertilised eggs of the sea urchin *Paracentrotus lividus*. Also a component of the struct. of adrenochrome, an Fe (III) contg. peptide from *Octopus vulgaris*

-----文献-----

Palumbo, A. et al., Tet. Lett., 1982, 23, 3207, (分離, UV, H-NMR, C13-NMR, 構造決定, 誘導体)

§ Octopamine; (R)-form

[CAS No.] 876-04-0
 [化合物分類] アルカロイド化合物 (Simple tyramine alkaloid)
 [構造式]
 [基原] 次の植物から得られるアルカロイド: *Capsicum frutescens*, *Citrus spp.*, *Cyperus rotundus*, *Cyperus papyrus* (ナス科, ミカン科, カヤツリグサ科). 多くの動物組織に見られる; found in high concs. in the posterior salivary gland of *Octopus vulgaris*
 [用途] Invertebrate neurotransmitter. In vertebrates, prob. a cotransmitter with noradrenaline. Adrenergic
 [性状] 結晶 (H₂O)
 [融点] Mp 約 160 °C
 [比旋光度]: [α]_D²⁵ -37.4 (c, 1 in H₂O). [α]_D²⁵ -56 (c, 1 in 1M HCl)



-----文献-----

Hengstmann, J.H. et al., Naunyn-Schmiedeberg's Arch. Pharmacol., 1974, 283, 93, (代謝)

Axelrod, J. et al., Nature (London), 1977, 265, 501, (レビュー)
 Smith, T.A., Phytochemistry, 1977, 16, 9, (生育)
 Doetsch, P.W. et al., J. Chromatogr., 1980, 189, 79, (生育, 誘導体)
 Yoshihara, T. et al., Agric. Biol. Chem., 1981, 45, 2593, (cinnamoyl deriv)
 Redouane, K. et al., Agressologie, 1984, 25, 3, (レビュー)
 Negwer, M., Organic-Chemical Drug and their Synonyms, 6th edn., Akademie-Verlag, 1987, 945
 Midgley, J.M. et al., J.C.S. Perkin 2, 1989, 963, (結晶構造, 絶対構造, 成書)
 Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1250
 Matsuda, F. et al., Biosci., Biotechnol., Biochem., 2000, 64, 625, (N-Coumaroyloctopamine)
 Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, AKT250

§ Octopine

[化学名・別名] *N*²-(1-Carboxyethyl) arginine (CAS 名). Arginine- α -propionic acid. Pectenin

[CAS No.] 34522-32-2

[化合物分類] アミノ酸とペプチド (Miscellaneous modified amino acid)

[構造式]

[分子式] $C_9H_{18}N_4O_4$

[分子量] 246.266

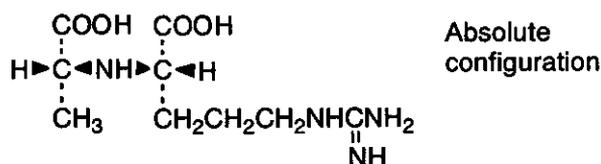
[正確な分子量] 246.132806

[基原] 次の植物から分離: *Octopus vulgaris*, *Pecten magellanicu*, *Eledone moschata*

[性状] 針状結晶 (H₂O or EtOH 溶液)

[融点] Mp 281-282 °C (261-264 °C)

[比旋光度]: $[\alpha]_D^{17} +20.94$ (H₂O)



-----文献-----

Izumiya, N. et al., J.A.C.S., 1957, 79, 652, (合成法)

Biellmann, J.F. et al., Bioorg. Chem., 1977, 6, 89, (合成法, 絶対構造)

Goto, K. et al., Bull. Chem. Soc. Jpn., 1982, 55, 261, (合成法, 絶対構造)

§ $\alpha, \alpha', 2$ -Triamino- $\gamma, \gamma', 3$ -trioxo-3*H*-phenoxazine-1,9-dibutanoic acid (CAS 名)

[化合物分類] アルカロイド化合物 (Phenoxazine)

[構造式]

[分子式] $C_{20}H_{18}N_4O_8$

[分子量] 442.384

[正確な分子量] 442.112466

[一般的性質] 推定構造式.

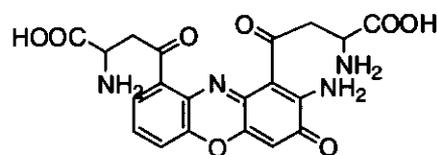
[基原] *Loligo vulgaris*, *Sepia officinalis*, *Octopus vulgaris*

[性状] 黄色

[溶解性] 不溶

[UV]: [neutral] λ_{max} 430 () (溶媒の報告はない)

[その他のデータ] λ_{max} 420-440 nm.



-----文献-----

Bolognese, A. et al., J. Het. Chem., 1988, 25, 1243, (成書)

§ § マダコ科イイダコ (*Octopus ocellatus* Gray) の可食部。

該当物質なし

§ § マダコ科テナガダコ (*Octopus minor* (Sasaki)) の可食部。

該当物質なし

§ § マダコ科ミズダコ (*Paroctopus dofleini dofleini* (Wulker)) の可食部。

該当物質なし

*****タデ (Tade, Water pepper) *****

§ § タデ科ヤナギタデ (*Polygonum hydropiper* Opiz) の全草。

§ 6,8-Dihydroxy-3,4-dimethyl-1H-2-benzopyran-1-one; 6-Me ether

[化学名・別名] 8-Hydroxy-6-methoxy-3,4-dimethyl-1H-2-benzopyran-1-one.

8-Hydroxy-6-methoxy-3,4-dimethylisocoumarin. Polygonolide

[CAS No.] 100560-66-5

[化合物分類] ベンゾピラノイド (Isocoumarin)

[構造式]

[分子式] $C_{12}H_{12}O_4$

[分子量] 220.224

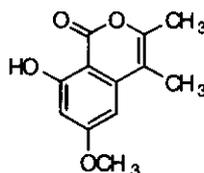
[正確な分子量] 220.07356

[基原] *Polygonum hydropiper*

[用途] 抗炎症薬

[性状] 結晶

[融点] Mp 142 °C



-----文献-----

Tanaka, A.K. et al., *Agric. Biol. Chem.*, 1974, 38, 1311, (合成法, UV)

Furuta, T. et al., *Phytochemistry*, 1986, 25, 517, (分離)

§ 7-Drimene-11,12-diol; (5 α , 9 α)-form, 11,12-Dialdehyde

[化学名・別名] Isopolygodial. Isotadeonal

[CAS No.] 5956-39-8

[化合物分類] テルペノイド (Drimane sesquiterpenoid)

[構造式]

[分子式] $C_{15}H_{22}O_2$

[分子量] 234.338

[正確な分子量] 234.16198

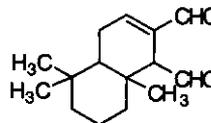
[基原] *Polygonum hydropiper*, その他の植物属

[性状] オイル

[沸点] Bp₁ 145-153 °C

[比旋光度]: $[\alpha]_D^{25}$ -237.4 (EtOH)

[UV]: [neutral] λ_{max} 227 (ϵ 10000) (MeOH)



-----文献-----

Ohsuka, A. et al., *Nippon Kagaku Zasshi*, 1963, 84, 748, (Isotadeonal)

Ohsuka, A. et al., *Chem. Lett.*, 1979, 63, (合成法, Isotadeonal)

§ 7-Drimene-11,12-diol; (5 α , 9 β)-form, 11,12-Dialdehyde

[化学名・別名] 7-Drimene-11,12-dial. Polygodial. Tadeonal

[CAS No.] 6754-20-7

[化合物分類] テルペノイド (Drimane sesquiterpenoid)

[構造式]

[分子式] $C_{15}H_{22}O_2$

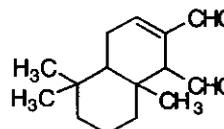
[分子量] 234.338

[正確な分子量] 234.16198

[基原] 次の植物から分離: *Polygonum hydropiper*, *Drimys lanceolata*

[用途] 抗痛覚物質活性を示す。抗菌, 抗カビ活性を示す。植物成長調節剤。昆虫の成長を制御する。茎葉を食する昆虫の予防効果を有する

[性状] 針状結晶 (petrol)



[融点] Mp 57 °C (50 °C)

[沸点] Bp_{0.8} 138-140 °C

[比旋光度]: [α]_D -210 (90% EtOH)

[溶解性] BERDY SOL: メタノール, ベンゼンに可溶; 水, ヘキサンに難溶

[UV]: [neutral] λ_{max} 223 (ε 6000) (MeOH) [neutral] λ_{max} 231 (ε 11800); 295 (ε 76) (MeOH)

[傷害・毒性] 皮膚を刺激する

-----文献-----

Kubo, I. et al., Chem. Comm., 1976, 1013, (分離, 構造決定)

Fukuyama, Y. et al., Phytochemistry, 1985, 24, 1521, (Polygonic acid)

Van Beek, T.A. et al., Phytochem. Anal., 1994, 5, 19, (分離, HPLC)

Brown, G.D., Phytochemistry, 1994, 35, 975, (分離, H-NMR, C13-NMR)

Filho, V.C. et al., J. Ethnopharmacol., 1998, 62, 223, (活性, Polygordial)

§ 7-Drimen-11,12-diol; (5 α,9 β)-form, 11-Carboxylic acid, 12-aldehyde

[化学名・別名] 12-Oxo-7-drimen-11-oic acid. Polygonic acid

[CAS No.] 98204-84-3

[化合物分類] テルペノイド (Drimane sesquiterpenoid)

[構造式]

[分子式] C₁₅H₂₂O₃

[分子量] 250.337

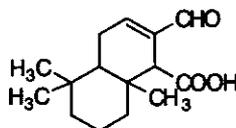
[正確な分子量] 250.156895

[基原] *Polygonum hydropiper*

[性状] 結晶

[融点] Mp 96-97 °C

[比旋光度]: [α]_D²³ -31 (c, 1.06 in CHCl₃)



-----文献-----

Fukuyama, Y. et al., Phytochemistry, 1985, 24, 1521, (Polygonic acid)

§ 7-Drimen-11,12-olide; 11 α-Alcohol

[化学名・別名] 11,12-Epoxy-7-drimen-11 α-ol. Isodrimeninol

[CAS No.] 72581-69-2

[化合物分類] テルペノイド (Drimane sesquiterpenoid)

[構造式]

[分子式] C₁₅H₂₄O₂

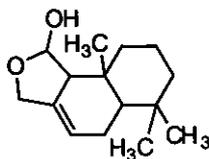
[分子量] 236.353

[正確な分子量] 236.17763

[基原] *Polygonum hydropiper*

[性状] オイル

[比旋光度]: [α]_D -37 (c, 1.5 in CHCl₃)



-----文献-----

Asakawa, Y. et al., Experientia, 1979, 35, 1420, (Isodrimeninol)

§ 1,4-Epoxy-p-menthane (旧 CAS 名)

[化学名・別名] 1-Methyl-4-(1-methylethyl)-7-oxabicyclo[2.2.1]heptane (CAS 名).

1-Isopropyl-4-methylbicyclo[2.2.1]heptane. 1,4-Cineole. Isocineole

[CAS No.] 470-67-7

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

[構造式]

[分子式] C₁₀H₁₈O

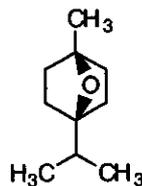
[分子量] 154.252

[正確な分子量] 154.135765

[基原] *Alpinia speciosa*, *Juniperus* spp., *Polygonum hydropiper*, *Artemisia* spp., *Shorea maranti* の木部, *Piper cubeba* と *Cannabis sativa* のオイル

[用途] 香水の芳香物質. Together with 1,8-Epoxy-p-menthane

[沸点] Bp 173-174 °C



[濃度] d^{20}_D 0.9
[屈折率] n^{20}_D 1.447
[化学物質毒性データ総覧(RTEC)登録番号] OS9274000

-----文献-----

Wallach, O., *Annalen*, 1907, 356, 197, (分離, 構造決定)
Naves, Y.R. et al., *Bull. Soc. Chim. Fr.*, 1950, 673, (分離)
Matsubara, Y. et al., *Nippon Kagaku Zasshi*, 1970, 91, 762; *CA*, 73, 120762a, (分離, purifn)
Takahashi, H. et al., *Chem. Lett.*, 1979, 373, (合成法, H-NMR)

RTECS (化学物質毒性データ)

健康障害に関するデータ

急性毒性に関するデータ

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 経口投与.

被験動物 : げっ歯類-ラット.

投与量・期間 : 3100 mg/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- [Vol.,頁,年(19-)]26,291,1988

<<試験方法>> LD50 試験 (50%致死量試験).

曝露経路 : 皮膚への塗布

被験動物 : げっ歯類-ウサギ.

投与量・期間 : >5 gm/kg

毒性影響 : 致死量以外に毒性影響に関する報告はない.

参照文献

FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- [Vol.,頁,年(19-)]26,291,1988

§ 11-Hydroxy-7-drimen-12,11-olide; 11 α -form, Et ether

[化学名・別名] 11 α -Ethoxycinnamolide

[化合物分類] テルペノイド (Drimane sesquiterpenoid)

[構造式]

[分子式] $C_{17}H_{26}O_3$

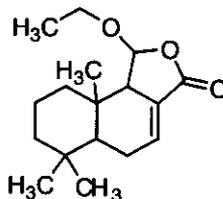
[分子量] 278.391

[正確な分子量] 278.188195

[基原] *Polygonum hydropiper*

[性状] 結晶

[融点] Mp 45-47 $^{\circ}C$



-----文献-----

Fukuyama, T. et al., *Phytochemistry*, 1985, 24, 1521, (分離, H-NMR, C13-NMR)

Paul, V.J. et al., *J. Nat. Prod.*, 1997, 60, 1115, (Ac)

§ Polygodial acetal

[CAS No.] 98204-88-7

[化合物分類] テルペノイド (Drimane sesquiterpenoid)

[構造式]

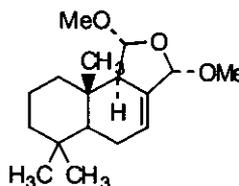
[分子式] $C_{17}H_{28}O_3$

[分子量] 280.406

[正確な分子量] 280.203845

[基原] *Polygonum hydropiper*, *Casella winterana*

[性状] 黄色のオイル



-----文献-----

Fukuyama, Y. et al., *Phytochemistry*, 1985, 24, 1521

Ying, B.-P. et al., *Phytochemistry*, 1995, 38, 909, (分離, H-NMR, C13-NMR)

§ Polygonal

[化学名・別名] 7- α -Hydroxy-11-nor-8-drimen-12-al

[CAS No.] 72537-20-3

[化合物分類] テルペノイド (Nor- and secodrimane sesquiterpenoid)

[構造式]

[分子式] $C_{14}H_{22}O_2$

[分子量] 222.237

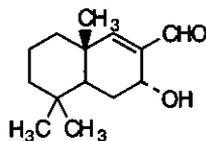
[正確な分子量] 222.16198

[基原] *Polygonum hydropiper*

[性状] 結晶

[融点] Mp 116-117 °C

[比旋光度]: $[\alpha]_D -7.3$ (c, 7.4 in $CHCl_3$)



-----文献-----

Asakawa, Y. et al., *Experientia*, 1979, 35, 1420, (Polygonal)

Fukuyama, Y. et al., *Phytochemistry*, 1985, 24, 1521, (Isopolygonal, Polygonone)

Errington, S.G. et al., *J. Chem. Res., Synop.*, 1987, 47, (分離, 誘導体)

Janaki, S. et al., *Indian J. Chem., Sect. B*, 1988, 27, 505, (合成法, 誘導体)

Cortecacutes, M. et al., *Nat. Prod. Lett.*, 1993, 2, 37, (合成法)

§ Polygonal; 7-Epimer

[化学名・別名] Isopolygonal

[CAS No.] 98204-83-2

[化合物分類] テルペノイド (Nor- and secodrimane sesquiterpenoid)

[構造式]

[分子式] $C_{14}H_{22}O_2$

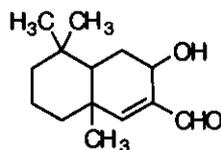
[分子量] 222.327

[正確な分子量] 222.16198

[基原] *Polygonum hydropiper*

[性状] オイル

[比旋光度]: $[\alpha]_D^{24} +73$ (c, 1.88 in $CHCl_3$)



-----文献-----

Fukuyama, Y. et al., *Phytochemistry*, 1985, 24, 1521, (Isopolygonal, Polygonone)

§ Polygonal; 7-Ketone

[化学名・別名] 7-Oxo-11-nor-8-drimen-12-al. Polygonone

[CAS No.] 72581-67-0

[化合物分類] テルペノイド (Nor- and secodrimane sesquiterpenoid)

[構造式]

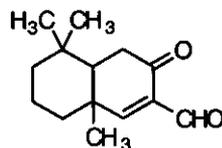
[分子式] $C_{14}H_{20}O_2$

[分子量] 220.311

[正確な分子量] 220.14633

[基原] *Polygonum hydropiper*

[性状] オイル



-----文献-----

Fukuyama, Y. et al., *Phytochemistry*, 1985, 24, 1521, (Isopolygonal, Polygonone)

§ 3,3',5,7-Tetrahydroxy-4'-methoxyflavone; 3-O- β -D-Glucopyranoside, 7-O-sulfate

[CAS No.] 156606-91-6

[化合物分類] フラボノイド (Flavonol; 5 \times O-置換基)

[構造式]

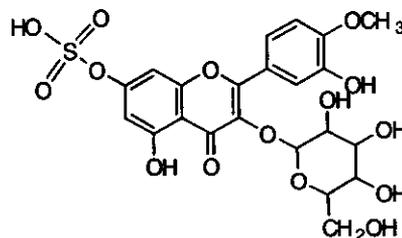
[分子式] $C_{22}H_{22}O_{15}S$

[分子量] 558.473

[正確な分子量] 558.067945

[基原] *Polygonum hydropiper* の葉

[性状] 黄色の粉末 (MeOH 溶液)



[比旋光度]: $[\alpha]_D^{17} -27.6$ (c, 0.6 in H₂O)

-----文献-----

- Gupta, S.R. et al., J.C.S., 1954, 3063, (Tamarixin)
Jurd, L., J.O.C., 1962, 27, 1294, (合成法)
Chakrabarty, G. et al., Indian J. Chem., 1965, 3, 171, (Tamarixin)
Audier, H., Bull. Soc. Chim. Fr., 1966, 2892, (Mas)
Bahl, C.P. et al., Indian J. Chem., 1967, 5, 171, (Tamarixetin)
Gunasegaran, R. et al., Indian J. Chem., Sect. B, 1981, 20, 832, (Thevefolin, 成書)
Norbedo, C. et al., Phytochemistry, 1984, 23, 2698, (分離)
McCormick, S. et al., Phytochemistry, 1985, 24, 2133, (分離)

§ 1',3',6'-Tris(4-hydroxycinnamoyl) sucrose

[化学名・別名] 1,3,6-Tris-O-[3-(4-hydroxyphenyl)-1-oxo-2-propeny]-β-D-fructofuranosyl α-D-glucopyranoside (CAS 名). 1',3',6'-Tricoumaroylsucrose. Hydropiperoside

[CAS No.] 87611-93-6

[化合物分類] 炭水化物 (Disaccharide)

[構造式]

[分子式] C₃₉H₄₆O₁₇

[分子量] 780.735

[正確な分子量] 780.226555

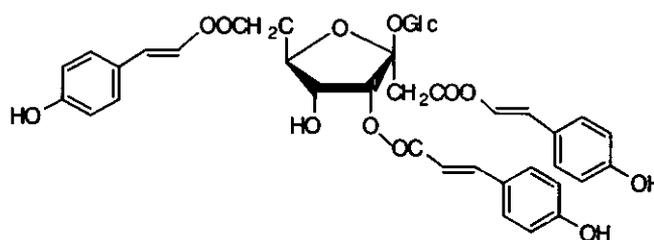
[基原] 次の植物の根から分離: *Polygonum*

hydropiper

[用途] Constit. of folk medicinal plant with anticancer allelopathic effects

[性状] 無定型

[UV]: [neutral] λ_{max} 228 (ε 15000); 315 (ε 26000) (MeOH)



-----文献-----

Fukuyama, Y. et al., Phytochemistry, 1983, 22, 549, (分離, UV, IR, H-NMR, C13-NMR, Mas)

*****ダバナ (Davana) *****

§ § キク科ダバナ (*Artemisia pallens* Wallich) の全草。

§ Artedouglasiaoxide

[CAS No.] 54783-60-7

[関連 CAS No.] 86575-88-4, 115403-96-8, 115403-97-9, 115403-98-0, 115403-99-1

[化合物分類] テルペノイド (Furanoid farnesane sesquiterpenoid)

[構造式]

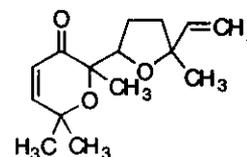
[分子式] C₁₅H₂₂O₃

[分子量] 250.337

[正確な分子量] 250.156895

[基原] 次の植物から分離: *Artemisia douglasiana*, *Artemisia pallens*, *Artemisia laciniata*

[性状] ガム



-----文献-----

Bohlmann, F. et al., Phytochemistry, 1982, 21, 2691, (分離, 構造決定)

Weyerstahl, P. et al., Annalen, 1988, 917, (分離, 構造決定)

§ Artemone

[化学名・別名] 2-(5-Ethenyltetrahydro-5-methyl-2-furanyl)

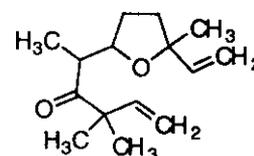
-4,4-dimethyl-5-hexen-3-one (CAS 名)

[CAS No.] 30925-48-5

[化合物分類] テルペノイド (Irregular acyclic sesquiterpenoid)

[構造式]

[分子式] C₁₅H₂₄O₂



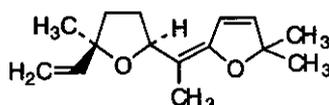
[分子量] 236.353
[正確な分子量] 236.17763
[基原] *Artemisia pallens*
[性状] 液体
[比旋光度]: $[\alpha]_D^{21} +41.4$ (c, 1.9 in CHCl₃)

-----文献-----

Naegeli, P. et al., Tet. Lett., 1970, 5021, (分離, 構造決定)
Akhila, A. et al., Tet. Lett., 1986, 27, 5885, (合成)

§ Davana ether

[CAS No.] 35470-57-6
[化合物分類] テルペノイド (Furanoid farnesane sesquiterpenoid)
[構造式]
[分子式] C₁₅H₂₀O₂
[分子量] 234.338
[正確な分子量] 234.16198
[基原] *Artemisia pallens*
[沸点] Bp_{0.001} 71-75 °C

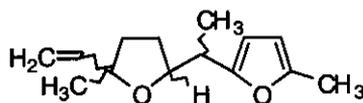


-----文献-----

Thomas, A.F. et al., Helv. Chim. Acta, 1974, 57, 2076

§ Davanafuran

[化学名・別名] 2-Ethenyltetrahydro-2-methyl-5-[1-(5-methyl-2-furanyl) ethyl] furan (CAS 名). Davanafuran
[関連 CAS No.] 56469-38-6, 56586-05-1, 56586-06-2, 56586-07-3
[化合物分類] テルペノイド (Furanoid farnesane sesquiterpenoid)
[構造式]
[分子式] C₁₄H₂₀O₂
[分子量] 220.311
[正確な分子量] 220.14633
[基原] *Artemisia pallens* のオイル
[沸点] Bp_{0.06} 42-50 °C

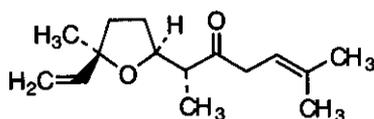


-----文献-----

Thomas, A.F. et al., Helv. Chim. Acta, 1974, 57, 2066, (分離, 合成法)
Ger. Pat., 1975, 2 452 083; CA, 83, 96998, (合成法)

§ Davanone

[化学名・別名] 2-(5-Ethenyltetrahydro-5-methyl-2-furanyl) -6-methyl-5-hepten-3-one (CAS 名)
[CAS No.] 30810-99-2
[化合物分類] テルペノイド (Furanoid farnesane sesquiterpenoid)
[構造式]
[分子式] C₁₅H₂₄O₂
[分子量] 236.353
[正確な分子量] 236.17763
[基原] *Artemisia pallens*
[比旋光度]: $[\alpha]_D^{21} +77.7$ (neat)

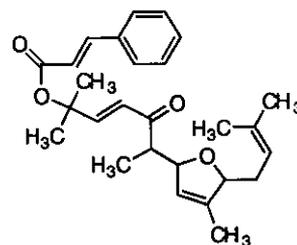


-----文献-----

Thomas, A.F. et al., Helv. Chim. Acta, 1974, 57, 2055, (分離, 構造決定)
Bartlett, P.A. et al., Tet. Lett., 1983, 24, 1365, (合成法)

§ 2,5-Dihydro-2-(5-hydroxy-1,5-dimethyl-2-oxo-3-hexenyl) -4-methyl-3-(3-methyl-2-butenyl) furan; O-Cinnamoyl

[化合物分類] テルペノイド (Furanoid farnesane sesquiterpenoid)
[構造式]
[分子式] C₂₇H₃₄O₄
[分子量] 422.563



[正確な分子量] 422.24571

[基原] *Artemisia pallens*

[性状] オイル

-----文献-----

Chandra, A. et al., Tet. Lett., 1987, 28, 6377, (分離, H-NMR)

§ 2,5-Dihydro-2-hydroxy-3-methyl-2-(3-methyl-2-butenyl) furan

[CAS No.] 133594-20-4

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

[構造式]

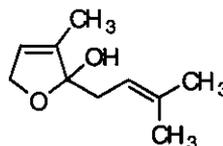
[分子式] $C_{10}H_{16}O_2$

[分子量] 168.235

[正確な分子量] 168.11503

[基原] *davana oil* (*Artemisia pallens*)

[性状] オイル



-----文献-----

Misra, L.N. et al., Phytochemistry, 1991, 30, 549, (分離, H-NMR)

§ 2,5-Dihydro-3-methyl-2-(3-methyl-2-butenyl) furan

[化学名・別名] α -Dihydorosefuran, 2,5-Dihydro-3-methyl-2-prenylfuran

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

[構造式]

[分子式] $C_{10}H_{16}O$

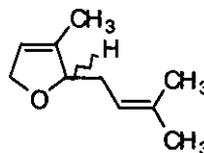
[分子量] 152.236

[正確な分子量] 152.120115

[基原] 次の植物から分離: *Artemisia pallens* (*davana oil*)

[用途] Floral odorant

[性状] オイル



-----文献-----

Chandra, A. et al., Tet. Lett., 1987, 28, 6377, (分離, H-NMR)

Misra, L.N. et al., Phytochemistry, 1991, 30, 549; 4212, (分離, H-NMR, C13-NMR)

§ 2,5-Dihydro-4-methyl-2-(3-methyl-2-butenyl) furan

[化学名・別名] β -Dihydorosefuran

[化合物分類] テルペノイド (Irregular acyclic monoterpeneoid)

[構造式]

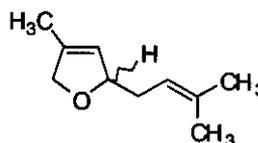
[分子式] $C_{10}H_{16}O$

[分子量] 152.236

[正確な分子量] 152.120115

[基原] 次の植物から分離: *Artemisia pallens* (*davana oil*)

[性状] オイル



-----文献-----

Misra, L.N. et al., Phytochemistry, 1991, 30, 549; 4212, (分離, H-NMR, C13-NMR)

§ 4,5-Epoxy-10-hydroxy-3-oxo-1-germacren-12,6-olide; (1E,4 ξ ,5 β ,6 α ,10 α ,11 α H)-form

[CAS No.] 174231-77-7

[化合物分類] テルペノイド (12,6-Germacranolide sesquiterpeneoid)

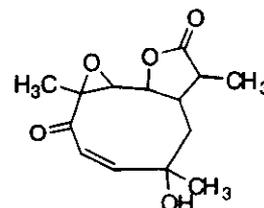
[構造式]

[基原] *Artemisia pallens*

[性状] 結晶

[融点] Mp 160-162 °C

[比旋光度]: $[\alpha]_D^{27} -19$ (c, 0.14 in MeOH)



-----文献-----

Rojatkar, S.R. et al., Phytochemistry, 1996, 41, 1105, (分離, H-NMR, C13-NMR)

§ Hydroxydavanone

[化学名・別名] 2-(5-Ethenyltetrahydro-5-methyl-2-furanyl)-6-hydroxy-6-methyl-4-hepten-3-one (CAS 名).

7,10-Epoxy-2-hydroxy-2,6,10-trimethyl-3,11-dodecadien-5-one

[CAS No.] 73395-08-1

[化合物分類] テルペノイド (Furanoid farnesane sesquiterpenoid)

[構造式]

[分子式] $C_{15}H_{24}O_3$

[分子量] 252.353

[正確な分子量] 252.172545

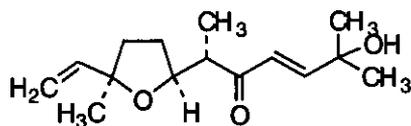
[基原] *Artemisia herba* and of *davana* oil

Artemisia pallens)

[性状] オイル

[沸点] $Bp_{0.05}$ 140 °C

[比旋光度]: $[\alpha]_D^{25} +43.7$ (c, 1.65 in $CHCl_3$)



Relative configuration (

-----文献-----

Thomas, A.F. et al., *Helv. Chim. Acta*, 1974, 57, 2081, (Isodavanone)

Gordon, M.M. et al., *J. Nat. Prod.*, 1981, 44, 432

Khafag, S.M. et al., *Phytochemistry*, 1983, 22, 1821, (Arteincultone)

Misra, L.N. et al., *Phytochemistry*, 1991, 30, 549, (分離, H-NMR, C13-NMR)

§ Hydroxydavanone; 11-Deoxy

[化学名・別名] Isodavanone. 2-(5-Ethenyltetrahydro-5-methyl-2-furanyl)-6-methyl-4-hepten-3-one (CAS 名)

[CAS No.] 54927-85-4

[化合物分類] テルペノイド (Furanoid farnesane sesquiterpenoid)

[構造式]

[分子式] $C_{15}H_{24}O_2$

[分子量] 236.353

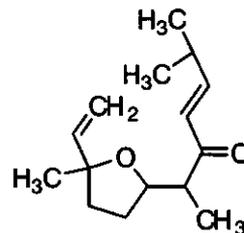
[正確な分子量] 236.17763

[基原] 次の植物から分離: *Artemisia pallens*

[性状] オイル

[比旋光度]: $[\alpha]_D^{20} +29.7$ (c, 10 in $CHCl_3$)

[その他のデータ] 立体構造は完全に決定していない。



-----文献-----

Thomas, A.F. et al., *Helv. Chim. Acta*, 1974, 57, 2081, (Isodavanone)

Gordon, M.M. et al., *J. Nat. Prod.*, 1981, 44, 432

§ Nordavanone

[化学名・別名] 3-(5-Ethenyltetrahydro-5-methyl-2-furanyl)-2-butanone (CAS 名)

[CAS No.] 54933-91-4

[化合物分類] テルペノイド (Furanoid farnesane sesquiterpenoid)

[構造式]

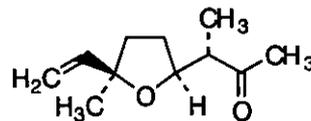
[分子式] $C_{11}H_{18}O_2$

[分子量] 182.262

[正確な分子量] 182.13068

[基原] *Artemisia pallens*

[比旋光度]: $[\alpha]_D^{20} +54$ ($CHCl_3$)



-----文献-----

Thomas, A.F. et al., *Helv. Chim. Acta*, 1974, 57, 2062

*****タマゴ (Egg) *****

§ § キジ科ニワトリ (*Gallus gallus* var. *domesticus* (Brisson)) の卵 (全部または卵黄, 乾燥または発酵処理したものを含む)。

該当物質なし

§ § キジ科ウズラ (*Coturnix coturnix* (L.)) の卵 (全部または卵黄, 乾燥または発酵処理したものを含む)。

該当物質なし

§ § ガンカモ科アヒル (*Anas platyrhyncha* var. *domestica* L.) の卵 (全部または卵黄, 乾燥または発酵処理したものを含む)。

該当物質なし

*****タマゴタケ (Royal agaric) *****

§ § テングタケ科タマゴタケ (*Amanita caesarea* (Scopoli) Persoon (*A. hemibapha* (Berk. et Br.) Sacc)) の子実体。

該当物質なし

*****タマネギ (Onion) *****

§ § ユリ科タマネギ (*Allium cepa* L.) の鱗茎。

§ **Astragalin; 2''-O-β-D-Glucopyranosyl, 7-O-β-D-glucuronopyranoside**

[化学名・別名] Kaempferol 3-sophoroside 7-glucuronide

[CAS No.] 140163-56-0

[化合物分類] フラボノイド (Flavonol; 4 × O-置換基)

[構造式]

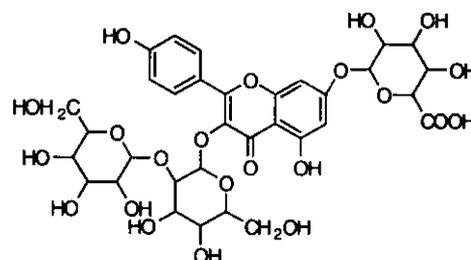
分子式] $C_{33}H_{38}O_{22}$

[分子量] 786.65

[正確な分子量] 786.18548

[基原] 次の植物から分離: *Allium cepa*

[性状] 黄-緑色の粉末



-----文献-----

Pavlii, O.I. et al., *Farm. Zh.* (Kiev), 1967, 22, 50, (Sorboside)

Markham, K.R. et al., *Phytochemistry*, 1990, 29, 3919, (Kaempferol 3-sophoroside 7-arabinoside)

Neilsen, J.K. et al., *Phytochemistry*, 1993, 34, 539, (3-acylsophoroside 7-glucoside)

§ **Butyl isopropyl disulfide**

[化学名・別名] Butyl 1-methylethyl disulfide (CAS 名), 2-Methyl-3,4-dithiooctane

[CAS No.] 72437-53-7

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

[構造式] $(H_3C)_2CH-S-S-(CH_2)_3CH_3$

[分子式] $C_7H_{16}S_2$

[分子量] 164.335

[正確な分子量] 164.06934

[基原] *Allium cepa*

-----文献-----

Gupta, D. et al., *Can. J. Chem.*, 1980, 58, 1350; 1981, 59, 543, (合成法, Mas)

Misharina, T.A. et al., *CA*, 1994, 120, 132679j, (分離)

§ **Butyl propyl disulfide**

[化学名・別名] 4,5-Dithianonane

[CAS No.] 72437-64-0

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

[構造式] $\text{H}_3\text{CCH}_2\text{CH}_2\text{-S-S-(CH}_2\text{)}_3\text{CH}_3$

[分子式] $\text{C}_7\text{H}_{16}\text{S}_2$

[分子量] 164.335

[正確な分子量] 164.06934

[基原] *Allium cepa*, *Azadirachta indica* と *Nigella sativa* の種子

-----文献-----

Gupta, D. et al., *Can. J. Chem.*, 1980, 58, 1350; 1981, 59, 543, (合成法, Mas)

Balandrin, M.F. et al., *J. Agric. Food Chem.*, 1988, 36, 1048, (分離)

§ Cycloalliin

[化学名・別名] 5-Methyl-3-thiomorpholinecarboxylic acid 1-oxide (CAS 名)

[CAS No.] 455-41-4

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

[構造式]

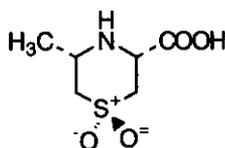
[分子式] $\text{C}_6\text{H}_{11}\text{NO}_3$

[分子量] 177.224

[正確な分子量] 177.045964

[基原] タマネギ (*Allium cepa*)

[比旋光度]: $[\alpha]_D^{20}$ -17.4 (H₂O)



Absolute
configuration

-----文献-----

Virtanen, A.I. et al., *Acta Chem. Scand.*, 1959, 19, 2257, (合成法, 生合成)

Palmer, K.J. et al., *Acta Cryst. B*, 1972, 28, 2615, (結晶構造, 絶対構造)

§ Dimethyl disulfide (CAS 名)

[化学名・別名] Methyl disulfide

[CAS No.] 624-92-0

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

[構造式] Me-S-S-Me

[分子式] $\text{C}_2\text{H}_6\text{S}_2$

[分子量] 94.201

[正確な分子量] 93.99109

[基原] 次の植物から分離: ニンニクオイル (*Allium sativum*), also in *Allium cepa* and *Allium ursinum*. ハムスター雌性フェロモンの成分

[性状] 液体

[融点] Mp -98 °C

[沸点] Bp 110 °C (116-118 °C). Bp_{12} 40 °C

[濃度] d_4^{16} 1.057

[屈折率] n_D^{16} 1.5219

[傷害・毒性] 50%致死濃度 (LC₅₀) (ラット, 吸入) 約 16 mg (月 3 回 2 時間暴露). 発火しやすい, 発火温度: <21 °C

[化学物質毒性データ総覧 (RTEC) 登録番号] JO1927500

-----文献-----

Schultz, O.E. et al., *Pharmazie*, 1965, 20, 441, (分離)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, 8, 189; 9, 91; 281; 473, (用途)

Connell, R.J. et al., *Anal. Chem. Symp. Ser.*, (Chem. Sens.), 1990, 6, 725

Block, E. et al., *Pure Appl. Chem.*, 1993, 65, 625, (酸化物, 生育)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DRQ400

RTECS (化学物質毒性データ)

生体影響物質 : 一時刺激物質

健康障害に関するデータ

皮膚/眼の刺激に関するデータ

<<試験方法>> 標準ドライズ試験.

曝露経路 : 眼中への塗布

被験動物 : げっ歯類-ウサギ.