

Archives Internationales de Pharmacodynamie et de Therapie. (Heymans Institute of Pharmacology, De Pintelaan 185, B-9000 Ghent, Belgium) 106,164,1956

変異原性に関するデータ

〈〈試験方法〉〉 DNA 損傷

試験系 : げっ歯類-ハムスター線維芽細胞.

投与量・期間: 100 ppm

参照文献

Collection of Papers Presented at the Annual Symposium on Fundamental Cancer Research. (Baltimore, MD) 23,346,1970

§ § キジ科ニワトリ (*Gallus gallus domesticus* Brisson) の可食部並びにその加工品。
本調査研究では、成分に関する文献はなかった。

*****ミモザ (Mimosa) *****

§ § マメ科 (*Acacia decurrens* Willdenow) の花。

§ 10,11,12,14,18-Pentahydroxy-20-nor-8,11,13-abietatrien-7-one; 12-Me ether, 18-Ac

[CAS No.] 224790-60-7

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

[構造式]

[分子式] $C_{27}H_{40}O_7$

[分子量] 406.475

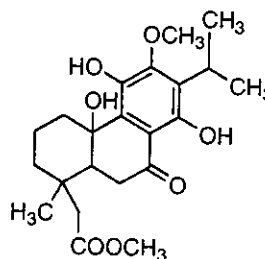
[基原] *Acacia decurrens*

[性状] 黄色の結晶

[融点] Mp 186-188 °C

[比旋光度]: $[\alpha]_D^{25} -16.2$ (c, 0.2 in MeOH)

UV: [neutral] λ_{max} 203 (log ϵ 3.92); 275 (log ϵ 3.66); 365 (log ϵ 3.21) (MeOH)



-----文献-----

Anam, E.M. et al., Indian J. Chem., Sect. B, 1998, 37, 1307-1309

§ 11,12,14,15-Tetrahydroxy-7-oxo-8,11,13-abietatrien-20-al; 12-Me ether

[化学名・別名] 11,14,15-Trihydroxy-12-methoxy-7-oxo-8,11,13-abietatrien-20-al

[CAS No.] 224790-58-3

[化合物分類] テルペノイド (Abietane diterpenoids)

[構造式]

[分子式] $C_{27}H_{40}O_8$

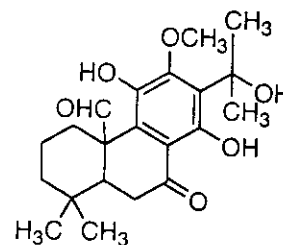
[分子量] 376.449

[基原] *Acacia decurrens* の根

[性状] 黄色の結晶 (Me:CO/petrol)

[比旋光度]: $[\alpha]_D^{25} +65.5$ (c, 0.1 in MeOH)

UV: [neutral] λ_{max} 215 (log ϵ 4.28); 273 (log ϵ 3.99); 365 (log ϵ 3.75) (MeOH)



-----文献-----

Anam, E.M. et al., Indian J. Chem., Sect. B, 1998, 37, 1307-1309

§ § マメ科ミモザアカシア (*Acacia decurrens* var. *dealbata* (Link) F. Mueller) の花。

本調査研究では、成分に関する文献はなかった。

*****ミヨウガ (Myoga) *****

本調査研究では、成分に関する文献はなかった。

*****ミルク (Milk) *****

§ § ウシ科ウシ (*Bos taurus* L.) の乳用家畜の乳汁。

「ミート」参照

§ § ウシ科ヤギ (*Capra hircus* L.) の乳用家畜の乳汁。

本調査研究では、成分に関する文献はなかった。

*****ミルテ (Myrtle) *****

§ § フトモモ科ギンバイカ (*Myrtus communis* L.) の茎葉、花または果実。

§ 3,6-Digalloylglucose; D -Pyranose-form

[CAS No.] 13186-20-4

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

[構造式]

[分子式] $C_{20}H_{20}O_{14}$

[分子量] 484.37

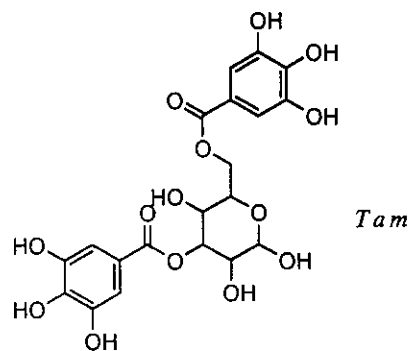
[基原] 次の植物から分離: *Geranium pratense* の根茎, *Polygonum bistorta*, *arix aphylla*, *Myrtus communis*, *Bergenia* sp.

[性状] 結晶 (H₂O)

[融点] Mp 185 °C

[比旋光度]: $[\alpha]_D^{20} +79$ (c, 2.3 in EtOH)

[その他のデータ] Equilibrated mixt. of α - and β -anomers in soln.



-----文献-----

Schmidt, O.T. et al., *Annalen*, 1951, 571, 19; 29, (構造決定, 合成法)

Gstirner, F. et al., *Arch. Pharm. (Weinheim, Ger.)*, 1962, 295, 823; 1966, 299, 640, (分離)

Diaz, A.M. et al., *Plant. Med. Phytother.*, 1987, 21, 317, (分離)

Nawwar, M.A.M. et al., *Phytochemistry*, 1994, 36, 1035, (分離)

Lin, T.-C. et al., *J. Chin. Chem. Soc. (Taipei)*, 1999, 46, 613-618, (分離, Me glycoside)

§ Myrtucommulone A

[CAS No.] 54247-21-1

[化合物分類] 単環芳香族 (Acylphloroglucinols)

[構造式]

[分子式] $C_{38}H_{52}O_{10}$

[分子量] 668.823

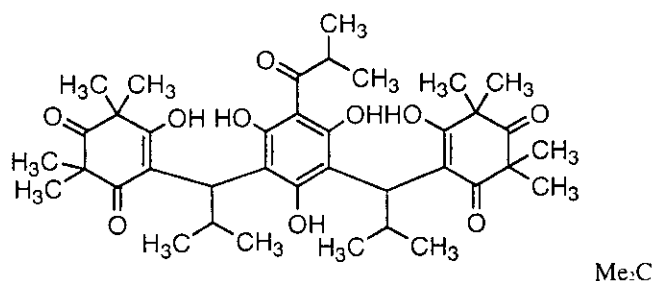
[基原] *Myrtus communis*, *Callistemon lanceolatus*

[用途] グラム陽性菌に対して強い抗菌活性を示す

[性状] 黄色の結晶 (MeOH, EtOAc, MeOH/CHCl₃ or O)

[融点] Mp 185-186 °C

UV: [neutral] λ_{max} 234 (ϵ 22000); 267 (ϵ 18500) (EtOH) (Berdy)



-----文献-----

Kashman, Y. et al., *Tetrahedron*, 1974, 30, 991, (分離, 構造)

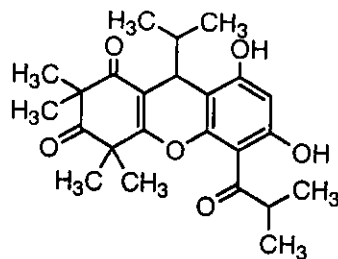
Rotstein, A. et al., *Antimicrob. Agents Chemother.*, 1974, 6, 539; *CA*, 82, 106871t, (分離)

Lounasmaa, M. et al., *Phytochemistry*, 1977, 16, 1851, (分離)

§ Myrtucommulone B

[化学名・別名] 4,9-Dihydro-6,8-dihydroxy-2,2,4,4-tetramethyl-9-(1-methylethyl)-5-(2-methyl-1-oxopropyl)-1H-xanthen-1,3(2H)-dione (CAS 名)

[CAS No.] 54247-23-3
 [化合物分類] 単環芳香族 (Dibenzo [b,e] pyrans)
 [構造式]
 [分子式] $C_{24}H_{30}O_6$
 [分子量] 414.497
 [基原] *Myrtus communis*
 [用途] 抗菌活性を持つ
 [性状] 無定型の粉末

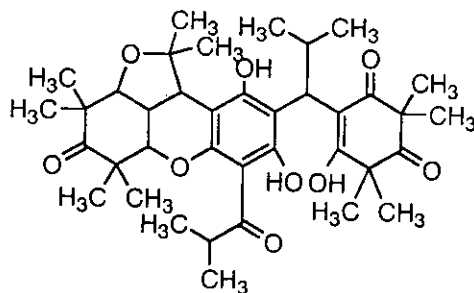


-----文献-----

Kashman, Y. et al., *Tetrahedron*, 1974, 30, 991, (分離, 構造)
 Rotstein, A. et al., *Antimicrob. Agents Chemother.*, 1974, 6, 539; *CA*, 82, 106871t, (分離)

§ **Myrtucommulone D**

[CAS No.] 126221-82-7
 [化合物分類] 単環芳香族 (Acylphloroglucinols)
 [構造式]



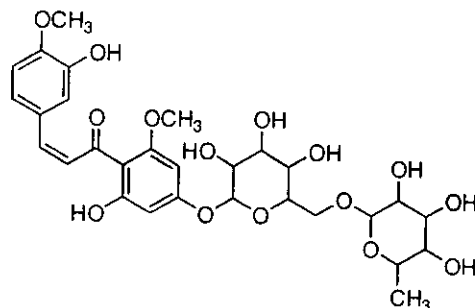
[分子式] $C_{38}H_{52}O_9$
 [分子量] 652.823
 [基原] *Myrtus communis* の葉
 [その他のデータ] Name incorr. spelt in abstract

-----文献-----

Davidyuk, L.P. et al., *CA*, 1990, 112, 195230m, (分離)

§ **2',3,4,4',6'-Pentahydroxychalcone; 2',4-Di-Me ether, 4'-O-[α -L-rhamnopyranosyl-(1 \rightarrow 6)- β -D-glucopyranoside]**

[化学名・別名] Hesperidin methylchalcone
 [CAS No.] 24292-52-2
 [その他の CAS No.] 25429-20-3
 [化合物分類] フラボノイド (Chalcone flavonoids; 5 \times O-置換基)
 [構造式]
 [分子式] $C_{29}H_{36}O_{15}$
 [分子量] 624.594
 [基原] *Myrtus communis* の果実

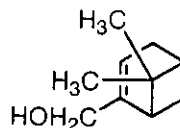


-----文献-----

Rimpler, H. et al., *Arch. Pharm. (Weinheim, Ger.)*, 1965, 298, 838, (配糖体)
 Wiermann, R., *Planta*, 1970, 95, 133, (分離)
 Fraser, A.W. et al., *Phytochemistry*, 1974, 13, 1561, (分離)
 Chibber, S.S. et al., *Curr. Sci.*, 1982, 51, 933, (分離, Tephron)
 Imperato, F., *Experientia*, 1982, 38, 67, (分離, 誘導体)
 Fukunaga, T. et al., *Chem. Pharm. Bull.*, 1987, 35, 3292, (配糖体)

§ **2-Pinen-10-ol; (+)-form**

[CAS No.] 6712-78-3
 [化合物分類] テルペノイド (Pinane monoterpenoids)
 [構造式]
 [分子式] $C_{10}H_{16}O$
 [分子量] 152.236
 [基原] 次の植物から分離: *Myrtus communis* のオイル, *Darwinia grandiflora*, *Leptospermum lanigerum*, *Chamaecyparis formosensis*, その他
 [性状] オイル
 [沸点] Bp_{11} 103-104 $^{\circ}C$
 [比旋光度]: $[\alpha]_D^{22} +44.3$ (c. 3.21 in $CHCl_3$)



-----文献-----

Couchman, F.M. et al., *Tetrahedron*, 1964, 20, 2037, (分離)
 Banthorpe, D.V. et al., *Chem. Rev.*, 1966, 66, 643, (レビュー)

Ford, R.A. et al., Food Chem. Toxicol., 1992, 30, 935, (レビュー, 毒性)

§ 2,3,6,23-Tetrahydroxy-12-oleanen-28-oic acid; (2 α , 3 β , 6 β)-form

[化学名・別名] Terminolic acid †

[CAS No.] 564-13-6

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

[構造式]

[分子式] $C_{30}H_{48}O_6$

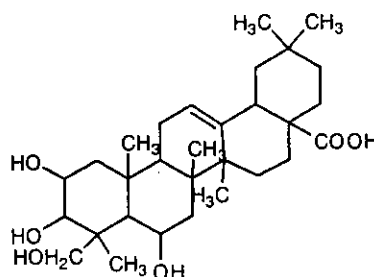
[分子量] 504.706

[基原] *Terminalia ivorensis*, *Myrtus communis*

[性状] 結晶 (Me₂CO)

[融点] Mp 347 °C

[比旋光度]: $[\alpha]_D +42$ (c, 0.11 in EtOH)



-----文献-----

King, F.E. et al., J.C.S., 1955, 1333; 1956, 4469, (Terminolic acid)

*****ミルフォイル (Milfoil) *****

§ § キク科セイヨウノコギリソウ (*Achillea millefolium* L.) の花または全草。

§ Achimilic acid

[化学名・別名] 3-[(2-Hydroxy-2-methyl-5-oxo-3-cyclopenten-1-ylidene)methyl]-2-methylene-6-oxoheptanoic acid (CAS 名)

[CAS No.] 110732-04-2

[化合物分類] 脂肪族化合物 (Monocarbocyclic carboxylic acids and lactones)

[構造式]

[分子式] $C_{15}H_{18}O_5$

[分子量] 278.304

[分子式] $C_{15}H_{18}O_5$

[分子量] 278.304

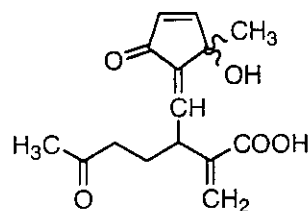
[基原] 次の植物から分離: *Achillea millefolium*

[用途] 強い抗腫瘍活性

[その他のデータ] Obt. as mixture of diastereoisomers

-----文献-----

Japan. Pat., 1987, 87 81 349; CA, 107, 161673, (分離, C13-NMR, IR, UV, Mass)



§ Achimilic acid A

[CAS No.] 157184-04-8

[化合物分類] テルペノイド (Seco-, cyclo-, abeo- and norguaiane sesquiterpenoids)

[構造式]

[分子式] $C_{15}H_{18}O_5$

[分子量] 278.304

[基原] *Achillea millefolium*

[性状] 針状結晶 (as Me ester)

[融点] Mp 76-77 °C (Me ester)

[比旋光度]: $[\alpha]_D -23.6$ (c, 1 in CHCl₃) (Me ester)

UV: [neutral] λ_{max} 245 (ϵ) (EtOH) (Derep)

-----文献-----

Tozoy, T. et al., Chem. Pharm. Bull., 1994, 42, 1096, (分離, H-NMR, C13-NMR, 結晶構造)

§ Achimilic acid A; 5Z-Isomer

[化学名・別名] Achimilic acid B

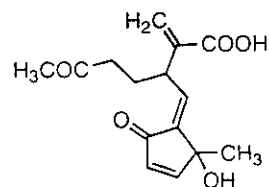
[CAS No.] 157184-05-9

[化合物分類] テルペノイド (Seco-, cyclo-, abeo- and norguaiane sesquiterpenoids)

[構造式]

[分子式] $C_{15}H_{18}O_5$

[分子量] 278.304



[基原] *Achillea millefolium*
[性状] オイル (as Me ester)
[比旋光度]: $[\alpha]_D -78.2$ (c, 1 in CHCl_3) (Me ester)
UV: [neutral] $\lambda_{\text{max}} 245$ (ϵ) (EtOH) (Derep)

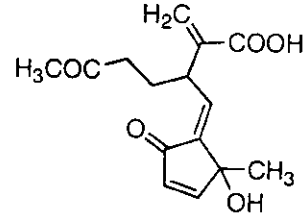
-----文献-----

Tozoy, T. et al., Chem. Pharm. Bull., 1994, 42, 1096, (分離, H-NMR, C13-NMR, 結晶構造)

§ Achimillic acid A; 4-Epimer

[化学名・別名] Achimillic acid C
[CAS No.] 157184-06-0
[化合物分類] テルペノイド (Seco-, cyclo-, abeo- and norguaiane sesquiterpenoids)
[構造式]
[分子式] $\text{C}_{15}\text{H}_{18}\text{O}_3$
[分子量] 278.304

[基原] *Achillea millefolium*
[性状] オイル (as Me ester)
[比旋光度]: $[\alpha]_D -87.3$ (c, 1 in CHCl_3) (Me ester)
UV: [neutral] $\lambda_{\text{max}} 245$ (ϵ) (EtOH) (Derep)

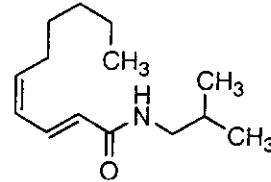


-----文献-----

Tozoy, T. et al., Chem. Pharm. Bull., 1994, 42, 1096, (分離, H-NMR, C13-NMR, 結晶構造)

§ 2,4-Decadienoic isobutylamide; (E,E)-form

[CAS No.] 18836-52-7
[化合物分類] アルカロイド化合物 (Simple isobutylamide alkaloids)
[構造式]
[分子式] $\text{C}_{11}\text{H}_{21}\text{NO}$
[分子量] 223.358



[基原] *Fagara xanthoxyloides*, *Piper sylvaticum*, *Piper nepalense*, その他数種の *Piper* spp., *Anacyclus pyrethrum*, *Achillea millefolium* and *Asiasarum heterotropoides* (ミカン科, コショウ科, キク科, ウマノスズクサ科)

[用途] Produces intense formication and local anaesthesia of the mucous membranes. 殺虫剤
[性状] 針状結晶 (petrol)
[融点] Mp 75 °C (69 °C). Mp 90-95 °C
[傷害・毒性] 強い刺激

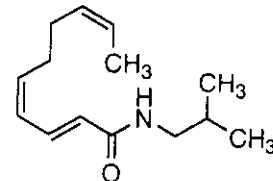
-----文献-----

Bowden, K. et al., J.C.S., 1963, 3503, (分離, UV, IR)
Loder, J.W. et al., Aust. J. Chem., 1969, 22, 1531, (分離, UV, IR, Mass, 合成法)
Banerji, A. et al., Experientia, 1974, 30, 223, (分離, 構造)
Mahanta, P.K. et al., J. Pharm. Sci., 1974, 63, 1160, (分離, UV, IR)
Dasgupta, S. et al., Indian J. Chem., Sect. B, 1979, 17, 538, (分離, UV, IR, H-NMR, Mass)
Yasusa, I. et al., Chem. Pharm. Bull., 1981, 29, 564, (分離, UV, IR, H-NMR, C13-NMR, Mass)

§ 2,4,8-Decatrienoic acid; (2E,4E,8Z)-form, 2-Methylpropylamide

[化学名・別名] *N*-Isobutyl-2,4,8-decatrienamamide. *N*-(2-Methylpropyl)-2,4,8-decatrienamamide (CAS 名).

2,4,8-Decatrienoic acid isobutylamide
[CAS No.] 52657-13-3
[化合物分類] アルカロイド化合物 (Simple isobutylamide alkaloids)
[構造式]
[分子式] $\text{C}_{17}\text{H}_{29}\text{NO}$
[分子量] 271.42



[基原] 次の植物の根から得られるアルカロイド: *Achillea millefolium* (キク科)
[性状] オイル

-----文献-----

Bohlmann, F. et al., Chem. Ber., 1974, 107, 1038. (分離, UV, IR, H-NMR, Mass, 構造)

§ 2,4,6-Decatrienoic acid dehydropiperidide; (2E,4E,6Z)-form

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

[構造式]

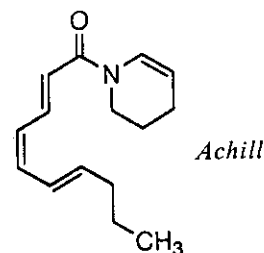
[分子式] $C_{15}H_{21}NO$

[分子量] 231.337

[基原] 次の植物から得られるアルカロイド: *Achillea nabelikii*, *Achillea millefolium*,
ea crithmifolia (キク科)

[性状] 黄色の結晶 (Et:O/petrol)

[融点] Mp 55 °C



-----文献-----

Bohlmann, F. et al., Chem. Ber., 1973, 106, 1328, (分離, UV, H-NMR, 構造決定, 合成法)

Greger, H. et al., Phytochemistry, 1981, 20, 2579, (分離, 誘導體)

Strunz, G.M. et al., Can. J. Chem., 1996, 74, 419, (合成法, 誘導體)

§ 2,4,6-Decatrienoic acid dehydropiperidide; (2E,4E,6Z)-form, 8,9-Didehydro

[化学名・別名] 2,4,6,8-Decatetraenoic acid dehydropiperidide

[CAS No.] 43110-68-5

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

[構造式]

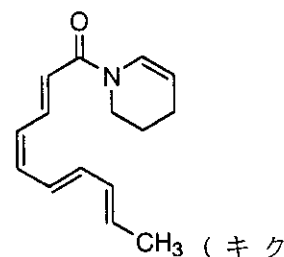
[分子式] $C_{15}H_{19}NO$

[分子量] 229.321

[基原] 次の植物から得られるアルカロイド: *Achillea nabelikii*, *Achillea millefolium*
科)

[性状] 黄色がかったオイル

[その他のデータ] 完全な純品は得られてない



-----文献-----

Bohlmann, F. et al., Chem. Ber., 1973, 106, 1328, (分離, UV, H-NMR, 構造決定, 合成法)

Greger, H. et al., Phytochemistry, 1981, 20, 2579, (分離, 誘導體)

Strunz, G.M. et al., Can. J. Chem., 1996, 74, 419, (合成法, 誘導體)

§ 3,8-Dihydroxy-1(10),4-germacradien-12,6-olide; (1(10)E,3 α,4E,6 α,8 α,11 ξ)-form, Di-Ac

[化学名・別名] Millefin

[CAS No.] 39262-27-6

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

[構造式]

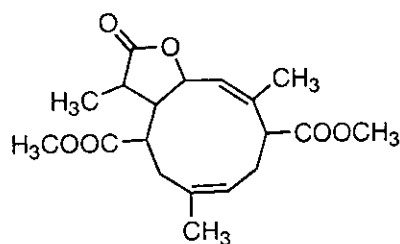
[分子式] $C_{19}H_{26}O_6$

[分子量] 350.411

[基原] *Achillea millefolium*

[性状] 結晶

[融点] Mp 209-210 °C



-----文献-----

Kasymov, Sh.Z. et al., Khim. Prir. Soedin., 1972, 8, 247; Chem. Nat. Compd. (Engl. Transl.), 1972, 8, 246.
(Millefin)

Gómez, G.F. et al., Phytochemistry, 1983, 22, 197, (Dihydroeucannabinolide)

Breton, J.L. et al., Tetrahedron, 1985, 41, 3141, (Heliangolidin)

Ohmura, K. et al., Phytochemistry, 1989, 28, 1919, (Hypochoeroside A)

Marco, A. et al., Phytochemistry, 1992, 31, 2163, (3 β-Hydroxybalchanolide)

§ 8,10-Dihydroxy-1,4-guaiadien-12,6-olide; (6 α,8 α,10 β,11 α)-form, 8-Ac

[化学名・別名] Achillicin. 8 α-Acetoxyartabsin

[CAS No.] 71616-00-7

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

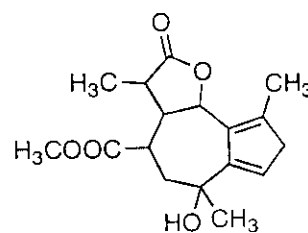
[構造式]

[分子式] $C_{17}H_{22}O_5$

[分子量] 306.358

[基原] *Achillea millefolium*, *Achillea collina*

[性状] 結晶



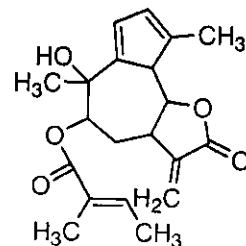
-----文献-----

----- 文献 -----

Banh-Nhu, C. et al., *Phytochemistry*, 1979, 18, 331, (分離)
Schroumlder, H. et al., *Phytochemistry*, 1994, 36, 1449, (構造決定, 成書)

§ **9,10-Dihydroxy-1,3,11(13)-guaiatrien-12,6-olide; (5 α ,6 α ,9 α ,10 α)-form, 9-Tigloyl**

[化学名・別名] Isoachifolidiene
[化合物分類]テルペノイド(12,6-Guaianolide sesquiterpenoids)
[構造式]
[分子式] C₂₀H₂₄O₅
[分子量] 344.407
[基原] *Achillea millefolium*
[性状] 結晶
[融点] Mp 153 °C

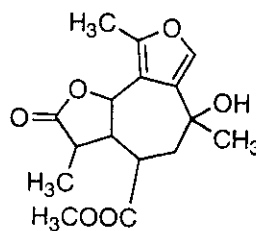


----- 文献 -----

Rücker, G. et al., *Planta Med.*, 1992, 58, 293, (分離, H-NMR, C13-NMR)

§ **Egelolide; 8-Ac**

[化学名・別名] 8-Acetylgegelolide. 3-Oxaachillicin
[CAS No.] 142449-62-5
[化合物分類]テルペノイド(Seco-, cyclo-, abeo- and norguaiiane sesquiterpenoids)
[構造式]
[分子式] C₁₆H₂₀O₆
[分子量] 308.33
[基原] *Achillea millefolium*
[性状] 結晶 (Et₂O)
[融点] Mp 219-221 °C

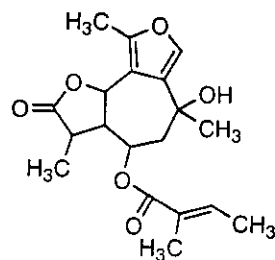


----- 文献 -----

Ochir, G. et al., *Phytochemistry*, 1991, 30, 4163-4165, (分離, H-NMR, C13-NMR)
Schroumlder, H. et al., *Phytochemistry*, 1994, 36, 1449-1451, (構造決定, 成書)

§ **Egelolide; 8-Angeloyl**

[化学名・別名] 8-Angeloylgegelolide. 8 α -Angeloyloxy-3-oxaartabsin
[CAS No.] 142449-63-6
[化合物分類]テルペノイド(Seco-, cyclo-, abeo- and norguaiiane sesquiterpenoids)
[構造式]
[分子式] C₁₉H₂₄O₆
[分子量] 348.395
[基原] *Achillea millefolium*
[性状] 結晶 (Et₂O)
[融点] Mp 152-154 °C
[比旋光度]: $[\alpha]_D^{20} +5.8$ (c, 0.34 in CHCl₃)



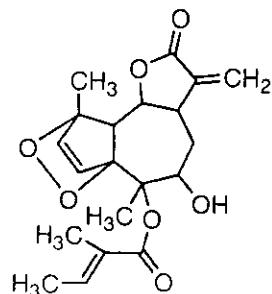
----- 文献 -----

Ochir, G. et al., *Phytochemistry*, 1991, 30, 4163-4165, (分離, H-NMR, C13-NMR)
Schroumlder, H. et al., *Phytochemistry*, 1994, 36, 1449-1451, (構造決定, 成書)

§ **1,4-Epidioxy-9,10-dihydroxy-2,11(13)-guaiadien-12,6-olide; (1 α ,4 α ,5 α ,6 α ,9 α ,10 α)-form, 10-Tigloyl**

[化学名・別名] α -Peroxyachifolide
[化合物分類]テルペノイド(12,6-Guaianolide sesquiterpenoids)
[構造式]

[分子式] C₂₀H₂₄O₇
[分子量] 376.405
[基原] *Achillea millefolium*
[性状] 針状結晶 (EtOH)

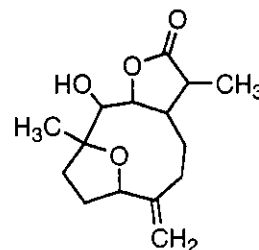


Rücker, G. et al., Arch. Pharm. (Weinheim, Ger.), 1991, 324, 979, (Peroxyachifolides)

§ 1,4-Epoxy-5-hydroxy-10(14)-germacren-12,6-olide; (1 α , 4 α , 5 β , 6 α , 11 β H)-form

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

[構造式]



[分子式] C₁₅H₂₂O₄

[分子量] 266.336

[基原] *Achillea millefolium*

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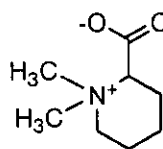
Ulubelen, A. et al., Phytochemistry, 1990, 29, 3948, (分離, H-NMR)

§ Homostachydrine; (S)-form

[CAS No.] 472-22-0

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

[構造式]



[分子式] C₉H₁₅NO₂

[分子量] 157.212

[基原] 次の植物の種子から分離: *Medicago sativa* (マメ科). また *Achillea millefolium*, *Moschata* sp.からも得られる (キク科)

[性状] 微細結晶

[融点] Mp 300 °Cで分解

[比旋光度]: [α]_D -9 (H₂O)

-----文献-----

Wiehler, G. et al., Can. J. Chem., 1958, 36, 339, (分離, 構造決定, 合成法)

Beyerman, H.C., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.), 1959, 78, 134, (絶対構造)

Pailer, M. et al., Arch. Pharm. (Weinheim, Ger.), 1960, 293, 646, (分離)

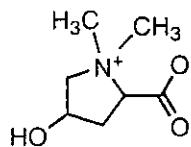
§ 4-Hydroxy-1,1-dimethylpyrrolidinium-2-carboxylate; (2S,4S)-form

[化学名・別名] Betonicine. Achillein

[CAS No.] 515-25-3

[化合物分類] アミノ酸とペプチド (Non-protein α -aminoacids), アルカロイド化合物 (Simple pyrrolidine alkaloids)

[構造式]



Marrubium vulgare

[分子式] C₇H₁₃NO₃

[分子量] 159.185

[基原] *Achillea millefolium*, *Betonica officinalis*, *Stachys sylvatica*, (horehound) (キク科, シソ科)

[用途] Possesses antiinflammatory activity

[性状] プリズム結晶 (EtOH)

[融点] Mp 252 °Cで分解 (244-245 °C)

[比旋光度]: [α]_D¹⁵ -36.6 (H₂O)

[販売元] Sigma:B6138

-----文献-----

Schulze, E. et al., Hoppe Seyler's Z. Physiol. Chem., 1911, 76, 258; 1912, 79, 236, (分離)

Goodson, J.A. et al., J.C.S., 1919, 115, 923, (分離)

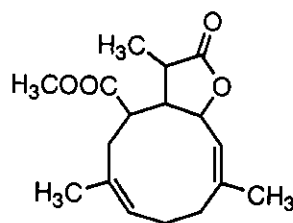
Paudler, W.W. et al., Chem. Ind. (London), 1963, 1693, (分離, 構造)

Mandava, N. et al., Annalen, 1970, 741, 167, (H-NMR, 構造)

§ 8-Hydroxy-1(10),4,11(13)-germacratrien-12,6-olide; (1(10)E,4E,6 α ,8 α)-form, 11 β ,13-Dihydro, Ac

[化学名・別名] Acetylbalchanolide

[化学名・別名] Acetylbalchanolide
 [化合物分類] テルペノイド (Elemene sesquiterpenoids)
 [構造式]
 [分子式] $C_{17}H_{24}O_4$
 [分子量] 292.374
 [基原] yarrow (*Achillea millefolium*)
 [性状] 結晶 (diisopropyl ether)
 [融点] Mp 125 °C
 [比旋光度]: $[\alpha]_D^{20} +128.1$ (c, 3.8 in $CHCl_3$)



-----文献-----

Hochmannová, J. et al., Coll. Czech. Chem. Comm., 1961, 26, 1826, (Balchanolide)
 Herout, V. et al., Coll. Czech. Chem. Comm., 1961, 26, 2612, (Balchanolide)
 Doskotch, R.W. et al., J.O.C., 1970, 35, 1928, (Balchanolide, Tulipinolide)
 Brozd, B. et al., Coll. Czech. Chem. Comm., 1972, 37, 1546, (分離)
 Lee, K.-H. et al., J. Pharm. Sci., 1972, 61, 629, (性質)
 Bohlmann, F. et al., Phytochemistry, 1978, 17, 471-474, (分離)
 Herz, W. et al., J.O.C., 1979, 44, 2784, (分離)
 Gao, F. et al., Phytochemistry, 1986, 25, 1231, (分離)
 Okunade, A.L. et al., Phytochemistry, 1994, 35, 191, (分離, H-NMR, C13-NMR, 結晶構造)

§ Millefolide

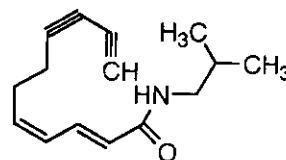
[化合物分類] テルペノイド (Terpenoids 構造は未知)
 [構造式] 不明
 [分子式] $C_{15}H_{22}O_3$
 [分子量] 250.337
 [一般的性質] Sesquiterpene monocyclic lactone contg. conjugated methylene, OH and CO groups
 [基原] 次の植物から分離: *Achillea millefolium* の花頭
 [性状] 繊維性針状結晶 (diisopropyl ether)
 [融点] Mp 138-140 °C
 [比旋光度]: $[\alpha]_D^{20} +107.2$ (c, 1.36 in $CHCl_3$)
 [その他のデータ] Readily polymerises

-----文献-----

Hochmannova, J. et al., Coll. Czech. Chem. Comm., 1961, 26, 1826

§ 2,4-Undecadiene-8,10-dienoic acid; (2E,4E)-form, 2-Methylpropylamide

[化学名・別名] 2,4-Undecadiene-8,10-dienoic acid isobutylamide. N-(2-Methylpropyl)-2,4-undecadiene-8,10-diyamide
 [CAS No.] 13891-74-2
 [化合物分類] アルカロイド化合物 (Simple isobutylamide alkaloids)
 [構造式]
 [分子式] $C_{15}H_{25}NO$
 [分子量] 229.321
 [基原] 次の植物から分離: *Chrysanthemum frutescens*, *Achillea macrophylla*, *Achillea ptarmica*, *Achillea millefolium*, *Otanthus maritimus*, *Anacyclus clavatus*, その他の属
 [性状] 結晶 (EtO/petrol)
 [融点] Mp 99-100 °C
 UV: [neutral] λ_{max} 252 (EtO)



-----文献-----

1974, 107, 1038; 1975, 108, 739, (分離, 合成法, UV, IR, H-NMR)
 Jente, R. et al., Chem. Ber., 1972, 105, 1694, (合成法, 分離, Mass, 構造決定, H-NMR, IR, UV)
 Bohlmann, F. et al., Phytochemistry, 1980, 19, 1535, (分離)
 Greger, H. et al., Phytochemistry, 1984, 23, 1503; 1989, 28, 2363, (分離)
 Martin, R. et al., Phytochemistry, 1985, 24, 2295, (分離, Mass, H-NMR)
 Kuropka, G. et al., Planta Med., 1986, 52, 244; 1987, 53, 440, (分離, UV, IR, H-NMR, Mass, 構造)
 Jakupovic, J. et al., Phytochemistry, 1988, 27, 1135, (分離)
 Bauer, R. et al., Phytochemistry, 1988, 27, 2339; 1989, 28, 505, (分離, H-NMR, Mass, IR, UV)
 Binns, S.E. et al., Planta Med., 2000, 66, 241-242, (活性, 2-methylpropylamide)

§ 2,4-Undecadiene-8,10-diyonic acid; (2E,4E)-form, 2,3-Didehydropiperidide

[化学名・別名] 2,4-Undecadiene-8,10-diyonic acid 2,3-dehydropiperidide

[CAS No.] 52704-38-8

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

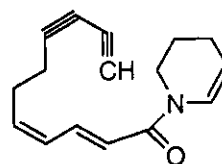
[構造式]

[分子式] C₁₅H₁₇NO

[分子量] 239.316

[基原] Alkamide from *Otanthus maritimus*, *Achillea millefolium*, *Achillea ptarmica* (キク科)

[性状] オイル



-----文献-----

- 1974, 107, 1038; 1975, 108, 739, (分離, 合成法, UV, IR, H-NMR)
Jente, R. et al., Chem. Ber., 1972, 105, 1694, (合成法, 分離, Mass, 構造決定, H-NMR, IR, UV)
Bohlmann, F. et al., Phytochemistry, 1980, 19, 1535, (分離)
Greger, H. et al., Phytochemistry, 1984, 23, 1503; 1989, 28, 2363, (分離)
Martin, R. et al., Phytochemistry, 1985, 24, 2295, (分離, Mass, H-NMR)
Kuroпка, G. et al., Planta Med., 1986, 52, 244; 1987, 53, 440, (分離, UV, IR, H-NMR, Mass, 構造)
Jakupovic, J. et al., Phytochemistry, 1988, 27, 1135, (分離)
Bauer, R. et al., Phytochemistry, 1988, 27, 2339; 1989, 28, 505, (分離, H-NMR, Mass, IR, UV)

§ § キク科ジャコウノコギリソウ (*Achillea moschata* Jacquin) の花または全草。

本調査研究では、成分に関する文献はなかった。

§ § キク科ノコギリソウ (*Achillea sibirica* Ledebour) の花または全草。

§ 2-Decene-4,6,8-triynoic acid; (E)-form, 2-Methylpropylamide

[化学名・別名] Dehydromatricaric acid isobutylamide

[CAS No.] 37064-10-1

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

[構造式]

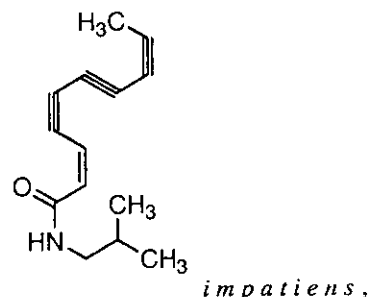
[分子式] C₁₄H₁₅NO

[分子量] 213.279

[基原] 次の植物から分離: *Achillea spinulifolia*, *Achillea ptarmica*, *Achillea sibirica*, *Anacyclus pyrethrum*, *Cladanthus arabicus*

[性状] 結晶 (CCl₄)

[融点] Mp 133-139 °C. Mp 144.5-145.5 °C



-----文献-----

- Stauholt, K. et al., Acta Chem. Scand., 1950, 4, 1567, (分離)
Sorensen, J.S. et al., Acta Chem. Scand., 1954, 8, 26, (分離)
Gardner, J.N. et al., J.C.S., 1960, 691, (分離)
Bohlmann, F. et al., Chem. Ber., 1962, 95, 1742; 1973, 106, 1328, (分離, 構造決定, 合成法)
Hodge, P. et al., J.C.S. (C), 1966, 1216, (成書)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 770
Greger, H., Phytochemistry, 1978, 17, 86; 1982, 21, 1071, (分離, 構造)
Bohlmann, F. et al., Phytochemistry, 1979, 18, 1736; 1980, 19, 841; 2655, (分離)
Japan. Pat., 1991, 03 287532; CA, 116, 181120w, (分離)
Lu, T. et al., Phytochemistry, 1993, 32, 1483, (結晶構造)

*****ミルラ (Myrrh) *****

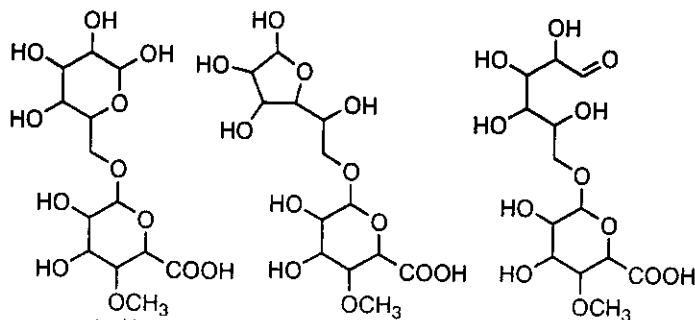
§ § カンラン科モツヤクジュ (*Commiphora myrrha* (Nees) Engler) の樹脂。

§ Acaciabiuronic acid; 4'-Me

[化学名・別名] 6-O-(4-O-Methyl-β-D-glucuronopyranuronosyl)-D-galactose (CAS 名) (旧 CAS 名)

[化学名・別名] 6-O-(4-O-Methyl-β-D-glucuronopyranuronosyl)-D-galactose (CAS名) (旧CAS名)
 [CAS No.] 13006-41-2
 [化合物分類] 炭水化物 (Glycuronic acids), 炭水化物 (Disaccharides)
 [構造式]

[分子式] C₁₃H₂₂O₁₂
 [分子量] 370.31
 [基原] Structural unit in plant gums, 例えば, *Prosopis juliflora*, *Commiphora myrrha*, *Boswellia carteri*
 [比旋光度]: [α]_D -1 (H₂O)



-----文献-----

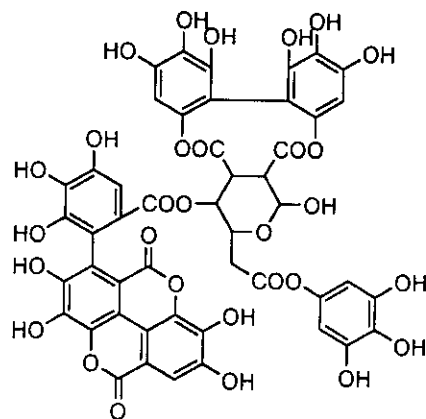
Hotchkiss, R.D. et al., J. Biol. Chem., 1936, 115, 285, (誘導體)
 Goebel, W.F. et al., J. Biol. Chem., 1938, 124, 207, (分離)
 Jackson, J. et al., J.C.S., 1940, 74, (α-Me pyr hexa-Me Me ester, 分離)
 Aspinall, G.O. et al., J.C.S., 1955, 1160; 1961, 3461, (分離)
 Mukherjee, S. et al., J.A.C.S., 1958, 80, 2536, (分離)
 Jones, J.K.N. et al., Can. J. Chem., 1961, 39, 162, (分離)
 Peciar, C. et al., Chem. Zvesti, 1974, 28, 83, (構造, H-NMR)
 Di Fabio, J.L. et al., Carbohydr. Res., 1982, 99, 41, (分離)

*****ミロバラン (Myrobalan) *****

§ § シクンシ科ミロバラン (*Terminalia chebula* Retzius) の果実。

§ Calamansanin; 1-O-Degalloyl

[化学名・別名] Terflavin A
 [CAS No.] 103744-85-0
 [化合物分類] タニン化合物 (Hexahydroxydiphenoyl ester tannins), タニン化合物 (Flavogallonoyl dilactone tannins)
 [構造式]



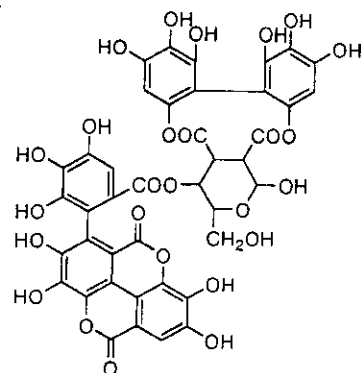
[分子式] C₄₈H₃₀O₃₁
 [分子量] 1086.747
 [基原] 次の植物から分離: *Terminalia catappa* の葉, *Terminalia chebula* の果実
 [性状] 青白い黄色の結晶粉末・四水和物 (H₂O)
 [融点] Mp 258 °C で分解
 [比旋光度]: [α]_D²⁰ +240.6 (c, 1.0 in MeOH)
 [その他のデータ] Equilibrated mixt. of anomers

-----文献-----

Tanaka, T. et al., Chem. Pharm. Bull., 1986, 34, 1039; 1991, 39, 60, (構造決定, H-NMR, C13-NMR)
 Liu, T.-C. et al., Chem. Pharm. Bull., 1990, 38, 3004, (Terflavins)

§ Calamansanin; 1,6-Bis-O-degalloyl

[化学名・別名] Terflavin C
 [CAS No.] 103744-92-9
 [化合物分類] タニン化合物 (Hexahydroxydiphenoyl ester tannins), タニン化合物 (Flavogallonoyl dilactone tannins)
 [構造式]
 [分子式] C₄₁H₂₆O₂₆
 [分子量] 934.641



[性状] 青白い黄色の結晶粉末・二水和物 (Me:CO 溶液)

[融点] Mp 225-227 °C

[比旋光度]: $[\alpha]_D^{22} +32.6$ (c, 1.2 in MeOH)

[その他のデータ] Equilibrated mixt. of anomers

-----文献-----

Tanaka, T. et al., Chem. Pharm. Bull., 1986, 34, 1039; 1991, 39, 60, (構造決定, H-NMR, C13-NMR)

Liu, T.-C. et al., Chem. Pharm. Bull., 1990, 38, 3004, (Terflavins)

§ Chebulagic acid

[CAS No.] 23094-71-5

[化合物分類] 薬物: 抗 HIV 薬 (Anti-HIV agents), 薬物: 抗ウイルス物質 (Antiviral agents), タンニン化合物 (Chebuloyl esters)

[構造式]

[分子式] $C_{41}H_{30}O_{27}$

[分子量] 654.672

[基原] 次の植物から誘導されたタンニン: divi-divi *Caesalpinia coriaria* の果実), myrobalans (*Terminalia chebula* 果実), *Geranium* spp. に存在

[用途] 抗 HIV 活性を示す. Potent DNA topoisomerase inhibitor

[性状] 斜方晶形・十水和物

[融点] Mp 240 °C で分解

[比旋光度]: $[\alpha]_D^{20} -57$ (H:O)

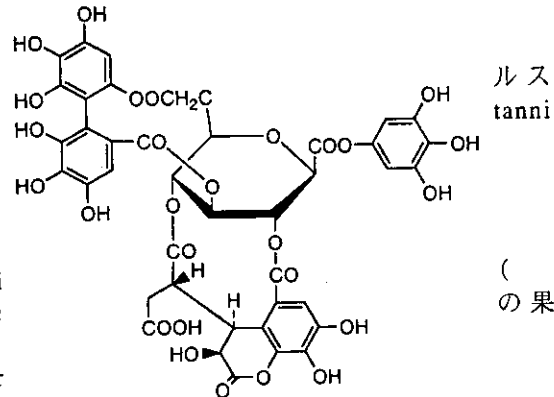
[Log P 計算値] Log P -1.2 (未確認値) (計算値)

-----文献-----

Haslam, E. et al., J.C.S. (C), 1967, 2381, (分離)

Yoshida, T. et al., Chem. Pharm. Bull., 1980, 28, 3713; 1982, 30, 2655, (構造決定, 絶対構造)

Hecht, S.M. et al., J. Nat. Prod., 1992, 55, 401, (薬理)



§ Chebulinic acid

[化学名・別名] Eutannin

[CAS No.] 18942-26-2

[化合物分類] タンニン化合物 (Chebuloyl ester tannins), 薬物: 抗 HIV 薬 (Anti-HIV agents), 薬物: 抗ウイルス物質 (Antiviral agents)

[構造式]

[分子式] $C_{41}H_{30}O_{27}$

[分子量] 956.688

[基原] 次の植物から誘導されたタンニン: divi-divi *Caesalpinia coriaria* の果実), myrobalans (*Terminalia ulia* の果実). Also obtainable from *Geranium thunbergii* the seeds of sal (*Shorea robusta*)

[用途] 抗 HIV 活性を示す

[性状] 針状結晶 (H:O)

[融点] Mp 234 °C

[比旋光度]: $[\alpha]_D^{20} -65.1$ (c, 1.0 in Me:CO)

[Log P 計算値] Log P -0.61 (未確認値) (計算値)

-----文献-----

Haslam, E. et al., J.C.S. (C), 1967, 2381, (分離, Mass)

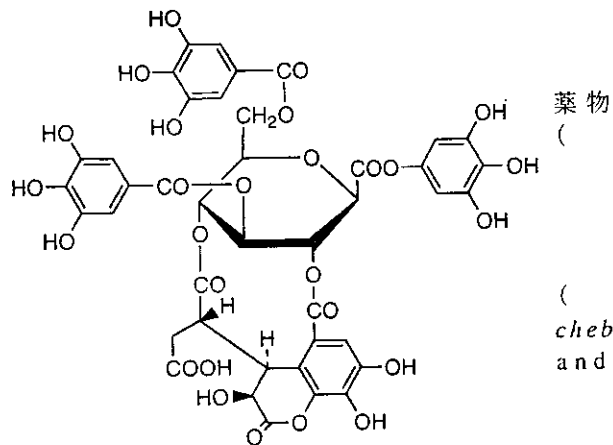
Yoshida, T. et al., Chem. Pharm. Bull., 1980, 28, 3713; 1982, 30, 2655, (構造決定, 絶対構造)

Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2535, (H-NMR, C13-NMR)

Weaver, J.L. et al., Biochem. Pharmacol., 1992, 43, 2479, (薬理)

Japan. Pat., 1995, 95 138 165; CA, 123, 152874j, (Chebularin)

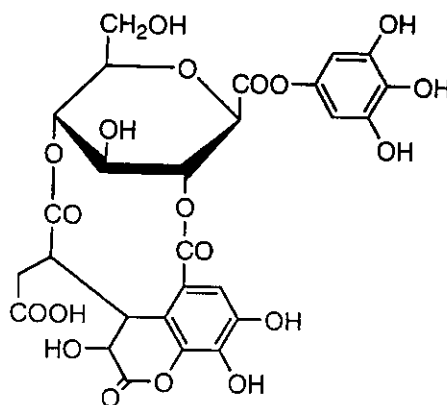
Liu, Y.Z. et al., Chin. Chem. Lett., 1998, 9, 827-828, (Terminalic acid)



§ Chebulinic acid; 3,6-Bis-O-degalloyl

[化学名・別名] Chebularin, Terminalic acid ‡

[化学名・別名] Chebulanin. Terminalic acid †
 [CAS No.] 166833-80-3
 [化合物分類] タンニン化合物 (Chebuloyl ester tannins)
 [構造式]



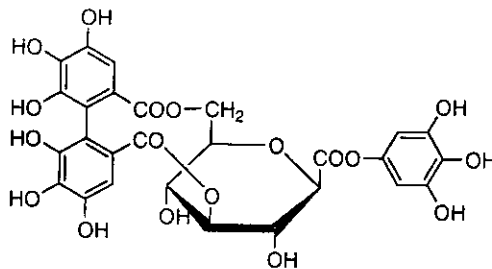
[分子式] $C_{27}H_{24}O_{16}$
 [分子量] 652.475
 [基原] *Terminalia chebula*
 [用途] Topoisomerase I 阻害因子
 [性状] 粉末
 [比旋光度]: $[\alpha]_D +9.1$ (MeOH)
 UV: [neutral] λ_{max} 221 (ϵ 42660) (溶媒の報告はない)

-----文献-----

Haslam, E. et al., J.C.S. (C), 1967, 2381, (分離, Mass)
 Yoshida, T. et al., Chem. Pharm. Bull., 1980, 28, 3713; 1982, 30, 2655, (構造決定, 絶対構造)
 Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2535, (H-NMR, C13-NMR)
 Nonaka, G., J. Nat. Prod., 1990, 53, 587, (anti-HIV activity)
 Weaver, J.L. et al., Biochem. Pharmacol., 1992, 43, 2479, (薬理)
 Japan. Pat., 1995, 95 138 165; CA, 123, 152874j, (Chebulanin)
 Liu, Y.Z. et al., Chin. Chem. Lett., 1998, 9, 827-828, (Terminalic acid)

§ Corilagin

[化学名・別名] 1-O-Galloyl-3,6-(R)-hexahydroxydiphenoyl- β -D-glucopyranose
 [CAS No.] 23094-69-1
 [化合物分類] タンニン化合物 (Hexahydroxydiphenoyl ester tannins)
 [構造式]



[分子式] $C_{27}H_{22}O_{16}$
 [分子量] 634.46
 [基原] 次の植物から分離: *Rhus* spp. の葉, *Eucalyptus* spp., *Angeissus latifolia*. また *Caesalpinia coriaria*, *Terminalia chebula*, *Schinopsis* spp., その他の植物からも得られる
 [性状] 針状結晶 (H₂O)

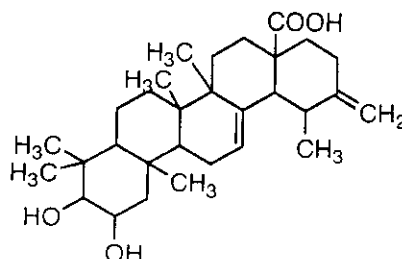
[融点] Mp 208 °C
 [比旋光度]: $[\alpha]_D^{20} -250$ (c, 0.3 in MeOH)
 [溶解性] BERDY SOL: Sol. H₂O
 UV: [base] λ_{max} 240 (ϵ); 326 (ϵ) (MeOH/NaOH) (Derep) [neutral] λ_{max} 220 (ϵ); 274 (ϵ) (MeOH) (Derep) [neutral] λ_{max} 218 (ϵ 16600); 270 (ϵ 14100) (MeOH) (Berdy) [neutral] λ_{max} 220; 274 (EtOH) (Berdy) [acid] λ_{max} 240; 326 (MeOH-HCl) (Berdy)

-----文献-----

Schmidt, O.T. et al., Annalen, 1951, 571, 232, (分離)
 Reddy, K.K. et al., Aust. J. Chem., 1964, 17, 238, (分離, 成書)
 Matsuda, H. et al., Chem. Pharm. Bull., 1966, 14, 877, (分離, UV)
 Seikel, M. et al., Phytochemistry, 1970, 9, 1115, (H-NMR, 構造)
 Nawwar, M.A.M. et al., Phytochemistry, 1994, 36, 793-798, (分離, H-NMR, C13-NMR)
 Latte, K.P. et al., Phytochemistry, 2000, 54, 701-708. (Isocorilagin)

§ 2,3-Dihydroxy-12,20(30)-ursadien-28-oic acid; (2 α ,3 β)-form

[化学名・別名] 2 α -Hydroxymicromeric acid
 [化合物分類] テルペノイド (Ursane triterpenoids)
 [構造式]



[分子式] $C_{30}H_{48}O_5$
 [分子量] 470.691

-----文献-----

- Kojima, H. et al., *Phytochemistry*, 1987, 26, 1107
Singh, C., *Phytochemistry*, 1990, 29, 2348, (分離, H-NMR, C13-NMR)
Lee, C.-K. et al., *Phytochemistry*, 1998, 49, 1119-1122, (3-hydroxycinnamoyl)
Sanoko, R. et al., *Phytochemistry*, 1999, 51, 1043-1047, (*Alternanthera repens* saponins)

§ Luteolic acid

[化学名・別名] 3,4,8,9,10-Pentahydroxy-6-oxo-6H-dibenzo[b,d]pyran-1-carboxylic acid (CAS名). Luteic acid

[CAS No.] 476-67-5

[化合物分類] 単環芳香族 (Dibenzo[b,d]pyrans)

[構造式]

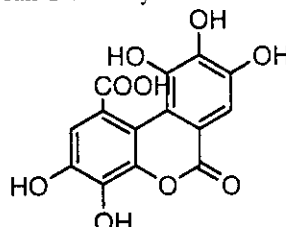
[分子式] $C_{15}H_8O_9$

[分子量] 320.212

[基原] 次の植物から分離: *Terminalia chebula* の果実

[性状] 赤みを帯びた針状結晶 (AcOH)

[融点] Mp 338-342 °C で分解



-----文献-----

- Nierenstein, M., *Ber.*, 1908, 41, 3015; 1909, 42, 353
Ishii, M., *CA*, 1951, 45, 2698, (配糖体)

§ 12-Oleanene-2,3,19,23,28-pentol; (2 α , 3 β , 19 α)-form

[化学名・別名] Chebupentol

[CAS No.] 143086-38-8

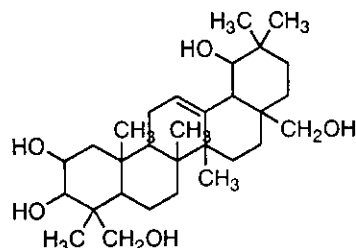
[化合物分類] テルペノイド (Oleanane triterpenoids)

[構造式]

[分子式] $C_{30}H_{50}O_5$

[分子量] 490.722

[基原] *Terminalia chebula*



-----文献-----

- Lu, P. et al., *Zhiwu Xuebao*, 1992, 34, 126; *CA*, 117, 108120n, (分離, H-NMR, C13-NMR)

§ Terchebin

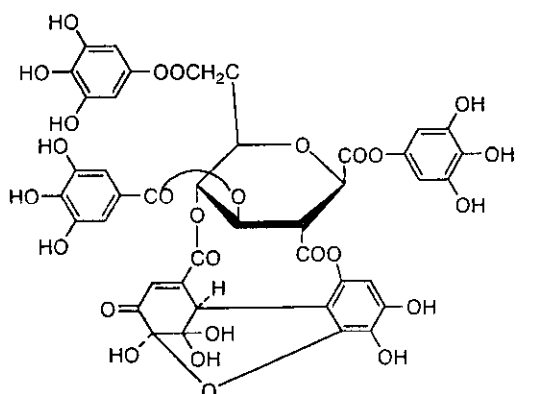
[CAS No.] 20598-45-2

[その他の CAS No.] 148077-28-5

[化合物分類] タンニン化合物

Dehydrohexahydroxydiphenoyl ester tannins)

[構造式]



[分子式] $C_{41}H_{30}O_{27}$

[分子量] 954.672

[一般的性質] 構造式は不明. Prob. in equilib. with an
ric struct.

[基原] 次の植物から分離: *Terminalia chebula* の果実, *Mallotus japonicus* の樹皮

[性状] やや緑がかった黄色のプリズム結晶・十水和物

[比旋光度]: $[\alpha]_D^{25} -39.4$ (c, 2 in EtOH)

[その他のデータ] Forms trihydrate on intensive drying

isome

-----文献-----

- Schmidt, O.T. et al., *Annalen*, 1967, 706, 169, (分離)
Okuda, T. et al., *Tet. Lett.*, 1980, 21, 4361, (構造決定)
Karl, C. et al., *Z. Naturforsch., C*, 1983, 38, 13, (構造決定, H-NMR)
Lin, J.-H. et al., *Chem. Pharm. Bull.*, 1990, 38, 1844, (3-Desgalloylterchebin)

§ Terchebulin

§ Terchebulin

[CAS No.] 132854-40-1

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

[構造式]

[分子式] $C_{48}H_{28}O_{50}$

[分子量] 1084.731

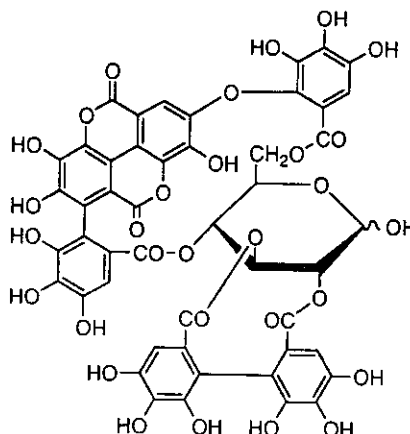
[一般的性質] 等量の α -, β -anomer の混合物として存在

[基原] 次の植物から分離されたタンニン: *Terminalia chebula* の果実

[性状] 褐色の結晶粉末・八水和物 (H₂O)

[融点] Mp 222-224 °C

[比旋光度]: $[\alpha]_D^{25} -136.2$ (c, 1.5 in MeOH)



----- 文献 -----

Lin, T.-C. et al., Chem. Pharm. Bull., 1990, 38, 3004-3008, (構造決定, H-NMR, C13-NMR)

§ Terflavin D

[CAS No.] 132839-27-1

[化合物分類] タンニン化合物 (Flavogallonoyl dilactone tannins)

[構造式]

[分子式] $C_{27}H_{20}O_{18}$

[分子量] 632.444

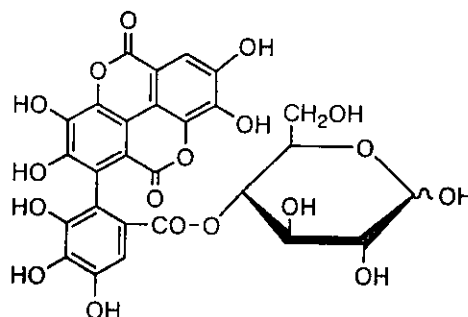
[一般的性質] 等量の α -, β -anomer の混合物として存在

[基原] 次の植物から分離: *Terminalia chebula* の葉

[性状] 青白い黄色の結晶粉末・五水和物 (Me₂CO)

[融点] Mp 215-218 °C で分解

[比旋光度]: $[\alpha]_D^{25} +11.2$ (c, 1.0 in 50% Me₂CO 溶液)



----- 文献 -----

Tanaka, T. et al., Chem. Pharm. Bull., 1986, 34, 1039, (構造決定, H-NMR, C13-NMR)

Lin, T.-C. et al., Chem. Pharm. Bull., 1990, 38, 3004, (構造決定, H-NMR, C13-NMR)

§ Terflavin D; 6'-O-(3,4,5-Trihydroxybenzoyl)

[化学名・別名] Terflavin B

[CAS No.] 103744-86-1

[化合物分類] タンニン化合物 (Flavogallonoyl dilactone tannins)

[構造式]

[分子式] $C_{33}H_{24}O_{22}$

[分子量] 784.55

[基原] 次の植物の葉から分離:

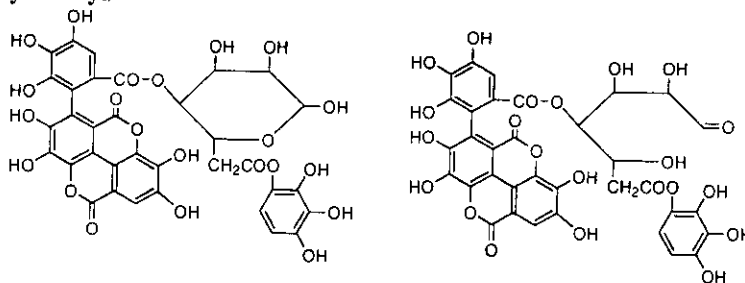
Terminalia catappa, *Terminalia chebula*

[性状] 青白い黄色の結晶粉末 + 4·1/2H₂O (Me₂CO 溶液)

[融点] Mp 232 °C で分解

[比旋光度]: $[\alpha]_D^{19} +178.2$ (c, 0.9 in MeOH)

[その他のデータ] アノマーの混合物



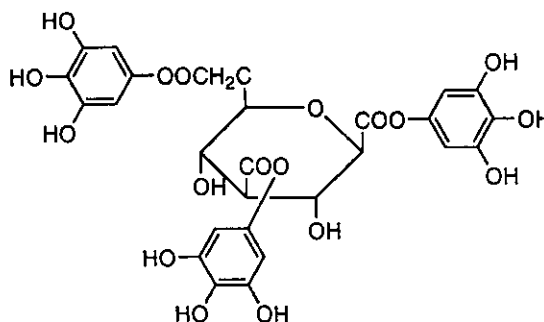
----- 文献 -----

Tanaka, T. et al., Chem. Pharm. Bull., 1986, 34, 1039, (構造決定, H-NMR, C13-NMR)

Lin, T.-C. et al., Chem. Pharm. Bull., 1990, 38, 3004, (構造決定, H-NMR, C13-NMR)

§ 1,3,6-Trigalloylglucose; β -D-Pyranose-form

[化合物分類] タンニン化合物 (Simple gallate ester tannins)
[構造式]



[分子式] $C_{27}H_{18}O_{18}$

[分子量] 636.476

[基原] 次の植物から分離: *Terminalia chebula* の果実

[性状] 灰白色の無定型粉末・三水和物

[比旋光度]: $[\alpha]_D^{25} +29$ (c, 3.0 in EtOH)

-----文献-----

Schmidt, O.T. et al., *Annalen*, 1967, 706, 169, (構造決定)

Haddock, E.A. et al., *J.C.S. Perkin 1*, 1982, 2515, (H-NMR, C13-NMR)

*****ムカゴニンジン (Skirret) *****

§ § セリ科ムカゴニンジン (*Sium sisarum* L.) の葉、茎または根。

§ 1,9-Heptadecadiene-4,6-diyne-3-one; (Z)-form

[化学名・別名] Falcarinone

[CAS No.] 4117-11-7

[化合物分類] 脂肪族化合物 (Miscellaneous acetylenes)

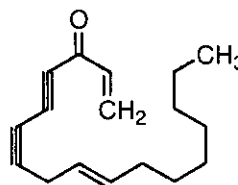
[構造式]

[分子式] $C_{17}H_{22}O$

[分子量] 242.36

[基原] 次の植物から分離: *Falcaria vulgaris*, *Oenanthe* spp. *Sium sisarum*, *Chaerophyllum temulum*, *Eryngium planum*, *Galinsoga paviflora*, *Hedera helix* 等

[性状] 青白い黄色のオイル



-----文献-----

Bohlmann, F. et al., *Chem. Ber.*, 1961, 94, 958; 1962, 95, 1320; 1965, 98, 3010

*****ムギチャ (Roasted barley) *****

§ § イネ科オオムギ (*Hordeum vulgare* L.) の種子 (焙煎)。

「コウジ」参照

§ § イネ科ロクジョウオオムギ (*Hordeum vulgare* L. var. *hexastichon* Aichison) の種子 (焙煎)。

本調査研究では、成分に関する文献はなかった。

§ § イネ科ハダカムギ (*Hordeum vulgare* L. var. *nudum* J. D. Hooker) の種子 (焙煎)。

§ Isovitexin; 7-O-[4-Hydroxy-3-methoxy-E-cinnamoyl-(→6)-β-D-glucopyranoside]

[化学名・別名] 6'''-O-Feruloylsaponarin

[化合物分類] フラボノイド (Flavones; 3 × O-置基)

[構造式]

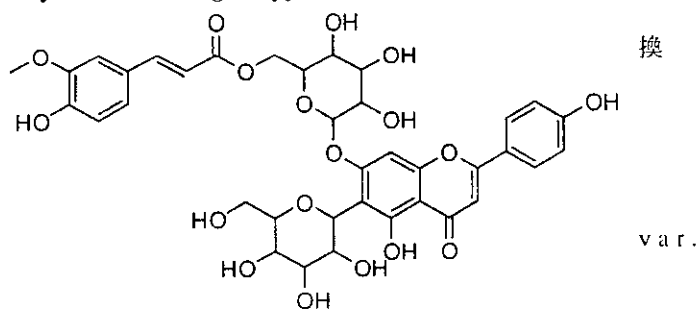
[分子式] $C_{27}H_{30}O_{18}$

[分子量] 770.696

[基原] 若い緑色のオオムギ (*Hordeum vulgare nudum*)

[性状] 無定型の粉末

[比旋光度]: $[\alpha]_D^{25} -141$ (c, 0.5 in MeOH 溶液)



換

var.

[比旋光度]: $[\alpha]_D^{25}$ -141 (c. 0.5 in MeOH 溶液)

-----文献-----

Ohkawa, M. et al., Chem. Pharm. Bull., 1998, 46, 1887, (*Hordeum vulgare* saponarins)

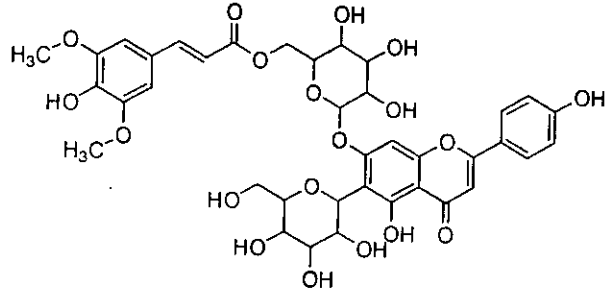
Haribal, M. et al., J. Nat. Prod., 1999, 62, 179, (hydroxydimethoxycinnamoylglucoside)

§ Isovitexin; 7-O-[4-Hydroxy-3,5-dimethoxy-E-cinnamoyl-(→6)-β-D-glucopyranoside]

[化学名・別名] 6'''-O-Sinapoylsaponarin

[化合物分類] フラボノイド (Flavones; 3 × O-置換基)

[構造式]



[分子式] C₃₉H₅₀O₁₉

[分子量] 800.723

[基原] 若い緑色のオオムギ (*Hordeum vulgare* var. *nudum*)

[性状] 無定型の粉末

[比旋光度]: $[\alpha]_D^{25}$ -144 (c. 0.5 in MeOH 溶液)

-----文献-----

Ohkawa, M. et al., Chem. Pharm. Bull., 1998, 46, 1887, (*Hordeum vulgare* saponarins)

Hoerhammer, L. et al., Tet. Lett., 1965, 1707, (*H-NMR*, 構造, Saponarin)

§ Isovitexin; 4',7-Di-O-β-D-glucopyranoside

[化学名・別名] Isovitexin 4',7-diglucoside

[化合物分類] フラボノイド (Flavones; 3 × O-置換基)

[構造式]

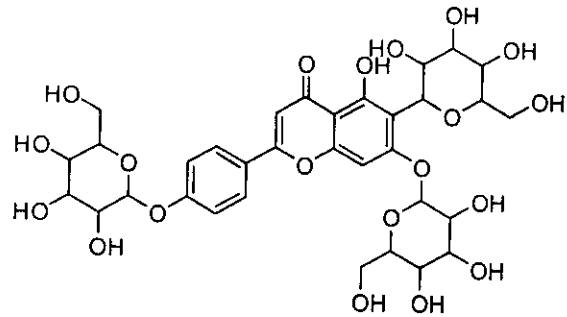
[分子式] C₃₃H₄₀O₂₀

[分子量] 756.667

[基原] 若い緑色のオオムギ (*Hordeum vulgare* var. *nudum*)

[性状] 無定型の塊

[比旋光度]: $[\alpha]_D^{25}$ -51 (c. 0.5 in MeOH)



-----文献-----

Ohkawa, M. et al., Chem. Pharm. Bull., 1998, 46, 1887, (*Hordeum vulgare* saponarins)

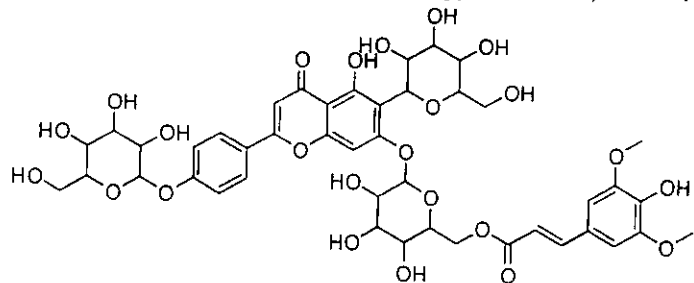
§ Isovitexin; 7-O-[4-Hydroxy-3,5-dimethoxy-E-cinnamoyl-(→6)-glucopyranoside], 4'-O-β-D-glucopyranoside

[CAS No.] 212271-13-1

[化合物分類] フラボノイド (Flavones;

3 × O-置換基)

[構造式]



[分子式] C₃₃H₅₀O₂₄

[分子量] 962.865

[基原] 若い緑色のオオムギ (*Hordeum vulgare* var. *nudum*)

[性状] 無定型の粉末

[比旋光度]: $[\alpha]_D^{25}$ -84 (c. 0.5 in MeOH 溶液)

-----文献-----

Ohkawa, M. et al., Chem. Pharm. Bull., 1998, 46, 1887, (*Hordeum vulgare* saponarins)

*****ムスク (Musk) *****

§ § ジャコウジカ科ジャコウジカ (*Moschus moschiferus* L.) の雄のジャコウ腺分泌物。

§ 3-Hydroxyandrost-4-en-17-one; 3 α-form

[構造式]

[分子式] $C_{19}H_{25}O_2$

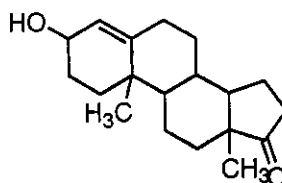
[分子量] 288.429

[基原] ジャコウ (*Moschus moschiferus*)

[性状] 結晶 (Et.O)

[融点] Mp 203-205 °C

[比旋光度]: $[\alpha]_D^{26} +230$ (c, 1.27 in $CHCl_3$)



-----文献-----

Sokolov, V.E. et al., J. Chem. Ecol., 1987, 13, 71-83, (分離)

§ Muscopyridine; (R)-form

[CAS No.] 501-08-6

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

[構造式]

[分子式] $C_{16}H_{23}N$

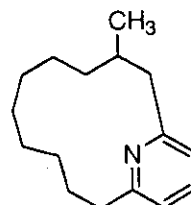
[分子量] 231.38

[基原] 次の植物から得られるアルカロイド: the scent gland of ジャコウジカ (*Moschus moschiferus*)

[性状] 液体

[沸点] Bp₁₂ 155-160 °C

[比旋光度]: $[\alpha]_D^{23} +17.4$ (c, 1.92 in $CHCl_3$)



-----文献-----

Schinz, H. et al., Helv. Chim. Acta, 1946, 29, 1524, (分離, UV)

Yu, D. et al., Planta Med., 1983, 49, 183, (Hydroxymuscopyridines)

§ Muscopyridine; (R)-form, 11-Hydroxy

[化学名・別名] Hydroxymuscopyridine A

[CAS No.] 89368-39-8

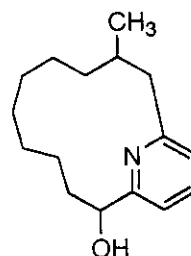
[化合物分類] アルカロイド化合物 (Miscellaneous pyridine alkaloids)

[構造式]

[分子式] $C_{16}H_{23}NO$

[分子量] 247.38

[基原] 次の植物から得られるアルカロイド: *Moschus moschiferus*



-----文献-----

Yu, D. et al., Planta Med., 1983, 49, 183, (Hydroxymuscopyridines)

§ Muscopyridine; (R)-form, 2-Hydroxy

[化学名・別名] Hydroxymuscopyridine B

[CAS No.] 89368-40-1

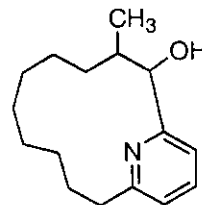
[化合物分類] アルカロイド化合物 (Miscellaneous pyridine alkaloids)

[構造式]

[分子式] $C_{16}H_{23}NO$

[分子量] 247.38

[基原] 次の植物から得られるアルカロイド: *Moschus moschiferus*



-----文献-----

Yu, D. et al., Planta Med., 1983, 49, 183, (Hydroxymuscopyridines)

*****ムラサキ (Murasaki, Gromwell) *****

§ § ムラサキ科ムラサキ (*Lithospermum officinale* L.) の葉または根茎。

§ 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione: (R)

m

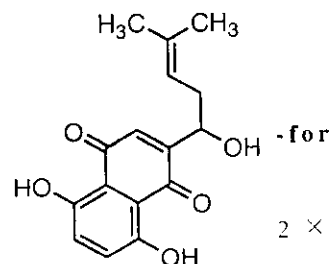
[CAS No.] 517-89-5

[化合物分類] 薬物: 抗菌性剤 (Antibacterial agents), 多環芳香族 (Naphthoquinones;

O-置換基)

[構造式]

[分子式] $C_{16}H_{16}O_5$



2 ×

[構造式]

[分子式] C₁₆H₁₆O₅

[分子量] 288.299

[基原] 次の植物から分離: *Lithospermum erythrorhizon*, *Lithospermum officinale*, *Lithospermum euchromum*, *Arnebia nobilis*, *Arnebia tibetana*

[用途] 抗菌性剤

[性状] 赤-茶色の結晶 (C₆H₆)

[融点] Mp 148 °C (143 °C)

[比旋光度]: [α]_D²⁰ +135 (C₆H₆)

[Log P 計算値] Log P 1.84 (計算値)

UV: [base] λ_{max} (溶媒は報告されていない) (Derep) [neutral] λ_{max} 276 (ε 20000); 488 (ε 1200); 525 (ε 8700); 563 (ε 5900) (MeOH) (Derep)

[その他のデータ] Component of Tokyo violet

[傷害・毒性] 50%致死量(LD₅₀) (マウス, 経口) >1000 mg/kg; 50%致死量(LD₅₀) (マウス, 腹膜内) 20 mg/kg

[化学物質毒性データ総覧(RTECS)登録番号] QL8000200

-----文献-----

Raudnitz, H. et al., Ber., 1934, 67, 1955; 1935, 68, 1479, (分離, 構造)

Brockmann, H., Annalen, 1935, 521, 1, (分離, 構造)

Arakawa, H. et al., Chem. Ind. (London), 1961, 947, (絶対構造)

Morimoto, I. et al., Tet. Lett., 1965, 3677; 4737; 1966, 3677, (分離, 誘導体)

Shcherbanovskii, L.R. et al., Khim. Prir. Soedin., 1971, 7, 517; Chem. Nat. Compd. (Engl. Transl.), 1971, 7, 491, (分離)

Shukla, Y.N. et al., Phytochemistry, 1971, 10, 1909, (分離, Arnebins)

Afzal, M. et al., J.C.S. Perkin 1, 1975, 1334, (分離)

Inouye, H. et al., Phytochemistry, 1979; 18, 1301, (合成)

Papageorgiou, V.P. et al., Planta Med., 1979, 35, 56, (分離, 構造決定, 用途)

Papageorgiou, V.P. et al., Angew. Chem., Int. Ed., 1999, 38, 271-300, (レビュー)

***RTECS (化学物質毒性データ) ***

生体影響物質 : 医薬品.

健康障害に関するデータ

急性毒性に関するデータ

<<試験方法>> LD50 試験(50%致死量試験).

曝露経路 : 腹腔内投与.

被験動物 : げっ歯類-マウス.

投与量・期間 : 20 mg/kg

毒性影響 : [行動] 活動度の変化(特定の試験).

[行動] 運動失調.

参照文献

Nippon Yakurigaku Zasshi. Japanese Journal of Pharmacology. 73,193,1977

§ Lithosenine

[CAS No.] 159903-58-9

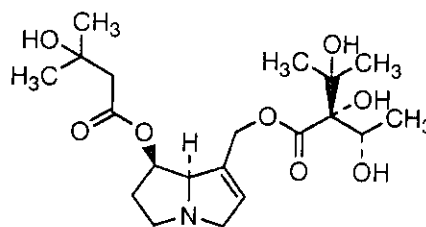
[化合物分類] アルカロイド化合物(Simple pyrrolizidine alkaloids)

[構造式]

[分子式] C₂₀H₃₃NO₈

[分子量] 415.483

[基原] 次の植物から得られるアルカロイド: *Lithospermum officinale* の地上部 (ムラサキ科)



-----文献-----

Krenn, L. et al., Phytochemistry, 1994, 37, 275, (Lithosenine, Acetylithosenine)

§ Lithosenine; O²-Ac

[化学名・別名] Acetylithosenine

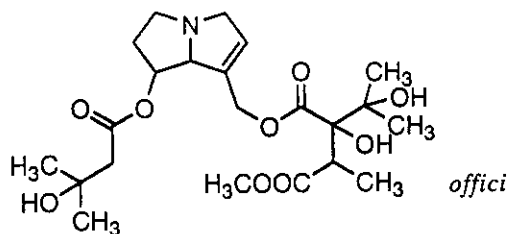
[CAS No.] 159690-29-6

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

[分子式] $C_{22}H_{33}NO_9$

[分子量] 457.52

[基原] 次の植物から得られるアルカロイド: *Lithospermum*
nale の地上部 (ムラサキ科)



-----文献-----

Krenn, L. et al., *Phytochemistry*, 1994, 37, 275, (Lithosenine, Acetyllithosenine)

§ Lithospermic acid A

[化学名・別名] 4-[3-[1-Carboxy-2-(3,4-dihydroxyphenyl) ethoxy]-3-oxo-1-propenyl]-2-(3,4-dihydroxyphenyl)-2,3-dihydro-7-hydroxy-3-benzofurancarboxylic acid (CAS 名). Lithospermic acid

[CAS No.] 28831-65-4

[化合物分類] 薬物: 抗甲状腺薬 (Antithyroid agents), 薬物: 強心剤 (Cardiac stimulants), リグナン化合物 (Neolignans)

[構造式]

[分子式] $C_{27}H_{22}O_{12}$

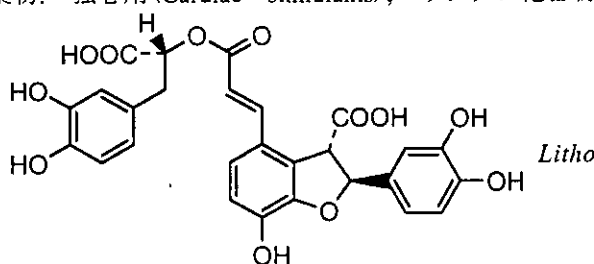
[分子量] 538.464

[基原] *Cynoglossum officinale*, *Lithospermum ruderales* と
spermum officinale の根

[用途] 強心剤, 抗性腺刺激, 抗甲状腺作用を示す

[性状] 無定型の粉末

[Log P 計算値] Log P 1.19 (未確認値) (計算値)



-----文献-----

Kelley, C.J. et al., *J.O.C.*, 1975, 40, 1804; 1976, 41, 449, (分離, 構造決定, C13-NMR)

§ Lithospermoside

[CAS No.] 63492-69-3

[化合物分類] 脂肪酸化合物 (Monocarboxylic alcohols)

[構造式]

[分子式] $C_{13}H_{19}NO_8$

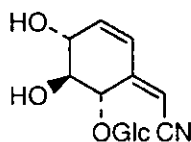
[分子量] 329.306

[基原] *Lithospermum officinale*, *Lithospermum caeruleum*

[性状] 結晶 (MeOH 溶液)

[融点] Mp 278-279 °C

[比旋光度]: $[\alpha]_D^{20} -156$ (c, 0.99 in H₂O)



-----文献-----

Sosa, A. et al., *Phytochemistry*, 1977, 16, 707, (分離, 構造)

Ueda, K. et al., *Chem. Lett.*, 1983, 149, (分離, 構造)

§ 4,8,12,15-Octadecatetraenoic acid (CAS 名)

[CAS No.] 67329-10-6

[関連 CAS No.] 81275-46-9, 106440-10-2

[化合物分類] 脂肪酸化合物 (Unbranched alkenic carboxylic acids and lactones)

[構造式] H₂C=CH:CH=CHCH:CH=CHCH:CH=CHCH:CH=CHCH:CH=CHCH:CH=CH:COOH

[分子式] $C_{18}H_{30}O_2$

[分子量] 276.418

[基原] 次の植物から分離: イワシオイル, *Lithospermum officinale* の種子, *Salpa thomsoni*

[販売元] Sigma:O4252

-----文献-----

Toyama, Y. et al., *Bull. Chem. Soc. Jpn.*, 1935, 10, 232, (分離)

Hörhammer, L. et al., *Arzneim.-Forsch.*, 1964, 14, 34, (分離)

Mimura, T. et al., *Chem. Pharm. Bull.*, 1986, 34, 4562, (分離)

§ 6,9,12,15-Octadecatetraenoic acid: (6Z,9Z,12Z,15Z)-form

[化学名・別名] Stearidonic acid