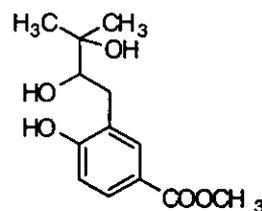


[CAS No.] 117176-70-2
 [化合物分類] 単環芳香族 (Simple benzoic acids and esters)
 [構造式]
 [分子式] $C_{13}H_{16}O_5$
 [分子量] 254.282
 [正確な分子量] 254.115425
 [基原] *Eriodictyon sessilifolium*, *Pandanus odoratissimus*
 [性状] 針状結晶
 [融点] Mp 143-144 °C
 [比旋光度]: $[\alpha]_D^{25} +12$ (c, 0.4 in EtOH)
 [UV]: [neutral] λ_{max} 220 (sh) (); 259 (); 290 (sh) () (溶媒の報告はない)



-----文献-----

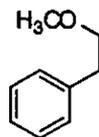
Shima, K. et al., *Yakugaku Zasshi*, 1972, 92, 1410, (分離, 合成法, UV, H-NMR)
 Diaz, D. et al., *Phytochemistry*, 1987, 26, 809, (分離, 誘導體)
 Arriaga-Giner, F.J. et al., *Z. Naturforsch., C*, 1988, 43, 337, (誘導體)
 Abraham, W.F. et al., *Phytochemistry*, 1990, 29, 2641, (分離)
 Venkatasubbaiah, P. et al., *J. Nat. Prod.*, 1991, 54, 1293, (分離, H-NMR, C13-NMR)
 Orjala, J. et al., *Planta Med.*, 1993, 59, 546, (分離, ester)
 Pereda-Miranda, R. et al., *J. Nat. Prod.*, 1997, 60, 282, (esters, 分離, H-NMR, C13-NMR, Mass)
 Terreaux, C. et al., *Phytochemistry*, 1998, 49, 461, (分離, 誘導體)
 Jong, T.-T. et al., *Phytochemistry*, 1998, 49, 2145, (分離, 誘導體)

§ 2-Phenylethanol; Me ether

[化学名・別名] (2-Methoxyethyl) benzene (CAS 名). 1-Methoxy-2-phenylethane. Methyl phenethyl ether.

Kewda ether

[CAS No.] 3558-60-9
 [化合物分類] 単環芳香族 (Phenylacetic acid derivatives)
 [構造式]
 [分子式] $C_9H_{10}O$
 [分子量] 136.193



[正確な分子量] 136.088815
 [基原] 次の植物のオイルから分離: *Tagetes signata*, *Pandanus odoratissimus*
 [性状] 香料, 液体
 [沸点] Bp 189-190 °C. Bp₂₅ 100-105 °C
 [化学物質毒性データ総覧 (RTECS) 登録番号] KO2230000

-----文献-----

C.Djerassi et al., *Dictionary of Natural Products*, Chapman, Hall, 2002
 Chopra, M.M. et al., *Perfum. Essent. Oil Res.*, 1963, 54, 238; *CA*, 59, 3714, (分離, 誘導體)
 Abramovitch, R.A. et al., *Can. J. Chem.*, 1966, 44, 2913, (分離)
 Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhauser Verlag, Basel, 1972, no. 251, (生育)
 Kozawa, M. et al., *Chem. Pharm. Bull.*, 1983, 31, 2712, (Phenethyl ferulate)

RTECS (化学物質毒性データ)

生体影響物質 : 天然物. 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>> 標準ドライブ試験.

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 : 500 mg/24 時間
 反応の症度 : 中等度.
 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-)] 20,807,1982

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 : 4100 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-)]20,807,1982

<<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 : 3970 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-)]20,807,1982

米国に於ける状況

EPA TSCA Section 8(b) CHEMICAL INVENTORY

*****バンレイシ (Sugar apple, Sweet sop) *****

§ § バンレイシ科バンレイシ (*Annona squamosa* L.) の果実.

§ Annonacin; 20-Epimer

[化学名・別名] Annonacin A. Annonacin 2

[CAS No.] 130853-76-8

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{35}H_{64}O_7$

[分子量] 596.886

[正確な分子量] 596.465205

[基原] 次の植物から分離: *Annona squamosa*

[性状] 無定型

[比旋光度]: $[\alpha]_D^{25} +23.8$ (c, 0.4 in $CHCl_3$)

[その他のデータ] C-4 と C-10 の立体化学は確定していない

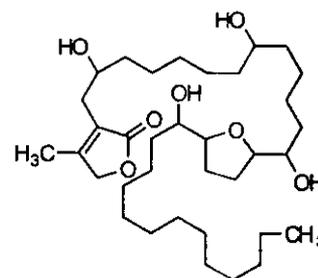
-----文献-----

Rieser, M.J. et al., J. Nat. Prod., 1996, 59, 100, (*cis*-Annonacins)

Ye, Q. et al., Nat. Prod. Lett., 1996, 8, 291, (4-Acetylannonacin)

Zeng, L. et al., Nat. Prod. Rep., 1996, 13, 275, (レビュー)

Cave, A. et al., Prog. Chem. Org. Nat. Prod., 1997, 70, 81, (レビュー)



§ Annonin XIV

[CAS No.] 129138-52-9

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_8$

[分子量] 638.924

[正確な分子量] 638.47577

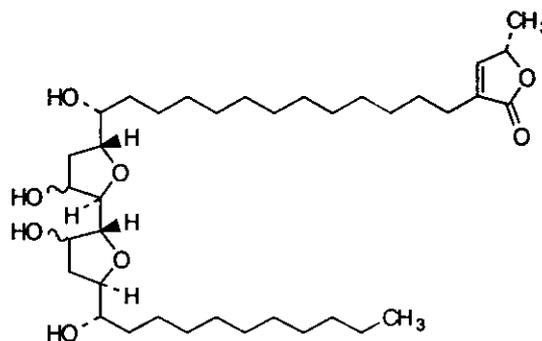
[一般的性質] 不正確な構造式が割り当てられている

[基原] *Annona squamosa*

[性状] 無定型のワックス

[比旋光度]: $[\alpha]_D^{25} +15.7$ (c, 0.3 in CH_2Cl_2)

-----文献-----



Nonfon, M. et al., *Phytochemistry*, 1990, 29, 1951, (分離, H-NMR, C13-NMR, Mass)

§ **Annorecticuin; 9-Ketone, stereoisomer (1)**

[化学名・別名] Mosin B

[CAS No.] 191876-89-8

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{35}H_{62}O_7$

[分子量] 594.871

[正確な分子量] 594.449555

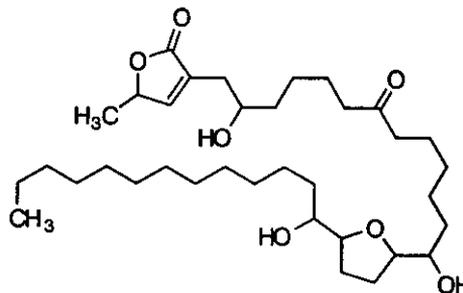
[基原] *Annona squamosa*

[用途] 細胞毒作用

[性状] ワックス様の塊

[比旋光度]: $[\alpha]_D^{23} +11.5$ (c, 0.005 in CH_2Cl_2)

[UV]: [neutral] λ_{max} 222 (log ϵ 3.57) (MeOH)



-----文献-----

Hopp, D.C. et al., *J. Nat. Prod.*, 1997, 60, 581, (Mosins, Annorecticuin-9-one)

§ **Annorecticuin; 9-Ketone, stereoisomer (2)**

[化学名・別名] Mosin C

[CAS No.] 191936-12-6

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{35}H_{62}O_7$

[分子量] 594.871

[正確な分子量] 594.449555

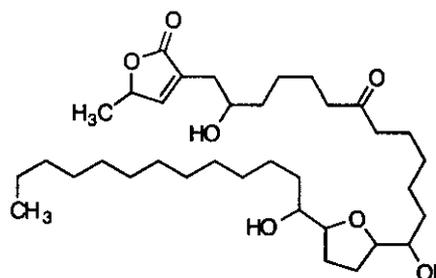
[基原] *Annona squamosa*

[用途] 細胞毒作用

[性状] ワックス様の塊

[比旋光度]: $[\alpha]_D^{23} -2.7$ (c, 0.007 in CH_2Cl_2)

[UV]: [neutral] λ_{max} 216 (log ϵ 3.56) (MeOH)



-----文献-----

Hopp, D.C. et al., *J. Nat. Prod.*, 1997, 60, 581, (Mosins, Annorecticuin-9-one)

§ **Annorecticuin; 4-Deoxy**

[化学名・別名] 4-Deoxyannorecticuin

[CAS No.] 206192-79-2

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{33}H_{56}O_6$

[分子量] 580.887

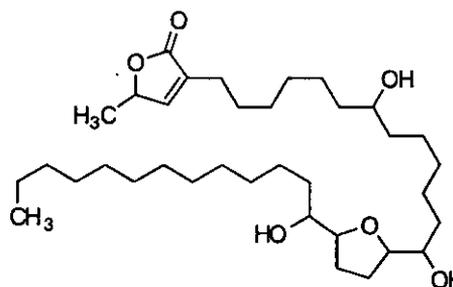
[正確な分子量] 580.47029

[基原] *Annona squamosa*

[性状] 無定形の粉末

[比旋光度]: $[\alpha]_D^{23} +6.8$ (c, 0.03 in CH_2Cl_2)

[UV]: [neutral] λ_{max} 215 (log ϵ 3.5) (MeOH) [neutral] λ_{max} 218 (ϵ 3162) (MeOH)



-----文献-----

Hopp, D.C. et al., *Phytochemistry*, 1998, 47, 803, (4-Deoxyannorecticuin)

§ Annoreticuin; 4-Deoxy, 19,20-diepimer

[化学名・別名] cis -4-Deoxyannoreticuin

[CAS No.] 206192-80-5

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{35}H_{64}O_6$

[分子量] 580.887

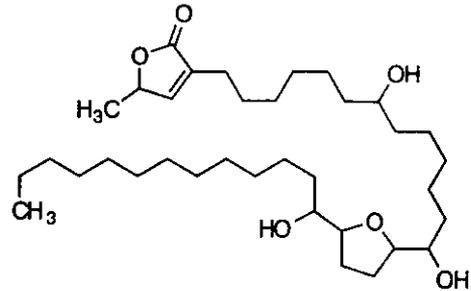
[正確な分子量] 580.47029

[基原] *Annona squamosa*

[性状] 無定型の粉末

[比旋光度]: $[\alpha]_D^{23} +6.8$ (c, 0.01 in CH_2Cl_2)

[UV]: [neutral] λ_{max} 218 (log ϵ 3.61) (MeOH) [neutral] λ_{max} 218 (ϵ 4070) (MeOH)



-----文献-----

Hopp, D.C. et al., *Phytochemistry*, 1998, 47, 803, (4-Deoxyannoreticuin)

§ Annosquamosin A

[CAS No.] 192584-48-8

[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)

[構造式]

[分子式] $C_{39}H_{60}N_8O_{11}S$

[分子量] 849.016

[正確な分子量] 848.410227

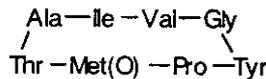
[一般的性質] 環状ペプチド

[基原] *Annona squamosa* の種子

[性状] 針状結晶 (MeOH)

[融点] Mp 215-216 °C

[比旋光度]: $[\alpha]_D^{24} -65.3$ (c, 0.4 in MeOH)



-----文献-----

Chao-Ming, L. et al., *Phytochemistry*, 1997, 45, 521, (分離, IR, H-NMR, C13-NMR, Mass)

§ Armepavine; (S)-form, Me ether

[化学名・別名] (+)-O-Methylarmepavine

[CAS No.] 3423-02-7

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

[構造式]

[分子式] $C_{20}H_{25}NO_3$

[分子量] 327.422

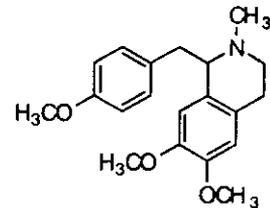
[正確な分子量] 327.183444

[基原] 次の植物から得られるアルカロイド: *Annona squamosa*, *Magnolia acuminata* (パンレイシ科, モクレン科)

[性状] 結晶 (petrol)

[融点] Mp 60-62 °C

[比旋光度]: $[\alpha]_D^{20} +85$



-----文献-----

C.Djerassi et al., *Dictionary of Natural Products*, Chapman, Hall, 2002

Kupchan, S.M. et al., *Tetrahedron*, 1963, 19, 227, (分離, UV, IR, H-NMR, 構造決定, Norarmepavine)

Yang, T.H. et al., *Yakugaku Zasshi*, 1963, 83, 22; *CA*, 59, 3974d, (分離, UV, IR, 構造決定, Norarmepavine)

Kapadia, G.J. et al., *J. Pharm. Sci.*, 1964, 53, 1140, (誘導体, 分離, H-NMR, 構造決定)

Bishay, D.W. et al., *Phytochemistry*, 1973, 12, 693, (分離, UV, IR, H-NMR, Mass)

Torres, R. et al., *J. Nat. Prod.*, 1979, 42, 430, (誘導体, 分離, UV, IR, H-NMR, Mass)

Bhaumik, P.K. et al., *Phytochemistry*, 1979, 18, 1584, (誘導体, 分離, UV, H-NMR)

Marek, R. et al., *Coll. Czech. Chem. Comm.*, 1997, 62, 1623, (分離, H-NMR, N-15 nmr, 結晶構造)

§ Asimicin

[化学名・別名] 3-[2,13-Dihydroxy-13-[octahydro-5'-(1-hydroxyundecyl) [2,2'-bifuran]-5-yl] tridecyl]-5-methyl-2(5H)-furanone (CAS 名). Annonastatin. Squamocin H.

Annonareticin

[関連 CAS No.] 123805-39-0, 129138-51-8, 130851-93-3

[化合物分類] 薬物: 抗腫瘍薬 (Antineoplastic agents), ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_7$

[分子量] 622.924

[正確な分子量] 622.480855

[一般的性質] 絶対構造はまだ完全に確立しておらず。

[基原] 次の植物から分離: *Annona squamosa*, *Annona purpurea*, *Asimina triloba*, *Rollinia mucosa*

[用途] Pesticidal. 強いミトコンドリア NADH 抑制因子: ubiquinone oxidoreductase. 抗腫瘍作用。

Defensive agent against bird predation

[性状] 結晶

[融点] Mp 70-72 °C

[比旋光度]: $[\alpha]_D +21.8$ (c, 0.6 in MeOH)

[UV]: [neutral] λ_{max} 208 (ϵ 14300) (MeOH)

-----文献-----

Lieb, F. et al., *Planta Med.*, 1990, 56, 317, (Annonastatin)

Sahai, M. et al., *Chem. Pharm. Bull.*, 1994, 42, 1163, (Squamocins)

§ Asimicin; 24-Epimer

[化学名・別名] Bullatacin. Rolliniastatin 2. Annonin VI. Squamocin G

[CAS No.] 123123-32-0

[その他の CAS No.] 121917-13-3, 129212-94-8

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_7$

[分子量] 622.924

[正確な分子量] 622.480855

[基原] 次の植物から分離: *Annona bullata*, *Annona squamosa*, *Annona reticulata*, *Rollinia mucosa*

[用途] 殺虫剤. 生体内で抗腫瘍活性を示す. Defensive agent against bird predation

[性状] 結晶 (EtOAc)

[融点] Mp 69-70 °C

[比旋光度]: $[\alpha]_D^{25} +13$ (c, 0.004 in $CHCl_3$). $[\alpha]_D^{27} +5.3$ (c, 0.27 in $CHCl_3$)

[UV]: [neutral] λ_{max} 208 (ϵ 14300) (MeOH) (Derep)

-----文献-----

Pettit, G.R. et al., *Heterocycles*, 1989, 28, 213, (Rolliniastatin 2)

Hui, Y.H. et al., *J. Nat. Prod.*, 1989, 52, 463; 1990, 53, 81, (分離, H-NMR, C13-NMR, Bullatacin)

Li, X.H. et al., *J. Nat. Prod.*, 1990, 53, 81, (Bullatacin)

Rupprecht, J.K. et al., *J. Nat. Prod.*, 1990, 53, 237, (レビュー)

Cortes, D. et al., *Tetrahedron*, 1991, 47, 8195, (Rolliniastatin 2)

Ahmadshahib, K.I. et al., *Life Sci.*, 1993, 53, 1113, (Bullatacin, 薬理)

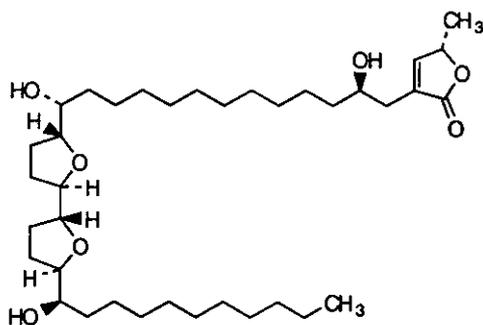
Cortes, D. et al., *Phytochemistry*, 1993, 32, 1467; 1475, (レビュー)

Hoye, T.R. et al., *Tet. Lett.*, 1993, 34, 5043; 1995, 36, 1981, ((-)-Bullatacin, 合成法)

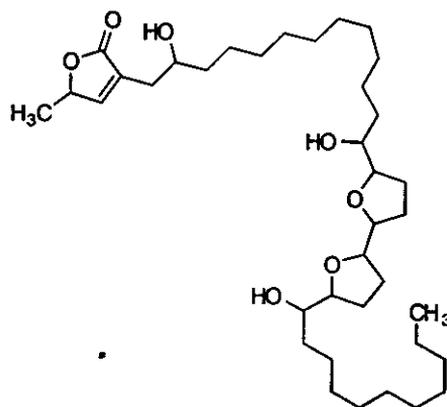
Holschneider, C.H. et al., *Cancer Chemother. Pharmacol.*, 1994, 34, 166, (Bullatacin, 薬理)

Sahai, M. et al., *Chem. Pharm. Bull.*, 1994, 42, 1163, (Squamocins)

Naito, H. et al., *J.O.C.*, 1995, 60, 4419, (Bullatacin, 合成法, IR, H-NMR)



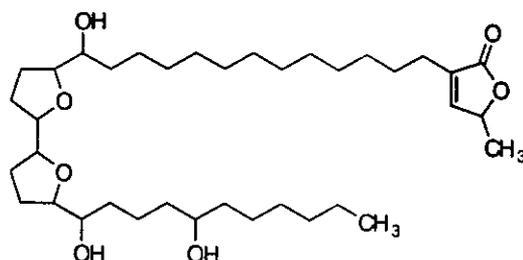
(4R,15R,16R,19R,20R,23R,24R,36S)-form



Morreacute, D.J. et al., Life Sci., 1995, 56, 343, (Bullatacin)
 Gu, Z.-M. et al., Phytochemistry, 1995, 40, 467, (Hydroxybullatacins)
 Liu, X.-X. et al., J. Nat. Prod., 1999, 62, 848, (27-Hydroxybullatacin)

§ **Asitribin; 20-Epimer**

[化学名・別名] Asiminacin. Squamocin D
 [CAS No.] 156199-51-8
 [化合物分類] ポリケチド (Annonaceae acetogenins)
 [構造式]
 [分子式] $C_{37}H_{66}O_7$
 [分子量] 622.924
 [正確な分子量] 622.480855
 [基原] *Asimina triloba*, *Annona squamosa*
 [用途] 細胞毒作用
 [性状] ワックス
 [比旋光度]: $[\alpha]_D +21.1$ (CHCl₃)
 [UV]: [neutral] λ_{max} 215 () (MeOH)

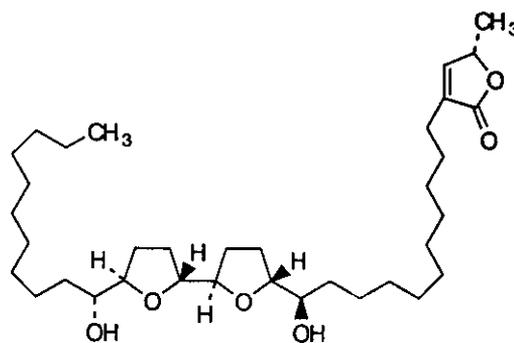


-----文献-----

Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163, (Squamocin D)
 Emde, U. et al., Tet. Lett., 1999, 40, 5979, (合成法, Asiminacin)
 Emde, U. et al., Eur. J. Org. Chem., 2000, 1889, (合成法, Asiminacin)

§ **Atemoyin**

[化学名・別名] Squamocin K
 [CAS No.] 161169-70-6
 [関連 CAS No.] 161025-06-5
 [化合物分類] ポリケチド (Annonaceae acetogenins)
 [構造式]
 [分子式] $C_{33}H_{62}O_6$
 [分子量] 578.871
 [正確な分子量] 578.45464
 [基原] *Annona atemoya* と *Annona squamosa* の種子
 [性状] ワックス
 [比旋光度]: $[\alpha]_D^{25} +20.5$ (c, 0.5 in MeOH)

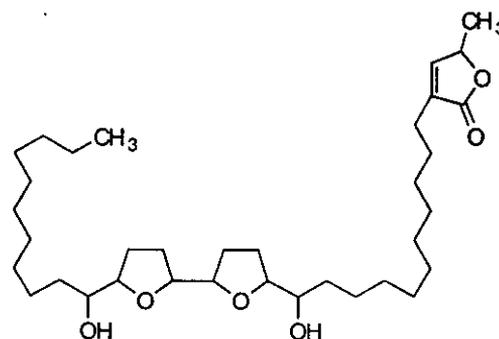


-----文献-----

Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163, (Squamocins)
 Duret, P. et al., Nat. Prod. Lett., 1995, 5, 295, (分離, UV, H-NMR, C13-NMR, Mass)
 Queiroz, E.F. et al., J. Nat. Prod., 1998, 61, 34, (Carolin C)

§ **Atemoyin; 13-Epimer**

[化学名・別名] Squamocin I
 [CAS No.] 159993-37-0
 [化合物分類] ポリケチド (Annonaceae acetogenins)
 [構造式]
 [分子式] $C_{33}H_{62}O_6$
 [分子量] 578.871
 [正確な分子量] 578.45464
 [基原] *Annona squamosa*
 [性状] 針状結晶 (MeOH 溶液)
 [融点] Mp 68.5-71 °C
 [比旋光度]: $[\alpha]_D^{25} +22.2$ (c, 0.5 in MeOH)



-----文献-----

Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163, (Squamocins)
 Duret, P. et al., Nat. Prod. Lett., 1995, 5, 295, (分離, UV, H-NMR, C13-NMR, Mass)
 Queiroz, E.F. et al., J. Nat. Prod., 1998, 61, 34, (Carolin C)

§ Benzo[h]quinazolin-4-ol

[化学名・別名] Benzo[h]quinazolin-4(3H)-one. 4-Hydroxybenzo[h]quinazoline. Samoquazine A

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

[構造式]

[分子式] $C_{12}H_8N_2O$

[分子量] 196.208

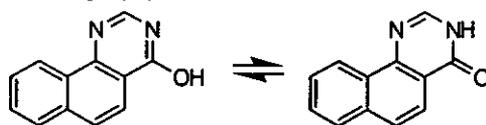
[正確な分子量] 196.063663

[基原] 次の植物の種子から得られるアルカロイド: *Annona squamosa*

[性状] 針状結晶

[UV]: [neutral] λ_{max} 244 (log ϵ 3.7); 251 (log ϵ 3.6); 322 (log ϵ 3.1); 337 (log ϵ 3.1); 353 (log ϵ 3.1) (MeOH)

[その他のデータ] $Mp > 300^\circ C$



-----文献-----

Morita, H. et al., J. Nat. Prod., 2000, 63, 1707

§ Bullacin B

[CAS No.] 210230-74-3

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_7$

[分子量] 622.924

[正確な分子量] 622.480855

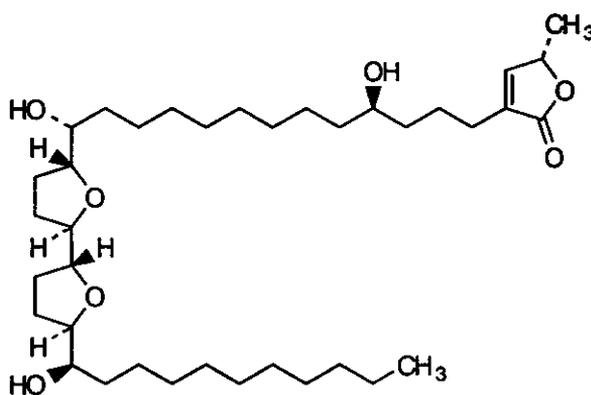
[基原] *Annona squamosa*

[用途] 細胞毒

[性状] 無定型の粉末

[比旋光度]: $[\alpha]_D^{25} +43.8$ (c, 0.03 in CH_2Cl_2)

[UV]: [neutral] λ_{max} 211 (log ϵ 3.79)



-----文献-----

Hopp, D.C. et al., Bioorg. Med. Chem., 1998, 6, 569

§ Bullatacinone

[化学名・別名] Isorolliniastatin 2. Isoannonareticin

[CAS No.] 123012-00-0

[化合物分類] 薬物: 抗腫瘍薬 (Antineoplastic agents), ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_7$

[分子量] 622.924

[正確な分子量] 622.480855

[基原] *Annona bullata*, *Annona reticulata*, *Annona squamosa*

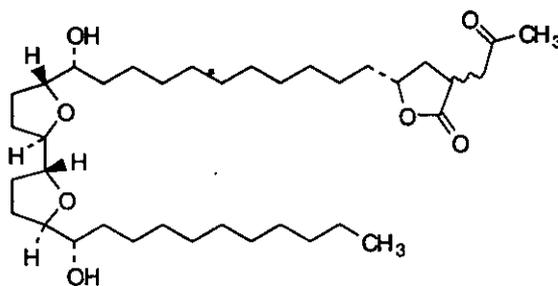
[用途] 細胞毒作用

[性状] 結晶 (MeOH)

[融点] Mp 90.5-90.7 $^\circ C$

[比旋光度]: $[\alpha]_D^{25} +12$ (c, 0.4 in $CHCl_3$)

[Log P 計算値] Log P 8 (未確認値) (計算値)



-----文献-----

Yu, J.G. et al., Chin. Chem. Lett., 1996, 7, 19, (Isoannonareticin)

§ Bullatacinone; 24-Epimer, 9-oxo

[化学名・別名] 9-Oxoasimicinone

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{64}O_8$

[分子量] 636.908

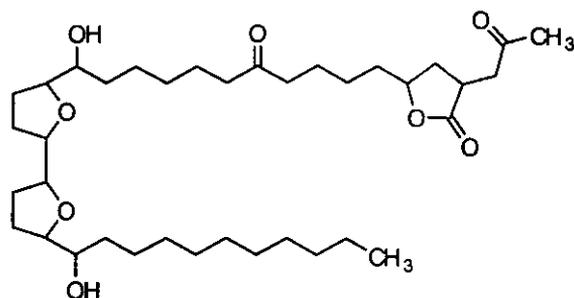
[正確な分子量] 636.46012

[基原] *Annona squamosa*

[性状] 無定形の粉末

[比旋光度]: $[\alpha]_D^{25} +19.7$ (c, 0.1 in CH_2Cl_2)

[UV]: [neutral] λ_{max} 203 (log ϵ 3.55) (MeOH) [neutral] λ_{max} 203 (ϵ 3550) (MeOH)



-----文献-----

Hopp, D.C. et al., *Bioorg. Med. Chem.*, 1998, 6, 569, (9-Oxoasimicinone)

§ Bullatacinone; 24-Epimer, 9R-hydroxy

[化学名・別名] 9-Hydroxyasimicinone

[CAS No.] 255900-36-8

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_8$

[分子量] 638.924

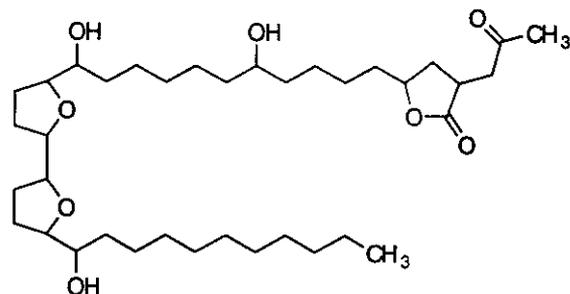
[正確な分子量] 638.47577

[基原] *Annona squamosa*

[性状] ワックス

[比旋光度]: $[\alpha]_D^{25} +19.3$ (c, 0.26 in CH_2Cl_2)

[UV]: [neutral] λ_{max} 203 (log ϵ 2.98) (MeOH)



-----文献-----

Hui, Y.-H. et al., *J. Nat. Prod.*, 1989, 52, 463; 1990, 53, 81, (分離, H-NMR, C13-NMR)

Gu, Z.-M. et al., *J. Nat. Prod.*, 1993, 56, 870, (Hydroxybullatacinones)

Gu, Z.-M. et al., *Nat. Toxins*, 1994, 2, 49

Laprevote, O. et al., *Tetrahedron*, 1994, 50, 8479, (Mass, 構造決定)

Gu, Z.-M. et al., *Phytochemistry*, 1995, 40, 467

Yu, J.G. et al., *Chin. Chem. Lett.*, 1996, 7, 19, (Isoannonareticin)

Zhao, G.-X. et al., *Nat. Toxins*, 1996, 4, 128, (Asimicinone)

Hopp, D.C. et al., *Bioorg. Med. Chem.*, 1998, 6, 569, (9-Oxoasimicinone)

§ Bullatanocin

[化学名・別名] Annonin IV. Cherimolin 2. Crassiflorin. Purpureacin 1. Squamostatin C

[関連 CAS No.] 125882-64-6

[その他の CAS No.] 150134-21-7, 151637-38-6, 157184-02-6, 159249-82-8

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_8$

[分子量] 638.924

[正確な分子量] 638.47577

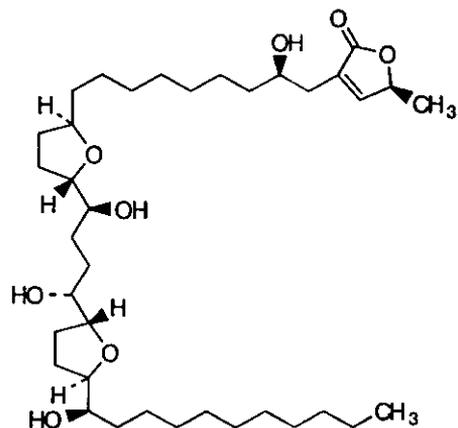
[基原] *Annona squamosa*, *Annona bullata*, *Annona cherimolia*, *Annona glabra*, *Annona crassiflora*, *Annona purpurea*

[性状] 無定形のワックス

[融点] Mp 107-109 °C (95-97 °C)

[比旋光度]: $[\alpha]_D^{25} +13.6$ (c, 0.28 in CH_2Cl_2)

[UV]: [neutral] λ_{max} 215 (ϵ 5000) (EtOH) (Derep)



-----文献-----

Nonfon, M. et al., *Phytochemistry*, 1990, 29, 1951, (分離, H-NMR, C13-NMR, Mass)
 Cortes, D. et al., *Phytochemistry*, 1993, 32, 1467; 1475, (レビュー)
 Fujimoto, Y. et al., *Chem. Pharm. Bull.*, 1994, 42, 1175, (Squamostatins)
 Pinheiro-Santos, L. et al., *Quim. Nova*, 1994, 17, 387, (Crassiflorin)
 Shimada, H. et al., *Tet. Lett.*, 1994, 35, 3961, (絶対構造, Squamostatins)
 Gu, Z.-M. et al., *J. Nat. Prod.*, 1995, 41, 229, (*cis*-Bullatanocin, *cis*-Bullatalicin)
 Marshall, J.A. et al., *J.O.C.*, 1998, 63, 7066, (合成法, Squamostatin D)
 Martin, J.M. et al., *J. Nat. Prod.*, 1999, 62, 2, (活性, Bullatalicin)
 Chang, F.-R. et al., *Phytochemistry*, 1999, 51, 883, (*cis*-Squamostatin D)

§ Bullatanocin; 4-Deoxy

[化学名・別名] Squamostatin E. 4-Desoxycherimolin 2

[CAS No.] 158515-34-5

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] C₃₇H₆₆O₇

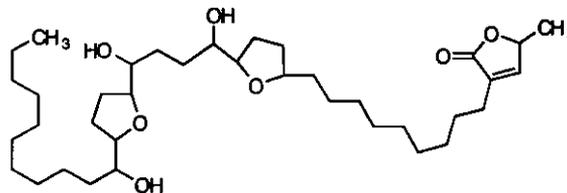
[分子量] 622.924

[正確な分子量] 622.480855

[基原] *Annona glabra*, *Annona squamosa*

[融点] Mp 105-106 °C

[比旋光度]: [α]_D +14.7 (c, 0.5 in MeOH)



-----文献-----

Cortes, D. et al., *Phytochemistry*, 1993, 32, 1467; 1475, (レビュー)
 Fujimoto, Y. et al., *Chem. Pharm. Bull.*, 1994, 42, 1175, (Squamostatins)
 Shimada, H. et al., *Tet. Lett.*, 1994, 35, 3961, (絶対構造, Squamostatins)
 Marshall, J.A. et al., *J.O.C.*, 1998, 63, 7066, (合成法, Squamostatin D)
 Chang, F.-R. et al., *Phytochemistry*, 1999, 51, 883, (*cis*-Squamostatin D)

§ Bullatanocin; 24-Epimer

[化学名・別名] Bullatalicin. Annonin VIII. Cherimolin 1. Squamostatin B

[CAS No.] 152323-84-7

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] C₃₇H₆₆O₈

[分子量] 638.924

[正確な分子量] 638.47577

[基原] *Annona squamosa*, *Annona bullata*, *Annona cherimolia*

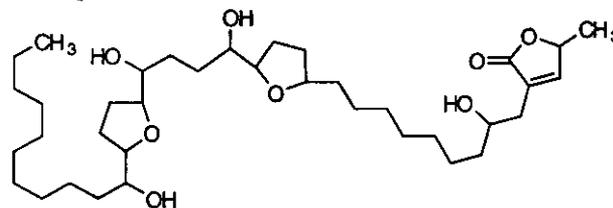
[用途] Defensive agent against bird predation

[性状] 無定型のワックス

[融点] Mp 120-121 °C (113-116 °C)

[比旋光度]: [α]_D +64 (c, 0.3 in MeOH). [α]_D²⁵ +9.8 (c, 0.29 in CH₂Cl₂)

[UV]: [neutral] λ_{max} 215 (ε 5000) (EtOH) (Derp)

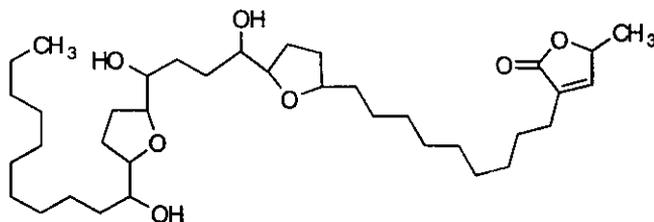


-----文献-----

Cortes, D. et al., *Phytochemistry*, 1993, 32, 1467; 1475, (レビュー)
 Fujimoto, Y. et al., *Chem. Pharm. Bull.*, 1994, 42, 1175, (Squamostatins)
 Shimada, H. et al., *Tet. Lett.*, 1994, 35, 3961, (絶対構造, Squamostatins)
 Gu, Z.-M. et al., *J. Nat. Prod.*, 1995, 41, 229, (*cis*-Bullatanocin, *cis*-Bullatalicin)
 Marshall, J.A. et al., *J.O.C.*, 1998, 63, 7066, (合成法, Squamostatin D)
 Martin, J.M. et al., *J. Nat. Prod.*, 1999, 62, 2, (活性, Bullatalicin)
 Chang, F.-R. et al., *Phytochemistry*, 1999, 51, 883, (*cis*-Squamostatin D)

§ Bullatanocin; 24-Epimer, 4-deoxy

[化学名・別名] Squamostatin D
 [CAS No.] 157184-03-7
 [化合物分類] ポリケチド (Annonaceae acetogenins)
 [構造式]
 [分子式] $C_{37}H_{56}O_7$
 [分子量] 622.924
 [正確な分子量] 622.480855
 [基原] *Annona squamosa*
 [融点] Mp 112-113.5 °C
 [比旋光度]: $[\alpha]_D +7.9$ (c, 0.5 in MeOH)

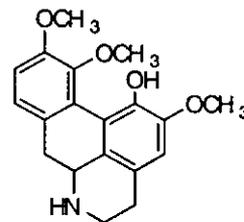


-----文献-----

Marshall, J.A. et al., J.O.C., 1998, 63, 7066, (合成法, Squamostatin D)
 Chang, F.-R. et al., Phytochemistry, 1999, 51, 883, (*cis*-Squamostatin D)

§ Corydine; (S)-form, N-De-Me

[化学名・別名] 1-Hydroxy-2,10,11-trimethoxynoraporphine. Norcorydine
 [CAS No.] 26931-78-2
 [化合物分類] アルカロイド化合物 (Aporphine alkaloids)
 [構造式]
 [分子式] $C_{19}H_{21}NO_4$
 [分子量] 327.379
 [正確な分子量] 327.147059
 [基原] 次の植物から得られるアルカロイド: *Annona squamosa*, *Popowia* sp. cf. *cyanocarpa*, *Stephania dinklagei*, *Laurelia philippiana*, *Glaucium fimbriigerum*, *Xylopia danguyella* (バンレイシ科, ツツラフジ科, アセロスペルマ科, ケシ科)
 [性状] 非結晶性
 [比旋光度]: $[\alpha]_D +156$ (MeOH). $[\alpha]_D^{23} +190$ (c, 0.2 in $CHCl_3$)

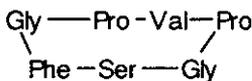


-----文献-----

Johns, S.R. et al., Aust. J. Chem., 1970, 23, 363, (分離, H-NMR, Mass, 構造決定)
 Bhakuni, D.S. et al., Phytochemistry, 1972, 11, 1819, (分離, UV, H-NMR, Mass)
 Tackie, A.N. et al., J. Nat. Prod., 1974, 37, 6, (分離, UV, H-NMR, Mass)
 Nieto, M. et al., Planta Med., 1976, 30, 48, (racemate)
 Karimova, S.U. et al., Khim. Prir. Soedin., 1980, 224; CA, 93, 110563p, (分離)
 Hocquemiller, R. et al., J. Nat. Prod., 1981, 44, 551, (生育)
 Urz acute u a, A. et al., Phytochemistry, 1982, 21, 773, (分離, IR, H-NMR, Mass)
 Shafiee, A. et al., Planta Med., 1998, 64, 489, (分離)

§ Cyclosquamosin A

[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)
 [構造式]
 [分子式] $C_{31}H_{45}N_7O_8$
 [分子量] 641.723
 [正確な分子量] 641.317313
 [基原] *Annona squamosa* の種子
 [性状] 粉末
 [比旋光度]: $[\alpha]_D^{20} -74.7$ (c, 0.83 in MeOH)

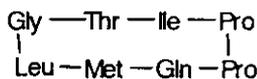


-----文献-----

Morita, H. et al., Tetrahedron, 1999, 55, 7509

§ Cyclosquamosin B

[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)
 [構造式]
 [分子式] $C_{38}H_{53}N_9O_{10}S$
 [分子量] 838.036



[正確な分子量] 838.441861
[基原] *Annona squamosa* の種子
[性状] 粉末
[比旋光度]: $[\alpha]_D^{20}$ -53.8 (c, 0.58 in MeOH)

-----文献-----

Morita, H. et al., *Tetrahedron*, 1999, 55, 7509

§ Cyclosquamosin B; S-Oxide

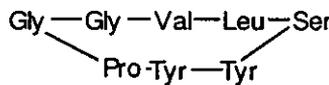
[化学名・別名] Cyclosquamosin C
[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)
[構造式] アミノ酸およびペプチド. 有効な構造式はない
[分子式] $C_{38}H_{63}N_9O_{11}S$
[分子量] 854.035
[正確な分子量] 853.436776
[基原] *Annona squamosa* の種子
[性状] 粉末
[比旋光度]: $[\alpha]_D^{20}$ -94 (c, 0.1 in MeOH)

-----文献-----

Morita, H. et al., *Tetrahedron*, 1999, 55, 7509

§ Cyclosquamosin D

[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)
[構造式]
[分子式] $C_{41}H_{56}N_8O_{11}$
[分子量] 836.94
[正確な分子量] 836.406857
[基原] *Annona squamosa* の種子
[性状] 粉末
[比旋光度]: $[\alpha]_D^{20}$ -36.4 (c, 0.11 in MeOH)
[UV]: [neutral] λ_{max} 278 (ϵ 2560) (MeOH)

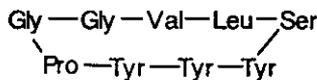


-----文献-----

Morita, H. et al., *Tetrahedron*, 1999, 55, 7509

§ Cyclosquamosin E

[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)
[構造式]
[分子式] $C_{50}H_{65}N_9O_{13}$
[分子量] 1000.116
[正確な分子量] 999.470186
[基原] *Annona squamosa* の種子
[性状] 粉末
[比旋光度]: $[\alpha]_D^{20}$ -10.9 (c, 1.4 in MeOH)
[UV]: [neutral] λ_{max} 278 (ϵ 7440) (MeOH)

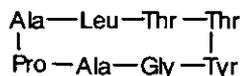


-----文献-----

Morita, H. et al., *Tetrahedron*, 1999, 55, 7509

§ Cyclosquamosin F

[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)
[構造式]
[分子式] $C_{36}H_{54}N_8O_{11}$
[分子量] 774.87
[正確な分子量] 774.391207
[基原] *Annona squamosa* の種子
[性状] 粉末
[比旋光度]: $[\alpha]_D^{20}$ -38.2 (c, 1.11 in MeOH)



[UV]:[neutral] λ_{\max} 278 (ϵ 1750) (MeOH)

-----文献-----

Morita, H. et al., Tetrahedron, 1999, 55, 7509

§ Cyclosquamosin G

[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)

[構造式]

[分子式] $C_{39}H_{60}N_8O_{10}S$

[分子量] 833.017

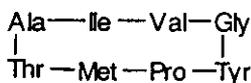
[正確な分子量] 832.415312

[基原] *Annona squamosa* の種子

[性状] 粉末

[比旋光度]: $[\alpha]_D^{20}$ -37.1 (c, 0.14 in MeOH)

[UV]:[neutral] λ_{\max} 278 (ϵ 1840) (MeOH)



-----文献-----

Morita, H. et al., Tetrahedron, 1999, 55, 7509

§ 17,19-Kauranediol; (*ent*-16 β)-form, 19-Aldehyde

[化学名・別名] *ent*-17-Hydroxy-16 β -kauran-19-al

[CAS No.] 41756-43-8

[化合物分類] テルペノイド (Kaurane diterpenoids)

[構造式]

[分子式] $C_{30}H_{52}O_2$

[分子量] 304.472

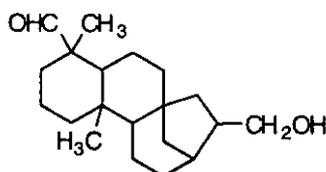
[正確な分子量] 304.24023

[基原] 次の植物から分離: *Annona squamosa*

[性状] 結晶 (Et.O/petrol)

[融点] Mp 148 °C

[比旋光度]: $[\alpha]_D^{25}$ -45.4 (c, 2.2 in $CHCl_3$)



-----文献-----

Jefferies, P.R. et al., Aust. J. Chem., 1964, 17, 915; 1965, 19, 1441, (分離, 構造決定)

Bohlmann, F. et al., Chem. Ber., 1973, 106, 841, (19-aldehyde)

§ 17,19-Kauranediol; (*ent*-16 β)-form, 19-Aldehyde, 17-Ac

[CAS No.] 41756-46-1

[化合物分類] テルペノイド (Kaurane diterpenoids)

[構造式]

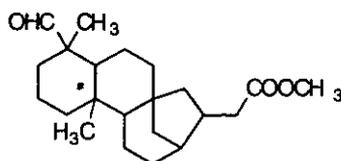
[分子式] $C_{32}H_{54}O_3$

[分子量] 346.509

「せいかく」 346.250795

[基原] 次の植物から分離: *Annona squamosa*

[性状] オイル



-----文献-----

Jefferies, P.R. et al., Aust. J. Chem., 1964, 17, 915; 1965, 19, 1441, (分離, 構造決定)

Bohlmann, F. et al., Chem. Ber., 1973, 106, 841, (19-aldehyde)

§ 16,17,19-Kauranetriol; (*ent*-16 α OH)-form, 19-Aldehyde, 17-Ac

[化学名・別名] Annosquamosin A

[CAS No.] 177742-55-1

[化合物分類] テルペノイド (Kaurane diterpenoids)

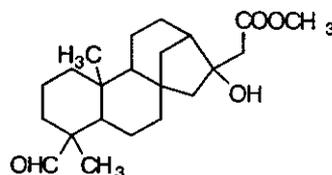
[構造式]

[分子式] $C_{32}H_{54}O_4$

[分子量] 362.508

[正確な分子量] 362.24571

[基原] *Annona squamosa*



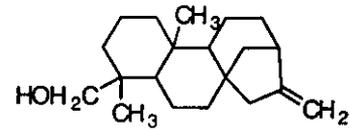
[性状] 針状結晶 (MeOH)
[融点] Mp 162-164 °C
[比旋光度]: $[\alpha]_D^{24}$ -64 (c, 0.2 in CHCl₃)

-----文献-----

Wu, Y.-C. et al., J. Nat. Prod., 1996, 59, 635, (Annosquamosin A, C13-NMR)

§ 16-Kauren-19-ol; *ent*-form

[CAS No.] 2300-11-0
[化合物分類] テルペノイド (Kaurane diterpenoids)
[構造式]
[基原] *Annona squamosa* の根。また *Cacalia bulbifera*, *Arctotis*,
Austroeupeatorium, *Helichrysum*, その他数種の属
[性状] 結晶 (MeOH 溶液)
[融点] Mp 141-142 °C
[比旋光度]: $[\alpha]_D$ -75 (c, 2.76 in CHCl₃)

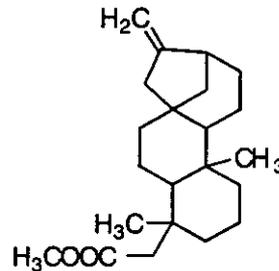


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C.Djerassi et al., Dictionary of Natural Products, Chapman, Hall, 2002
Kalinowskii, A.I. et al., Khim. Prir. Soedin., 1971, 7, 281; Chem. Nat. Compd. (Engl. Transl.), 1971, 7, 269, (Mass, acid)
Bohlmann, F. et al., Chem. Ber., 1973, 106, 841, (分離)
Bohlmann, F. et al., Phytochemistry, 1980, 19, 107; 267; 2399; 1981, 20, 1899; 1907; 1982, 21, 399, (16)
Aljancýic, I. et al., Phytochemistry, 1996, 43, 169, (19-Acetoxy-16,17-epoxykaurane) T
oyota, M. et al., J.O.C., 2000, 65, 4565, (合成法)

§ 16-Kauren-19-ol; *ent*-form, Ac

[CAS No.] 41756-45-0
[化合物分類] テルペノイド (Kaurane diterpenoids)
[構造式]
[分子式] C₂₂H₃₄O₂
[分子量] 330.509
[正確な分子量] 330.25588
[基原] *Annona squamosa*, *Espeletopsis guacharaca*
[性状] 結晶 (MeOH) もしくはガム
[融点] Mp 117-118 °C
[比旋光度]: $[\alpha]_D$ -74 (c, 2.3 in CHCl₃)

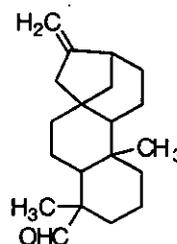


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C.Djerassi et al., Dictionary of Natural Products, Chapman, Hall, 2002
Kalinowskii, A.I. et al., Khim. Prir. Soedin., 1971, 7, 281; Chem. Nat. Compd. (Engl. Transl.), 1971, 7, 269, (Mass, acid)
Piozzi, F. et al., Phytochemistry, 1971, 10, 1164, (分離, aldehyde)
Bohlmann, F. et al., Chem. Ber., 1973, 106, 841, (分離)

§ 16-Kauren-19-ol; *ent*-form, 19-Aldehyde

[化学名・別名] *ent*-16-Kauren-19-al
[CAS No.] 14046-84-5
[化合物分類] テルペノイド (Kaurane diterpenoids)
[構造式]
[分子式] C₂₀H₃₀O
[分子量] 286.456
[正確な分子量] 286.229665
[基原] *Annona squamosa* の根, *Espeletia grandiflora*, *Cacalia bulbifera*, また数多くのその他の属
[性状] 結晶 (petrol)
[融点] Mp 113-116 °C
[比旋光度]: $[\alpha]_D^{24}$ -84.2 (c, 1.05 in CHCl₃)

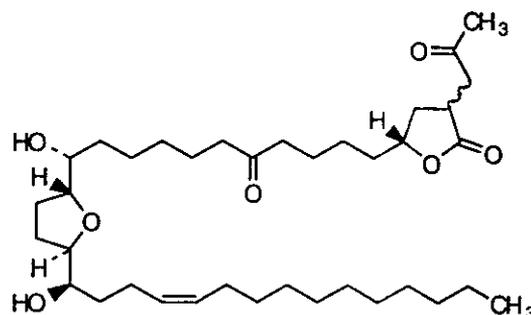


-----文献-----

C.Djerassi et al., Dictionary of Natural Products, Chapman, Hall, 2002
Piozzi, F. et al., Phytochemistry, 1971, 10, 1164, (分離, aldehyde)

§ Mosinone A

[CAS No.] 191800-47-2
[化合物分類] ポリケチド (Annonaceae acetogenins)
[構造式]
[分子式] $C_{37}H_{66}O_7$
[分子量] 620.908
[正確な分子量] 620.465205
[基原] *Annona squamosa*
[用途] 細胞毒作用
[性状] ワックス様の塊
[UV]: [neutral] λ_{max} 202 (2.96) (MeOH)

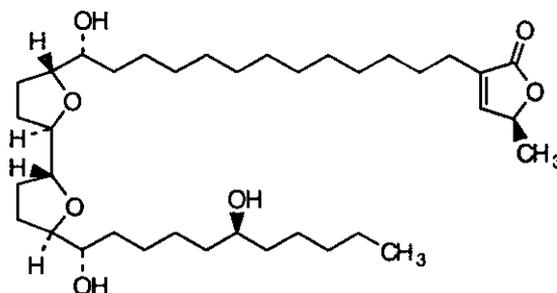


-----文献-----

Hopp, D.C. et al., J. Nat. Prod., 1997, 60, 581, (分離, UV)

§ Motrilin

[化学名・別名] Annonin III. Squamocin C
[CAS No.] 138551-27-6
[関連 CAS No.] 141505-62-6
[その他の CAS No.] 157084-75-8
[化合物分類] ポリケチド (Annonaceae acetogenins)
[構造式]



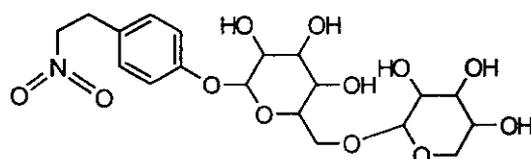
[分子式] $C_{37}H_{66}O_7$
[分子量] 622.924
[正確な分子量] 622.480855
[一般的性質] 化学構造は次の化合物とよく似ている: Narumicin I, Squamostatin A
[基原] 次の植物から分離: *Annona cherimolia*, *Annona squamosa*, *Asimina triloba*
[用途] 細胞毒作用
[融点] Mp 50-51 °C
[比旋光度]: $[\alpha]_D^{20} +19.5$ (c, 0.9 in MeOH)
[UV]: [neutral] λ_{max} 210 (ϵ 7000) (MeOH) [neutral] λ_{max} 211 (ϵ 11800) (EtOH)

-----文献-----

Cortes, D. et al., Tetrahedron, 1991, 47, 8195, (分離, H-NMR, C^{13} -NMR)
Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163, (Squamocin C)
Zhao, G.-X. et al., J. Med. Chem., 1994, 37, 1971, (Asiminecin)
Cave, A. et al., Prog. Chem. Org. Nat. Prod., 1997, 70, 81, (レビュー)

§ 4-(2-Nitroethyl) phenol; O-[β -D-Xylopyranosyl-(1 \rightarrow 6)- β -D-glucopyranoside]

[化学名・別名] 4-(2-Nitroethyl) phenyl primeveroside
[化合物分類] 炭水化物 (Disaccharides), 単環芳香族 (Simple phenols)
[構造式]
[分子式] $C_{19}H_{27}NO_{12}$
[分子量] 461.422
[正確な分子量] 461.153329
[基原] *Annona squamosa*
[性状] 結晶 (EtOH)
[融点] Mp 125 °C
[比旋光度]: $[\alpha]_D^{20} -70$ (c, 2 in EtOH)
[UV]: [neutral] λ_{max} 274 (log ϵ 3.05) (EtOH)

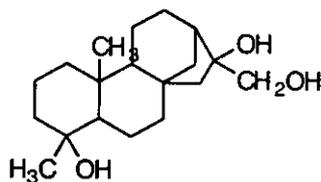


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Chirkunov, E.V. et al., *CA*, 1972, 77, 126172r, (合成法)
 Forgacs, P. et al., *Phytochemistry*, 1980, 19, 1251, (primeveroside)
 Ina, M. et al., *Chem. Pharm. Bull.*, 1986, 34, 726, (分離, 構造決定, 合成法, 誘導體)
 Miyase, T. et al., *Chem. Pharm. Bull.*, 1987, 35, 1109, (誘導體)
 Shimomura, H. et al., *Phytochemistry*, 1988, 27, 644, (誘導體)
 Yoshikawa, M. et al., *Chem. Pharm. Bull.*, 1996, 44, 492, (Arabinothalictoside)
 Hanawa, F. et al., *Phytochemistry*, 2000, 53, 55, (分離, Lysichitalalexin)

§ 19-Nor-4,16,17-kauranetriol; (*ent*-4 β , 16 α OH)-form

[化学名・別名] Annosquamosin B
 [CAS No.] 177742-56-2
 [化合物分類] テルペノイド (Norkaurane diterpenoids)
 [構造式]
 [基原] *Annona squamosa*
 [性状] 粉末
 [融点] Mp 263-266 °C
 [比旋光度]: $[\alpha]_D^{24}$ -47 (c, 0.2 in CHCl₃/MeOH)

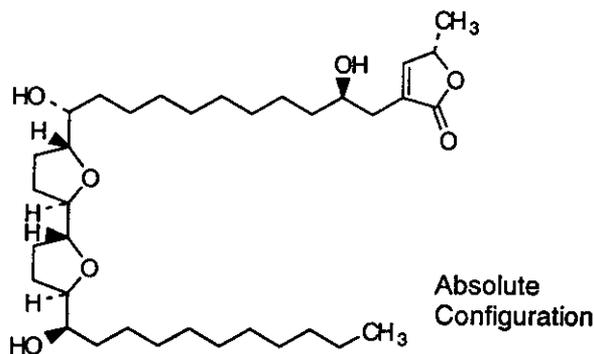


-----文献-----

Wu, Y.C. et al., *J. Nat. Prod.*, 1996, 59, 635, (分離, H-NMR, C13-NMR)

§ Parviflorin

[化学名・別名] Atemoyacin A. Squamocin E
 [CAS No.] 152378-19-3
 [その他の CAS No.] 166735-11-1
 [化合物分類] ポリケチド (Annonaceae acetogenins)
 [構造式]
 [分子式] C₃₅H₆₂O₇
 [分子量] 594.871
 [正確な分子量] 594.449555
 [基原] *Annona bullata*, *Annona squamosa*, *Annona atemoya*, *Asimina parviflora*
 [用途] 細胞毒作用
 [性状] ワックス
 [比旋光度]: $[\alpha]_D$ +20.9 (c, 0.2 in MeOH)
 [UV]: [neutral] λ_{max} 223 (ϵ 8405) (EtOH)

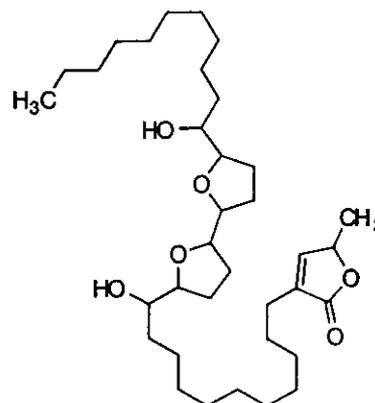


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Kawaza, K. et al., *Agric. Biol. Chem.*, 1989, 53, 2719, (Neoannonin)
 Gu, Z.-M. et al., *Heterocycles*, 1993, 36, 2221, (Bullacin)
 Ratnayake, S. et al., *Can. J. Chem.*, 1994, 72, 287, (分離)
 Sahai, M. et al., *Chem. Pharm. Bull.*, 1994, 42, 1163, (Squamocins)
 Chen, W.-S. et al., *Chin. J. Chem.*, 1995, 13, 263, (Atemoyacin A)
 Hoye, T.R. et al., *J.A.C.S.*, 1996, 118, 1801, (合成法)
 Duret, P. et al., *Phytochemistry*, 1997, 45, 1423, (Annonisin)
 Cave, A. et al., *Prog. Chem. Org. Nat. Prod.*, 1997, 70, 81, (レビュー)

§ Parviflorin; 22-Epimer, 4-deoxy

[化学名・別名] Neoannonin. Squamocin J
[CAS No.] 125205-43-8
[化合物分類] ポリケチド (Annonaceae acetogenins)
[構造式]
[分子式] $C_{35}H_{62}O_6$
[分子量] 578.871
[正確な分子量] 578.45464
[基原] *Annona squamosa*
[用途] 殺虫作用を示す
[性状] ワックス
[融点] Mp 85-86.5 °C (62-64 °C)
[比旋光度]: $[\alpha]_D^{22} +18.8$ (c, 1.35 in MeOH)
[溶解性] BERDY SOL: メタノール, ヘキサンに可溶; 水に難溶
[UV]: [neutral] λ_{max} 215 (ϵ 12000) (MeOH)

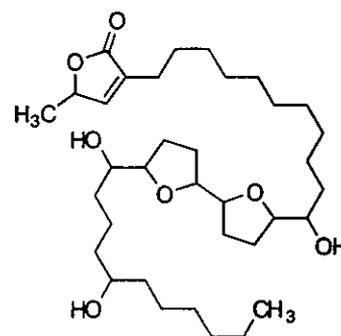


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Kawaza, K. et al., Agric. Biol. Chem., 1989, 53, 2719, (Neoannonin)
Gu, Z.-M. et al., Heterocycles, 1993, 36, 2221, (Bullacin)
Ratnayake, S. et al., Can. J. Chem., 1994, 72, 287, (分離)
Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163, (Squamocins)
Chen, W.-S, et al., Chin. J. Chem., 1995, 13, 263, (Atemoyacin A)
Hoye, T.R. et al., J.A.C.S., 1996, 118, 1801, (合成法)
Duret, P. et al., Phytochemistry, 1997, 45, 1423, (Annonisin)
Cave, A. et al., Prog. Chem. Org. Nat. Prod., 1997, 70, 81, (レビュー)

§ Parviflorin; 22-Epimer, 4-deoxy, 26S-hydroxy

[化学名・別名] Squamocin B
[CAS No.] 159934-23-3
[化合物分類] ポリケチド (Annonaceae acetogenins)
[構造式]



[分子式] $C_{35}H_{62}O_7$
[分子量] 594.871
[正確な分子量] 594.449555
[基原] *Annona squamosa*
[性状] ワックス
[比旋光度]: $[\alpha]_D^{25} +27.6$ (c, 0.2 in MeOH)

-----文献-----

Kawaza, K. et al., Agric. Biol. Chem., 1989, 53, 2719, (Neoannonin)
Gu, Z.-M. et al., Heterocycles, 1993, 36, 2221, (Bullacin)
Ratnayake, S. et al., Can. J. Chem., 1994, 72, 287, (分離)
Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163, (Squamocins)
Chen, W.-S, et al., Chin. J. Chem., 1995, 13, 263, (Atemoyacin A)
Hoye, T.R. et al., J.A.C.S., 1996, 118, 1801, (合成法)
Duret, P. et al., Phytochemistry, 1997, 45, 1423, (Annonisin)
Cave, A. et al., Prog. Chem. Org. Nat. Prod., 1997, 70, 81, (レビュー)

§ Reticulatain 1

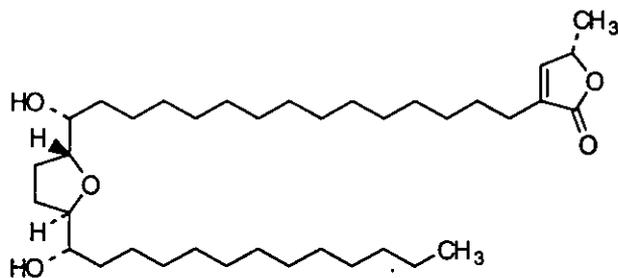
[化学名・別名] Neoreticulatacin A

[CAS No.] 166022-35-1

[その他の CAS No.] 170080-02-1

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]



[分子式] $C_{37}H_{66}O_5$

[分子量] 592.941

[正確な分子量] 592.506675

[基原] *Annona atemoya*, *Annona reticulata*, *Annona squamosa*

[性状] 無定型の塊

[比旋光度]: $[\alpha]_D^{25} +22$ (c, 1 in $CHCl_3$)

[UV]: [neutral] λ_{max} 207 (MeOH)

-----文献-----

Hisham, A. et al., Tet. Lett., 1990, 31, 4649, (分離)

Saad, J.M. et al., Tetrahedron, 1991, 47, 2751, (Reticulatacin, Uvariamicin II)

Sinha, S.C. et al., J.A.C.S., 1993, 115, 4891, (合成法)

Makabe, H. et al., J.C.S. Perkin 1, 1994, 1975, (合成法)

Tam, V.T. et al., Bull. Soc. Chim. Fr., 1995, 132, 324, (分離, UV, IR, H-NMR, C13-NMR, Mass)

Zheng, X.-C. et al., Zhiwu Xuebao, 1995, 37, 238, (分離)

Gleye, C. et al., J. Nat. Prod., 1998, 61, 576, (cis-Reticulatacin, cis-Reticulatacin-10-one)

§ Rollidecin A; 4-Deoxy, stereoisomer

[化学名・別名] Annonosilin A

[CAS No.] 164177-57-5

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_7$

[分子量] 622.924

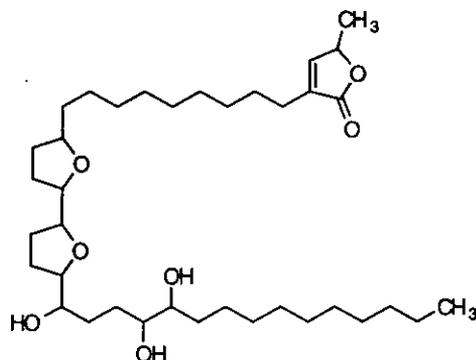
[正確な分子量] 622.480855

[基原] *Annona squamosa* の種子

[融点] Mp 107-109 °C

[比旋光度]: $[\alpha]_D^{25} +18.6$ (c, 1.7 in $CHCl_3$)

[その他のデータ] 立体構造に関する報告はない



-----文献-----

Yang, R.Z. et al., Zhiwu Xuebao, 1995, 37, 492; CA, 124, 170607z, (Annonosilin A)

Shi, G. et al., Bioorg. Med. Chem., 1996, 4, 1281, (分離, UV, IR, H-NMR, C13-NMR)

§ Squamin A

[CAS No.] 241486-93-1

[化合物分類] アミノ酸とペプチド (Cyclic oligo- and polypeptides)

[構造式]

[分子式] $C_{39}H_{66}N_8O_{11}S$

[分子量] 848.016

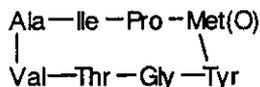
[正確な分子量] 848.410227

[基原] *Annona squamosa*

[性状] 結晶

[比旋光度]: $[\alpha]_D^{18} -48.4$ (MeOH)

[その他のデータ] Mp >300 °C



-----文献-----

Shi, J.X. et al., Chin. Chem. Lett., 1999, 10, 299

§ Squamocin F

[CAS No.] 159957-81-0

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_7$

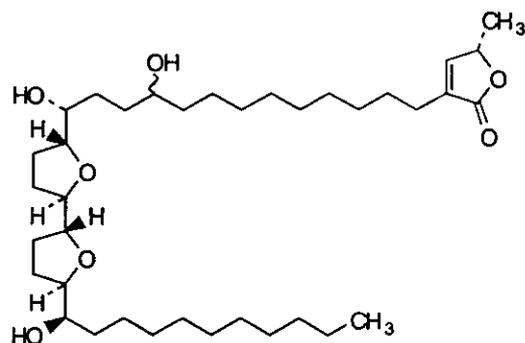
[分子量] 622.924

[正確な分子量] 622.480855

[基原] *Annona squamosa*

[性状] ワックス

[比旋光度]: $[\alpha]_D^{25} +21$ (c, 0.6 in MeOH)



-----文献-----

Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163-1174

§ Squamocin L

[化学名・別名] Desacetyluvaricin. Nedesacetyluvaricin. Squamocin L

[CAS No.] 98767-45-4

[その他の CAS No.] 145165-08-8

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_6$

[分子量] 606.925

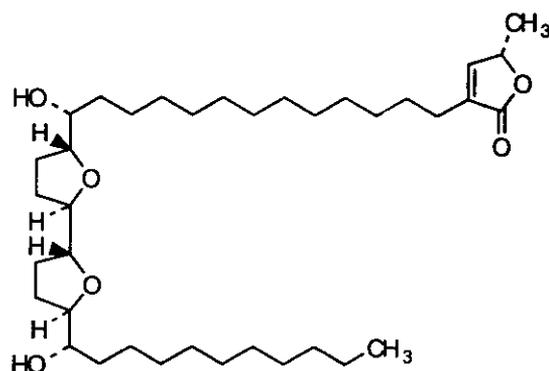
[正確な分子量] 606.48594

[基原] 次の植物から分離: *Uvaria acuminata*, *Annona bullata*, *Annona squamosa*

[融点] Mp 約 25 °C

[比旋光度]: $[\alpha]_D +21.1$ (c, 0.5 in $CHCl_3$)

[UV]: [neutral] λ_{max} 207 (ϵ 12700) (EtOH) (Derep) [neutral] λ_{max} 207 (ϵ 12730) (EtOH)



Absolute Configuration

-----文献-----

Gu, Z. et al., Tetrahedron, 1993, 49, 747, (Desacetyluvaricin)

Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163, (Squamocins)

§ Squamocin L; 19,20,24-Triepimer

[化学名・別名] Squamocin N

[CAS No.] 159993-40-5

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] $C_{37}H_{66}O_6$

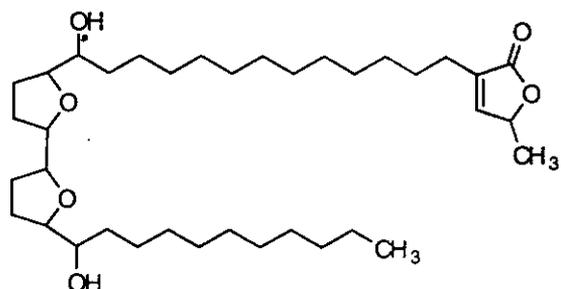
[分子量] 606.925

[正確な分子量] 606.48594

[基原] *Annona squamosa* の種子

[性状] オイル

[比旋光度]: $[\alpha]_D^{25} +40.6$ (c, 0.4 in MeOH)



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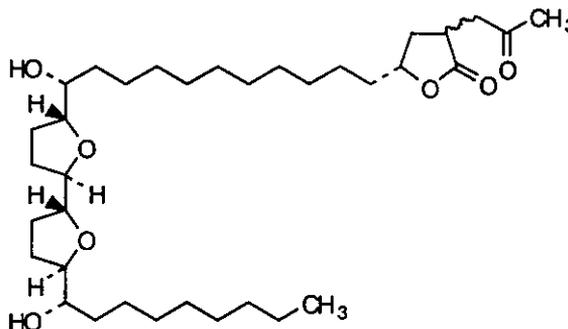
Sahai, M. et al., Chem. Pharm. Bull., 1994, 42, 1163, (分離, IR, H-NMR, C13-NMR)

§ Squamolone

[その他の CAS No.] 210230-72-1, 210230-73-2

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]



[分子式] C₃₃H₆₂O₇

[基原] *Annona squamosa*

[性状] 無定型の粉末

[比旋光度]: $[\alpha]_D^{25} +21.4$ (c, 0.07 in CH₂Cl₂)

[UV]: [neutral] λ_{max} 203 (log ϵ 2.85) (MeOH)

[その他のデータ] 2,4-*cis*- と *trans*-isomers の混合物として分離される

-----文献-----

Hopp, D.C. et al., Bioorg. Med. Chem., 1998, 6, 569

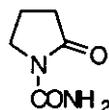
§ Squamolone

[化学名・別名] 2-Oxo-1-pyrrolidinecarboxamide (CAS 名). 1-Carbamoyl-2-pyrrolidone

[CAS No.] 40451-67-0

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

[構造式]



[分子式] C₅H₈N₂O₂

[分子量] 128.13

[正確な分子量] 128.058578

[基原] *Annona squamosa*, *Hexalobus crispiflorus* (パンレイシ科). また *Asimina triloba* から得られる

[性状] プリズム結晶 (C₅H₈)

[融点] Mp 148 °C

-----文献-----

Yang, T.H. et al., J. Chin. Chem. Soc. (Taipei), 1972, 19, 149; CA, 78, 16151w, (分離, UV, H-NMR, Mass)

Marquez, V.E. et al., J.O.C., 1980, 45, 5308, (構造決定, 合成法, IR, H-NMR, Mass)

Achenbach, H. et al., Annalen, 1982, 1623, (分離, C13-NMR)

Zhao, G.-X. et al., Phytochemistry, 1993, 33, 1065, (分離, 合成法)

Sahai, M. et al., Indian J. Chem., Sect. B, 1996, 35, 510, (分離, 合成法, IR, H-NMR, C13-NMR, Mass)

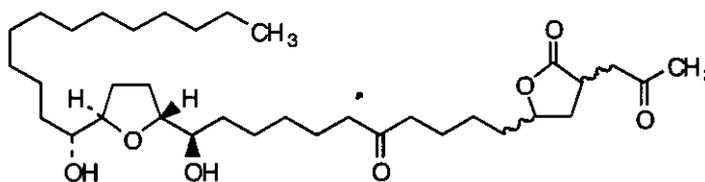
§ Squamone

[CAS No.] 126655-24-1

[化合物分類] ポリケチド (Annonaceae

acetogenins)

[構造式]



[分子式] C₃₃H₆₂O₇

[分子量] 594.871

[正確な分子量] 594.449555

[基原] *Annona squamosa*, *Annona reticulata*

[性状] ワックス様の塊

[融点] Mp 89 °C

[比旋光度]: $[\alpha]_D^{25} +7$ (c, 0.1 in CHCl₃)

[溶解性] BERDY SOL: メタノール, ヘキサンに可溶; 水に難溶

[UV]: [neutral] λ_{max} 0 (end) (ϵ) (MeOH) (Derep) [neutral] λ_{max} 204 (ϵ 10800) (MeOH)

[その他のデータ] 2,4-*cis*- と *trans*-isomers の混合物として分離される

-----文献-----

Li, X.-H. et al., J. Nat. Prod., 1990, 53, 81, (分離, H-NMR, C13-NMR, Mass)

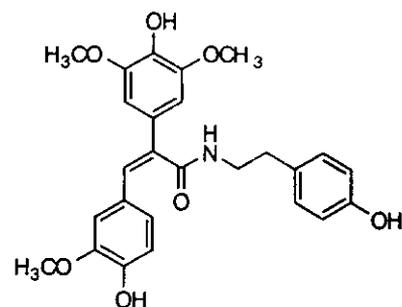
Chang, F.-R. et al., J. Nat. Prod., 1993, 56, 1688, (分離)

§ Squamosamide; (E)-form

[CAS No.] 142750-35-4

[化合物分類] アルカロイド化合物 (Simple tyramine alkaloids), アルカロイド化合物 (Cinnamic acid amides)

[構造式]



[基原] 次の植物から分離: *Annona squamosa* の枝 (バンレイシ科)

[融点] Mp 206-207 °C

-----文献-----

Yang, X.J. et al., *Yaoxue Xuebao*, 1992, 27, 185; CA, 117, 86699d, (分離, 構造決定)

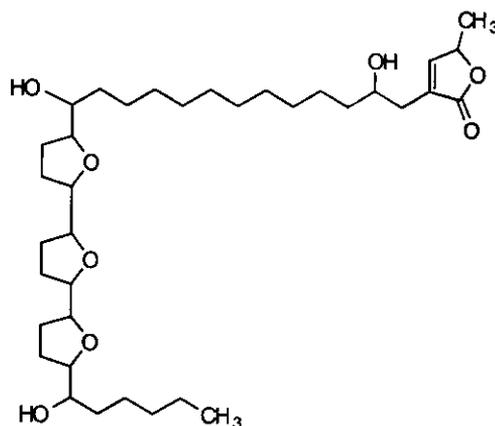
Ji, X. et al., *Chin. Chem. Lett.*, 1993, 4, 297, (合成法, H-NMR, C13-NMR)

§ Squamosinin A

[CAS No.] 163597-71-5

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]



[分子式] C₃₆H₆₂O₈

[分子量] 622.881

[正確な分子量] 622.44447

[基原] *Annona squamosa*

[比旋光度]: [α]_D +24.7 (c, 1.4 in CHCl₃)

-----文献-----

Yang, R. et al., *Zhiwu Xuebao*, 1994, 36, 809; CA, 123, 5595r, (分離, 構造決定)

§ Squamostatin A

[化学名・別名] Almunequin. Annonin XVI

[CAS No.] 129138-53-0

[関連 CAS No.] 128232-75-7

[化合物分類] ポリケチド (Annonaceae acetogenins)

[構造式]

[分子式] C₃₇H₆₆O₈

[分子量] 638.924

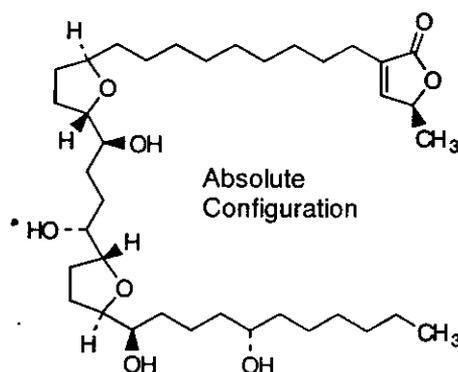
[正確な分子量] 638.47577

[基原] *Annona squamosa*, *Annona cherimola*

[性状] 無定型のワックス

[融点] Mp 105-126 °C (87-89 °C)

[比旋光度]: [α]_D +13.5 (c, 0.1 in CHCl₃). [α]_D +25 (c, 0.38 in MeOH)



-----文献-----

Kawazu, K. et al., *Agric. Biol. Chem.*, 1989, 53, 2719, (分離, Annonin)

Nonfon, M. et al., *Phytochemistry*, 1990, 29, 1951, (分離, H-NMR, C13-NMR, Mass)

Fujimoto, Y. et al., *Tet. Lett.*, 1990, 31, 535, (Squamostatin A)

Yu, J. et al., *Chin. Chem. Lett.*, 1993, 4, 423, (Squamostatin B)

Fang, X.-P. et al., *J. Nat. Prod.*, 1993, 56, 1095, (H-NMR, 構造決定)

Fujimoto, Y. et al., *Chem. Pharm. Bull.*, 1994, 42, 1175, (C13-NMR, H-NMR)

Shimada, H. et al., *Tet. Lett.*, 1994, 35, 3961, (絶対構造)

Laprevote, O. et al., *Tetrahedron*, 1994, 50, 8479, (Mass, 構造決定)

Zafra-Polo, M.C. et al., *Phytochemistry*, 1996, 42, 253, (レビュー)

Cave, A. et al., *Prog. Chem. Org. Nat. Prod.*, 1997, 70, 81, (レビュー)

Chang, F.-R. et al., *Phytochemistry*, 1999, 51, 883, (12,15-cis-Squamostatin A)