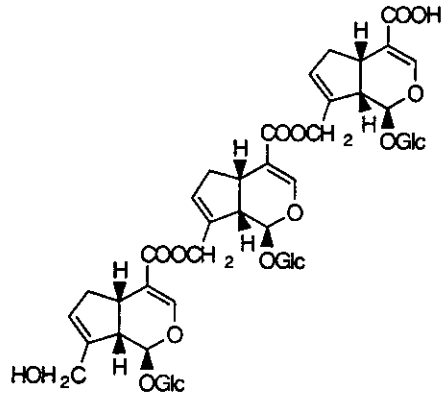


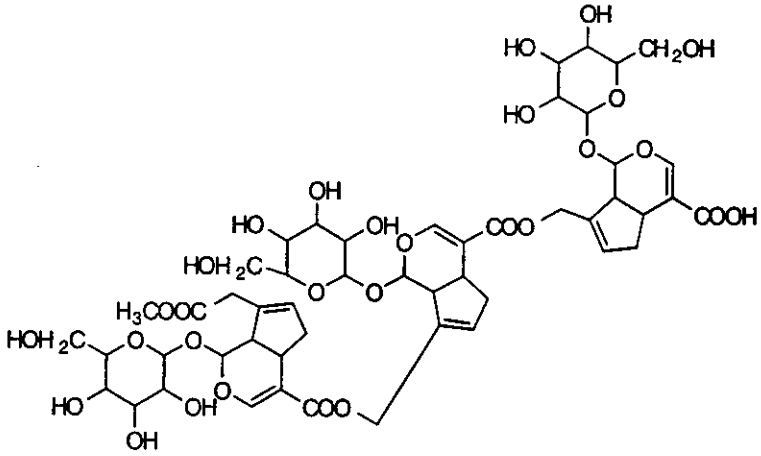
[分子式] $C_{48}H_{62}O_{28}$
[分子量] 1087.001
[正確な分子量] 1086.34277
[基原] *Eucommia ulmoides*
[性状] 粉末
[比旋光度]: $[\alpha]_D$ +7.5 (H2O)

----------文献----------

Yahara, S. et al., Chem. Pharm. Bull., 1990, 38, 267, (分離, H-NMR, C13-NMR)

§ Ulmoidoside A; 10-Ac

[化学名・別名] Ulmoidoside B
[CAS No.] 127214-80-6
[化合物分類] テルペノイド (Iridoid monoterpenoid)
[構造式]



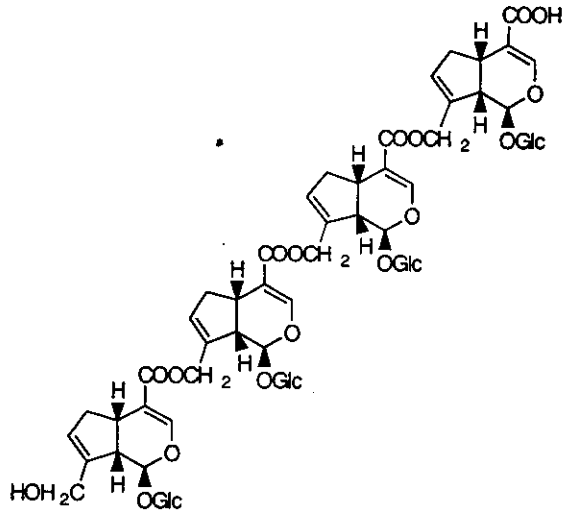
[分子式] $C_{50}H_{64}O_{29}$
[分子量] 1129.038
[正確な分子量] 1128.353335
[基原] *Eucommia ulmoides*
[性状] 粉末
[比旋光度]: $[\alpha]_D$ +8.3 (H_2O)

----------文献----------

Yahara, S. et al., Chem. Pharm. Bull., 1990, 38, 267, (分離, H-NMR, C13-NMR)

§ Ulmoidoside C

[CAS No.] 127214-81-7
[化合物分類] テルペノイド (Iridoid monoterpenoid)
[構造式]



[分子式] $C_{64}H_{82}O_{37}$
[分子量] 1443.33
[正確な分子量] 1442.453505
[基原] *Eucommia ulmoides*
[性状] 粉末
[比旋光度]: $[\alpha]_D$ +9.5 (H_2O)

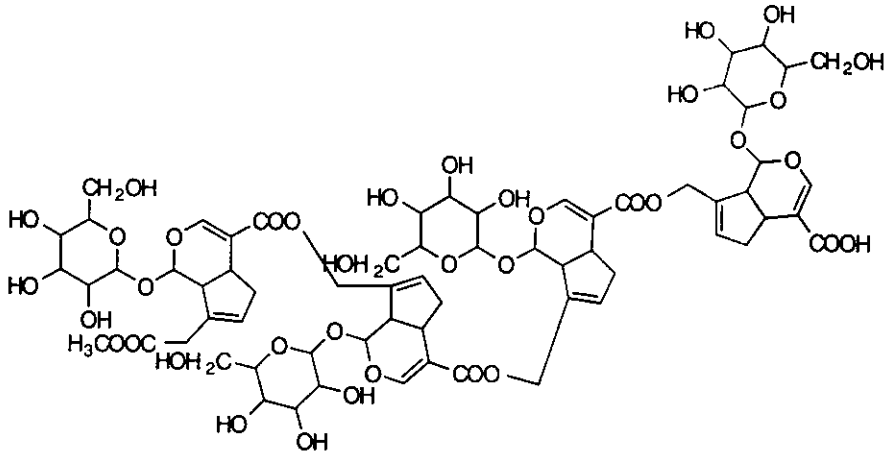
----------文献----------

Yahara, S. et al., Chem. Pharm. Bull., 1990, 38, 267, (分離, H-NMR, C13-NMR)

§ Ulmoidoside C; 10-Ac

[化学名・別名] Ulmoidoside D
[CAS No.] 127214-82-8

[化合物分類]テルペノイド(Iridoid monoterpenoid)
[構造式]

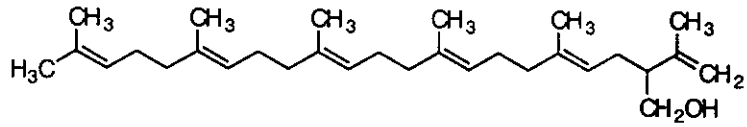


[分子式]$C_{66}H_{84}O_{38}$
[分子量]1485.367
[正確な分子量]1484.46407
[基原]*Eucommia ulmoides*
[性状]粉末
[比旋光度]:[α]$_D$ +15.4
(H_2O)

----------文献----------

Yahara, S. et al., Chem. Pharm. Bull., 1990, 38, 267, (分離, H-NMR, C13-NMR)

§ Ulmoprenol
[CAS No.]70475-06-8
[化合物分類]テルペノイド(Linear triterpenoid)
[構造式]



[分子式]$C_{30}H_{50}O$
[分子量]426.724
[正確な分子量]426.386165
[基原]*Eucommia ulmoides*
[性状]オイル
[沸点]$Bp_{0.00005}$ 180-185 ℃
[比旋光度]:[α]$_D^{20}$ -15

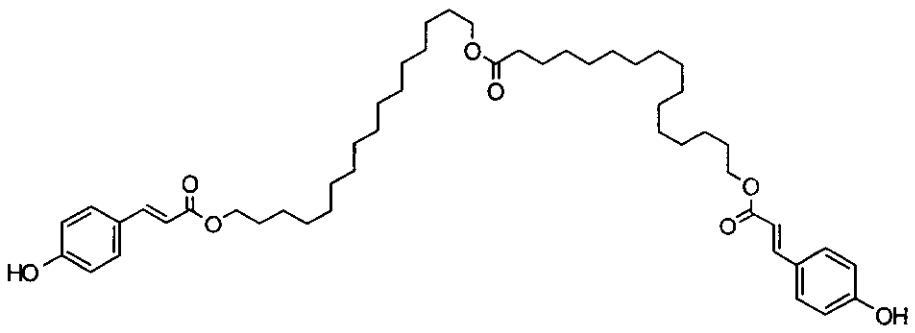
----------文献----------

Hori, Z.-I. et al., Tet. Lett., 1978, 5015

***********ドッググラス (Dog grass, Couch gras)***********

§§イネ科シバムギ(*Agropyron repens* Beauvoi)の根。

§ 16-[[3-(4-Hydroxyphenyl)-1-oxo-2-propenyl]oxy]hexadecyf 16-[[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy]hexadecanoate; (*E,E*)-form
[CAS No.]160388-67-0
[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]



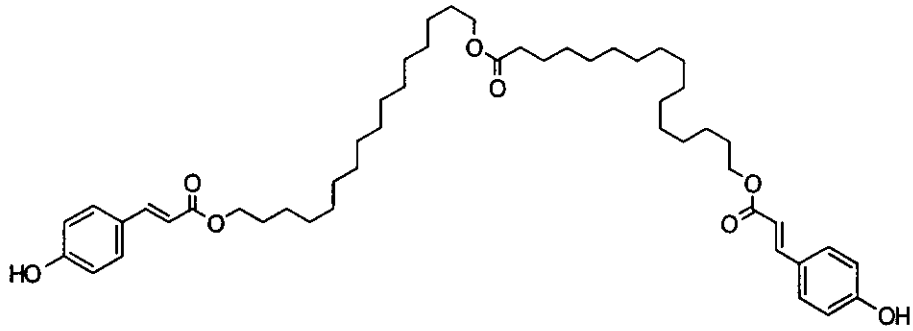
[基原]*Agropyron repens*
(イネ科)の根茎
[性状]ワックス様の塊
[融点]Mp 73-75 ℃
[UV]:[neutral] λ $_{max}$ 226 (); 308 () (MeCN)

----------文献----------

Koetter, U. et al., Planta Med., 1994, 60, 488, (分離, UV, IR, H-NMR, Mas)

§ 16-[[3-(4-Hydroxyphenyl)-1-oxo-2-propenyl]oxy]hexadecyl 16-[[3-(4-hydroxyphenyl)

-1-oxo-2-propenyl] oxy] hexadecanoate; (*Z,Z*)-form
[CAS No.] 160388-68-1
[化合物分類] 単環芳香族(Simple phenylpropanoid)
[構造式]

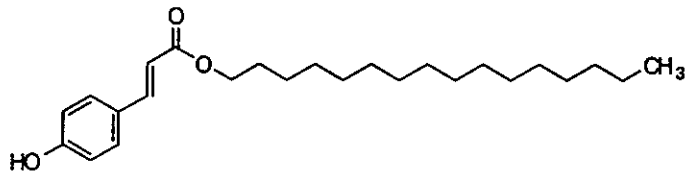


[基原] *Agropyron repens* (イネ科)の根茎
[性状] ワックス様の塊
[融点] Mp 48-56 ℃
[UV]:[neutral] λ max 212 (); 296 () (MeCN)

----------文献----------

Koetter, U. et al., Planta Med., 1994, 60, 488, (分離, UV, IR, H-NMR, Mas)

§ 3-(4-Hydroxyphenyl)-2-propenoic acid; (*E*)-form, Hexadecyl ester
[化学名・別名] Hexadecyl (*E*)-*p*-coumarate. Hexadecyl 4-hydroxycinnamate
[化合物分類] 単環芳香族(Simple phenylpropanoid)
[構造式]

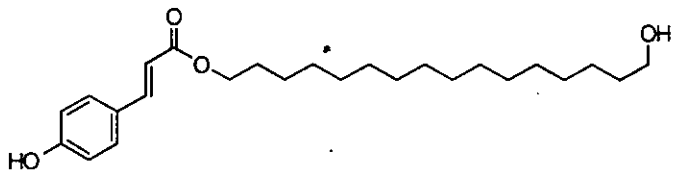


[分子式] $C_{25}H_{40}O_3$
[分子量] 388.589
[正確な分子量] 388.297745
[基原] *Agropyron repens*, *Argyreia speciosa*
[性状] 結晶
[融点] Mp 78 ℃ (63-65 ℃)
[UV]:[neutral] λ max 203 (); 225 (); 309 () (MeOH)

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 951; 953; 955, (生育)
Chatterjee, A. et al., Indian J. Chem., Sect. B, 1980, 19, 421, (Hexacosyl *p*-coumarate)
Srivastava, A. et al., Indian J. Chem., Sect. B, 1998, 37, 192, (hexadecyl ester)

§ 3-(4-Hydroxyphenyl)-2-propenoic acid; (*E*)-form, 16-Hydroxyhexadecyl ester
[化学名・別名] 16-Hydroxyhexadecyl (*E*)-*p*-coumarate
[化合物分類] 単環芳香族(Simple phenylpropanoid)
[構造式]

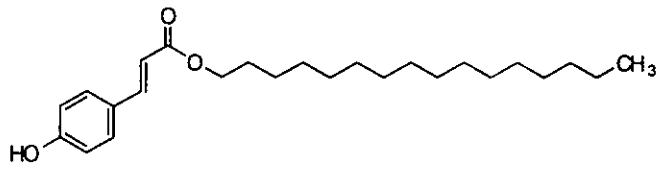


[分子式] $C_{25}H_{40}O_4$
[分子量] 404.589
[正確な分子量] 404.29266
[基原] *Agropyron repens*
[性状] ワックス様の塊
[融点] Mp 107-111 ℃

----------文献----------

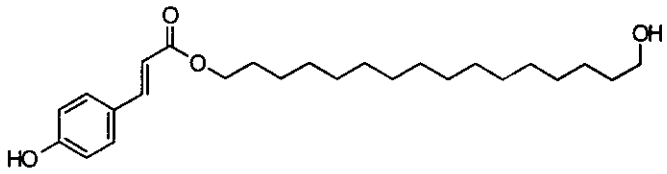
Zincke, T., Annalen, 1902, 322, 224, (分離)
Ogawa, S., Bull. Chem. Soc. Jpn., 1927, 2, 25, (分離)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 951; 953; 955, (生育)
Tachibana, S. et al., Holzforschung, 1980, 34, 131; CA, 93, 222098x, (生育, Me ester)
Chatterjee, A. et al., Indian J. Chem., Sect. B, 1980, 19, 421, (Hexacosyl *p*-coumarate)
Parmar, V.S. et al., Phytochemistry, 1994, 36, 507, (Hexacosanoyl *p*-coumarate)
Srivastava, A. et al., Indian J. Chem., Sect. B, 1998, 37, 192, (hexadecyl ester)

§ 3-(4-Hydroxyphenyl)-2-propenoic acid; (*Z*)-form, Hexadecyl ester
[化学名・別名] Hexadecyl (*Z*)-*p*-coumarate

[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]

[分子式]$C_{25}H_{40}O_3$
[分子量]388.589
[正確な分子量]388.297745
[基原]*Agropyron repens*
[性状]ワックス様の塊
[融点]Mp 42-47 ℃

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhä user Verlag, Basel, 1972, nos. 951; 953; 955, (生育)
Chatterjee, A. et al., Indian J. Chem., Sect. B, 1980, 19, 421, (Hexacosyl *p*-coumarate)
Weyerstahl, P. et al., Annalen, 1994, 1043, (誘導体)
Parmar, V.S. et al., Phytochemistry, 1994, 36, 507, (Hexacosanoyl *p*-coumarate)
Li, C.J. et al., Phytochemistry, 1997, 45, 571, (分離, ester)
Srivastava, A. et al., Indian J. Chem., Sect. B, 1998, 37, 192, (hexadecyl ester)

§ 3-(4-Hydroxyphenyl)-2-propenoic acid; (*Z*)-form, 16-Hydroxyhexadecyl ester
[化学名・別名]16-Hydroxyhexadecyl (*Z*)-*p*-coumarate
[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]

[分子式]$C_{25}H_{40}O_4$
[分子量]404.589
[正確な分子量]404.29266
[基原]*Agropyron repens*
[性状]ワックス様の塊
[融点]Mp 105-108 ℃

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhä user Verlag, Basel, 1972, nos. 951; 953; 955, (生育)
Chatterjee, A. et al., Indian J. Chem., Sect. B, 1980, 19, 421, (Hexacosyl *p*-coumarate)
Parmar, V.S. et al., Phytochemistry, 1994, 36, 507, (Hexacosanoyl *p*-coumarate)
Srivastava, A. et al., Indian J. Chem., Sect. B, 1998, 37, 192, (hexadecyl ester)

§ 1-Phenyl-2,4-hexadiyne
[化学名・別名]2,4-Hexadiynylbenzene(CAS 名). Capillene. Agropyrene. Capilline
[CAS No.]520-74-1
[化合物分類]脂肪族化合物(Miscellaneous acetylene), 単環芳香族(Miscellaneous aryl derivative), 薬物: 抗菌性剤(Antibacterial agent)
[構造式]$PhCH_2C \equiv CC \equiv CCH_3$
[分子式]$C_{12}H_{10}$
[分子量]154.211
[正確な分子量]154.07825
[基原]次の植物から分離: *Artemisia capillaris* のオイル, *Artemisia dracunculus*, *Artemisia scoparia*, *Agropyron repens* (as Agropyrene, impure Capillene)
[用途]抗菌性剤. 種子発芽抑制因子
[性状]オイル
[融点]凝固点: 0 ℃
[沸点]Bp_1 101-103 ℃
[濃度]d^{22}_0 0.977
[屈折率]n^{22}_D 1.581

[Log P 計算値] Log P 3.47(計算値)

----------文献----------

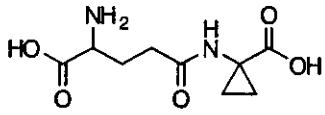
Harada, R. et al., Nippon Kagaku Kaishi, 1957, 78, 415; 1031; CA, 54, 347, (構造決定, 合成法)
Cymerman-Craig, J. et al., Chem. Ind. (London), 1959, 952
Bohlmann, F. et al., Chem. Ber., 1962, 95, 39, (分離)
Yano, K. et al., Phytochemistry, 1994, 37, 689, (分離)

*********トマト (Tomato) *********

§§ ナス科トマト(*Lycopersicon esculentum* Miller)の果実。

§ 1-Aminocyclopropanecarboxylic acid; *N*-(L-γ-Glutamyl)

[化学名・別名] 1-(γ-Glutamylamino)cyclopropanecarboxylic acid
[CAS No.] 171437-78-8
[化合物分類] アミノ酸とペプチド(Dipeptide)
[構造式]



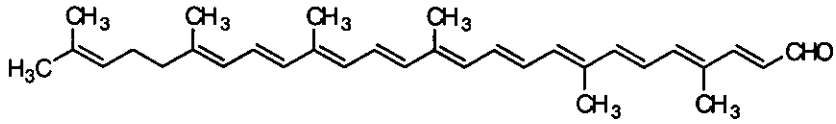
[分子式] $C_9H_{14}N_2O_5$
[分子量] 230.22
[正確な分子量] 230.090273
[基原] 次の植物から分離: トマトの果実(*Lycopersicon esculentum*)

----------文献----------

Baldwin, J.E. et al., Chem. Comm., 1985, 206, (性質)
Yang, S.F. et al., Conjugated Plant Horm.: Proc. Int. Symp., 1986 (1987), 1986, 92, (レビュー)
Amrhein, N. et al., Conjugated Plant Horm.: Proc. Int. Symp., 1986 (1987), 1986, 102
Wiesendanger, R. et al., Experientia, 1986, 42, 207, (生合成)
Vaidyanathan, G. et al., J.O.C., 1989, 54, 1810; 1815, (合成法, 誘導体, 成書)
Stammer, H., Tetrahedron, 1990, 46, 2231, (レビュー)
Alami, A. et al., Bull. Soc. Chim. Fr., 1993, 130, 5, (レビュー)

§ 6'-Apo-ψ-caroten-6'-al

[化学名・別名] Apo-6'-lycopenal. Lycopenal. Apo-2-lycopenal
[CAS No.] 22255-36-3
[化合物分類] テルペノイド(Apocarotenoid)
[構造式]



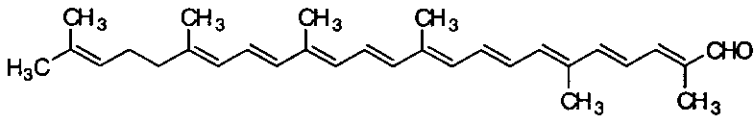
[分子式] $C_{32}H_{42}O$
[分子量] 442.683
[正確な分子量] 442.323565
[基原] 次の植物から分離: *Lycopersicon esculentum*
[性状] 暗赤色の板状結晶 (EtOH)
[融点] Mp 147 ℃
[その他のデータ] λ_{max} 475 nm (EtOH); 569 nm (CS_2); 455, 486, 519 nm (petrol)

----------文献----------

Winterstein, A. et al., Chem. Ber., 1960, 93, 2951, (分離)
Kjosen, H. et al., Phytochemistry, 1969, 8, 483, (Methyl apo-6'-lycopenate)
Ben-Aziz, A. et al., Phytochemistry, 1973, 12, 2759, (分離)

§ Apo-8'-lycopenal

[化学名・別名] 2,6,11,15,19,23-Hexamethyl-2,4,6,8,10,12,14,16,18,22-tetracosadecaenal. 8'-Apo-ψ-caroten-8'-al. Apo-3-lycopenal
[CAS No.] 2213-22-1
[化合物分類] テルペノイド(Linear triterpenoid), テルペノイド(Apocarotenoid)
[構造式]

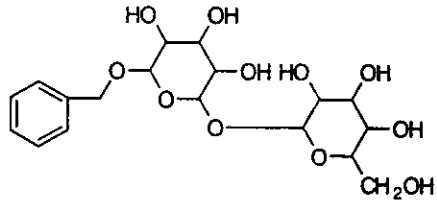


[分子式] $C_{30}H_{40}O$
[分子量] 416.645
[正確な分子量] 416.307915
[基原] 次の植物から分離: *Lycopersicon esculentum*. Oxidation prod. of Lycopene
[性状] 紫色の板状結晶 (C_6H_6/MeOH)
[融点] Mp 141 ℃
[その他のデータ] λ_{max} 280, 475, 505 nm (cyclohexane)

----------文献----------

Ben-Aziz, A. et al., Phytochemistry, 1973, 12, 2759, (分離)
Johansen, J.E. et al., Acta Chem. Scand., Ser. B, 1974, 28, 301, (合成法)

§ Benzyl alcohol; *O*-[β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranoside]
[化学名・別名] Benzyl gentiobioside
[CAS No.] 56775-64-5
[化合物分類] 炭水化物(Disaccharide), 単環芳香族(Simple benzyl alcohol)
[構造式]

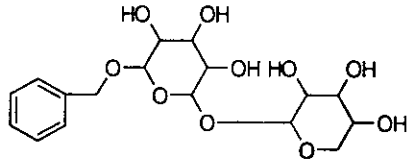


[分子式] $C_{19}H_{28}O_{11}$
[分子量] 432.424
[正確な分子量] 432.163165
[基原] *Lycopersicon esculentum* (ナス科)
[比旋光度]: $[\alpha]_D$ -76.2 (c, 0.01 in H_2O)

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 248, (生育)
Opdyke, D.L.J., Food Cosmet. Toxicol., 1973, 11, 1011, (レビュー, 毒性)
C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002

§ Benzyl alcohol; *O*-[α-L-Arabinopyranosyl-(1 → 6)-β-D-glucopyranoside]
[化合物分類] 単環芳香族(Simple benzyl alcohol), 炭水化物(Disaccharide)
[構造式]

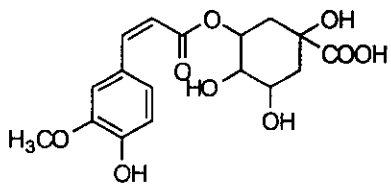


[分子式] $C_{18}H_{26}O_{10}$
[分子量] 402.397
[正確な分子量] 402.1526
[基原] *Lycopersicon esculentum* (ナス科)
[比旋光度]: $[\alpha]_D$ -39 (c, 0.02 in H_2O)

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 248, (生育)
C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002

§ 3-*O*-Caffeoylquinic acid; (*E*)-form, 3'-Me ether
[化学名・別名] 3-*O*-Feruloylquinic acid
[CAS No.] 62929-69-5
[化合物分類] 脂肪族化合物(Monocarbocyclic carboxylic acid andlactone)
[構造式]

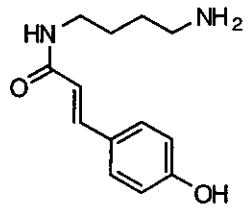


[分子式] $C_{17}H_{20}O_9$
[分子量] 368.34
[正確な分子量] 368.110735
[基原] コーヒー豆. また, *Lycopersicon esculentum*, *Helianthus annuus*, *Nicotiana tabacum*
[融点] Mp 196-197 ℃
[比旋光度]: $[\alpha]_D^{28}$ -42.8 (EtOH)
[UV]: [neutral] λ_{max} 325 (ε 19200) (EtOH)

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 990, (生育)
Ida, Y. et al., Phytochemistry, 1994, 35, 209, (3-Feruloylquinic acid)

§ 4-Coumaroylputrescine
[化学名・別名]4-Hydroxycinnamoylputrescine
[CAS No.]34136-53-3
[化合物分類]アルカロイド化合物(Putrescine alkaloid)
[構造式]

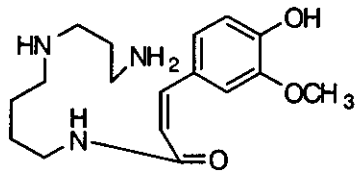


[分子式]$C_{13}H_{18}N_2O_2$
[分子量]234.297
[正確な分子量]234.136828
[基原]次の植物から得られるアルカロイド: *Pennisetum americanum*, *Triticum vulgare*, *Zea mays*, *Persea gratissima*, *Salix* sp., *Lycopersicon esculentum*, *Nicotiana tabacum*, *Petunia hybrid* (イネ科, クスノキ科, ヤナギ科, ナス科)
[性状]弱い黄色の針状結晶・一水和物 (H_2O)
[融点]Mp 182-183.5 ℃

----------文献----------

Stoessl, A. et al., Tet. Lett., 1969, 2807, (誘導体)
Mizusaki, S. et al., Phytochemistry, 1971, 10, 1347, (分離, 合成法)
Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927, (生育)

§ 4-Coumaroylspermidine; 3'-Methoxy
[化学名・別名]Feruloylspermidine
[CAS No.]70185-60-3
[化合物分類]アルカロイド化合物(Acyclic spermidine alkaloid)
[構造式]

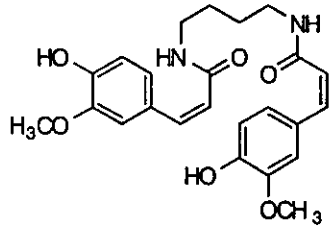


[分子式]$C_{17}H_{27}N_3O_3$
[分子量]312.419
[正確な分子量]312.205242
[基原]次の植物から得られるアルカロイド: *Ananas comosus*, *Lycopersicon esculentum* (パイナップル科, ナス科)

----------文献----------

Deleacutetang, J., Ann. Tab., Sect. 2, 1974, 11, 123; CA, 84, 147656m, (構造決定)
Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927, (生育)

§ Di-4-coumaroylputrescine; 3,3'-Dimethoxy
[化学名・別名]Diferuloylputrescine. *N,N'*-Bis(4-hydroxy-3-methoxycinnamoyl)-1,4-butanediamine
[CAS No.]42369-86-8
[化合物分類]アルカロイド化合物(Putrescine alkaloid)
[構造式]



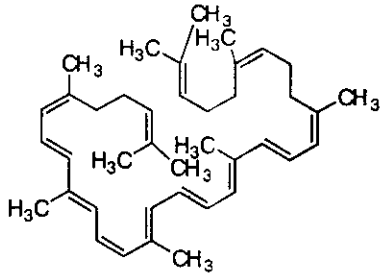
[分子式]$C_{24}H_{28}N_2O_6$
[分子量]440.495
[正確な分子量]440.194738
[基原]次の植物から得られるアルカロイド: *Ananas comosus*, *Triticum vulgare*, *Gomphrena globosa*, *Dianthus caryophyllus*, *Vicia faba*, *Lycopersicon esculentum*, *Petunia* sp., *Nicotiana tabacum* (パイナップル科, イネ科, ヒユ科, ナデシコ科, マメ科, ナス科)

----------文献----------

Martin-Tanguy, J. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1973, 276, 1433, (UV, 構造決定, 合成法, Diferuloylputrescine)
Cabanne, F. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1976, 282, 1959, (UV, 構造決定, Dicaffeoylputrescine)

§ 7,8-Dihydrolycopene; (9Z,7'Z,9'Z)-form

[CAS No.] 10467-46-6
[化合物分類] テルペノイド (Tetraterpenoid)
[構造式]

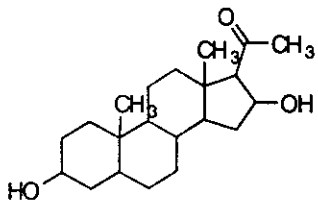


[基原] 次の植物から分離: *Lycopersicon esculentum* var. *'Tangella'*
[性状] 暗赤色の粘着性オイル
[その他のデータ] λ_{max} 410, 433 nm (hexane)

----------文献----------

Suzue, G. et al., Biochim. Biophys. Acta, 1969, 176, 653, (生合成)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1817b, (生育)
Frecknell, E.A. et al., Phytochemistry, 1984, 23, 1707, (分離, 生育)
Straub, O. et al., Key to Carotenoids, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 34, (成書)

§ 3,16-Dihydroxypregnan-20-one; (3 β,5 α,16 β)-form
[化学名・別名] Lycopersiconol
[CAS No.] 20745-29-3
[化合物分類] ステロイド (Pregnane steroid). (C21)
[構造式]

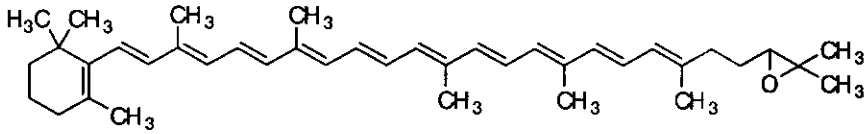


[基原] 次の植物から分離: *Lycopersicon esculentum*, *Lycopersicon hirsutum*
[性状] 結晶 (Me_2CO)
[融点] Mp 255-258 ℃ (分解) (202-204 ℃)
[比旋光度]: $[\alpha]_D^{27}$ +51.3 (c, 0.95 in MeOH/$CHCl_3$). $[\alpha]_D^{18}$ +58.3 (c, 0.309 in $CHCl_3$)

----------文献----------

Yoshihara, T. et al., Phytochemistry, 1988, 27, 3982, (Lycopersiconol)

§ 1',2'-Epoxy-1',2'-dihydro-β,ψ-carotene;
[CAS No.] 92008-21-4
[化合物分類] テルペノイド (Tetraterpenoid)
[構造式]

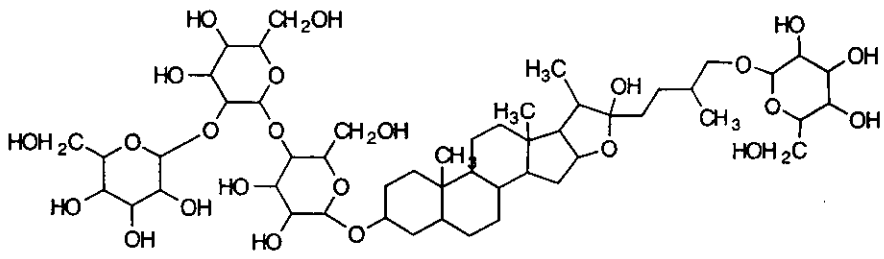


[基原] 次の植物から分離: トマト変異株 (*Lycopersicon esculentum*); 8'-Apo-β-caroten-8'-al から合成
[性状] 赤色の結晶 (CH_2Cl_2/MeOH)
[融点] Mp 142-143 ℃

----------文献----------

Britton, G. et al., Phytochemistry, 1975, 14, 2530, (分離)
Kamber, M. et al., Helv. Chim. Acta, 1984, 67, 968, (合成法, 絶対構造)
Straub, O. et al., Key to Carotenoids, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 215

§ Furostane-3,22,26-triol; (3 β,5 α,22 α,25)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside
[化学名・別名] Tomatoside A
[CAS No.] 75557-22-1
[化合物分類] ステロイド (Furostane steroid). (C27).
[構造式]



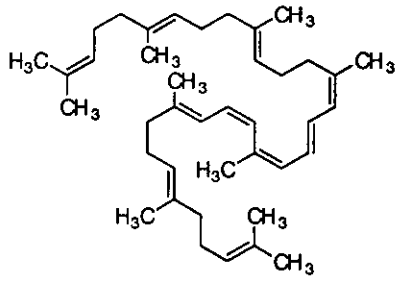
[分子式] $C_{51}H_{86}O_{24}$
[分子量] 1083.226
[正確な分子量] 1082.55091
[基原] *Lycopersicon esculentum* (トマト)
[性状] 結晶

[融点]Mp 247-250 ℃で分解
[比旋光度]:[α]$_D^{20}$ -29.3 (c, 1.18 in Py)

----------文献----------

Sato, H. et al., Agric. Biol. Chem., 1973, 37, 225, (Tomatoside A)
Shchelochkova, A.P. et al., Khim. Prir. Soedin., 1980, 16, 533; Chem. Nat. Compd. (Engl. Transl.), 1980, 16, 386, (Tomatoside A)

§ 7,7',8,8',11,12-Hexahydrolycopene; (15Z,9'Z)-form



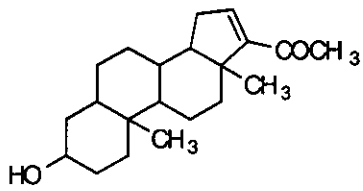
[CAS No.]72746-34-0
[化合物分類]テルペノイド(Tetraterpenoid)
[構造式]

[基原]次の植物から分離: *Lycopersicon esculentum* var. *'Tangella'*
[性状]強い青緑色の蛍光を伴う黄色オイル
[UV]:[neutral] λ $_{max}$ 249 (); 257 (); 331 (); 348 (); 367 () (hexane)

----------文献----------

Zechmeister, L. et al., Arch. Biochem. Biophys., 1953, 47, 160, (生育)
Davis, J.B. et al., J.C.S.(C), 1966, 2154, (分離, 構造決定)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1817, (生育)
Frecknall, E.A. et al., Phytochemistry, 1984, 23, 1707, (生育)
Ebenezer, W.J. et al., J.C.S. Perkin 1, 1993, 1869, (9Z-isomer)

§ 3-Hydroxypregn-16-en-20-one; (3 β,5 α)-form



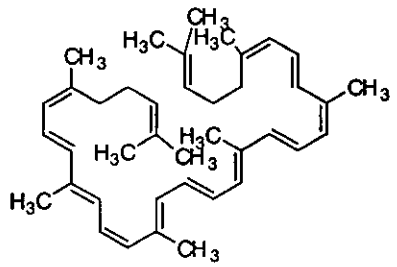
[CAS No.]566-61-0
[化合物分類]ステロイド(Pregnane steroid). (C21)
[構造式]

[基原]次の植物から分離: *Lycopersicon esculentum*
[性状]結晶(EtOAc)
[融点]Mp 207-209 ℃ (180-183 ℃)
[比旋光度]:[α]$_D^{25}$ +51 (c, 0.530 in $CHCl_3$)

----------文献----------

Djerassi, C. et al., Tetrahedron, 1957, 1, 22, (合成法, 3 β,5 α,8 α-form)
Hirschmann, H. et al., J. Biol. Chem., 1961, 236, 3141, (合成法, IR, 3 α,5 α-form)
Nagata, W. et al., Tetrahedron, 1961, 13, 295, (合成法, (±)-3 β,5 α-form)
Crabbeacute, P. et al., Can. J. Chem., 1963, 41, 156, (合成法, 3 β,5 α-form)
Tschesche, R. et al., Chem. Ber., 1965, 98, 1188, (合成法, 3 β,5 α-form)
Mukawa, C. et al., Bull. Chem. Soc. Jpn., 1972, 45, 574, (誘導体, 3 β,5 α,8 α,14 β-form)
Jankowski, K. et al., Steroids, 1972, 19, 189, (H-NMR, 3 β,5 α-form)
Baillie, T.A. et al., J. Labelled Compd., 1974, 10, 549, (合成法, Mass, 3 α,5 α-form)
Kirk, D.N. et al., J.C.S. Perkin 2, 1990, 1567, (H-NMR)

§ Lycopene; (7Z,7'Z,9Z,9'Z)-form



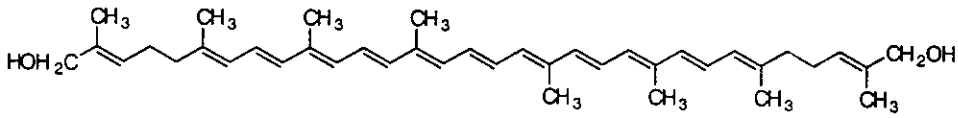
[化学名・別名]Prolycopene
[CAS No.]2361-24-2
[化合物分類]テルペノイド(Tetraterpenoid)
[構造式]
[基原]*Lycopersicon esculentum*. また他の果実
[性状]赤色のプリズム結晶 (C_6H_6/MeOH); 赤-橙色の薄片状の結晶 (hexane/EtOH)
[融点]Mp 111 ℃
[その他のデータ]λ $_{max}$ 232, 255, 295, 437 nm (hexane)

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag,

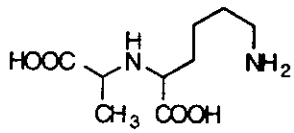
Basel, 1972, nos. 1818; 1820, (生育)
Ben-Aziz, A. et al., Phytochemistry, 1973, 12, 2759, (分離)
Clough, J.M. et al., J.C.S. Perkin 1, 1983, 3011, (Prolycopene)
Straub, O. et al., Key to Carotenoids, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 31, (成書)
Stahl, W. et al., Arch. Biochem. Biophys., 1996, 336, 1, (レビュー)
Bramley, P. M. et al., Phytochemistry, 2000, 54, 233, (レビュー)

§ Lycophyll

[化学名・別名] ψ,ψ-Carotene-16,16'-diol. 16,16'-Dihydroxylycopene
[CAS No.] 19891-75-9
[化合物分類] テルペノイド(Tetraterpenoid)
[構造式]

[分子式] $C_{40}H_{56}O_2$
[分子量] 568.881
[正確な分子量] 568.42803
[基原] ナス科の属. 例えば, *Solanum dulcamara*, *Lycopersicon esculentum*, また *Chromatium minutissimum* により生産される
[性状] 紫-赤色の結晶 (C_6H_6/MeOH)
[融点] Mp 191 ℃

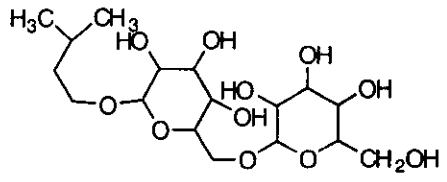
文献
Kelly, M. et al., Acta Chem. Scand., 1971, 25, 1607, (stereochem)
Kjosen, H. et al., Acta Chem. Scand., 1972, 26, 4121, (分離, 合成法)

§ Lysopine; L-form

[化合物分類] アミノ酸とペプチド(Miscellaneous modified aminoacid)
[構造式]

[基原] 試験管内でクラウンゴールドの組織培養で得られるアミノ酸. また *Nicotiana tabacum* と *Lycopersicon esculentum* (タバコ, トマト)の乾燥した組織から分離される
[性状] 針状結晶・二水和物 (EtOH 溶液)
[融点] Mp 157-160 ℃. Mp 240 ℃で分解 (double Mp)
[比旋光度]: $[\alpha]_D$ +18 (c, 1.40 in H_2O)
[その他のデータ] 天然及び合成品は共に光学異性体の混合物である

文献
Lioret, C., C. R. Hebd. Seances Acad. Sci., 1957, 244, 2171, (分離)
Biemann, K. et al., Biochim. Biophys. Acta, 1960, 40, 369, (構造決定, Mass, 合成法)
Kemp, J.D., Plant Physiol., 1978, 62, 26, (合成法, 生合成)

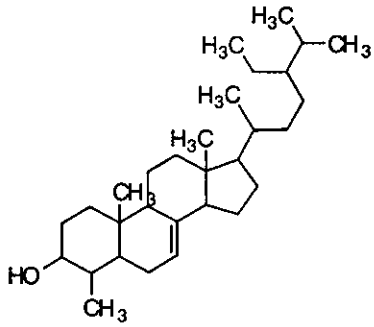
§ 3-Methyl-1-butanol; *O*-[β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranoside]

[化学名・別名] Isopentyl gentiobioside
[CAS No.] 178275-89-3
[化合物分類] テルペノイド(Hemiterpenoid), 脂肪族化合物(Branched aliphatic alcohol)
[構造式]

[分子式] $C_{17}H_{32}O_{11}$
[分子量] 412.433
[正確な分子量] 412.194465
[基原] トマトの組織細胞(*Lycopersicon esculentum*) (ナス科)
[比旋光度]: $[\alpha]_D$ -41.5 (c, 0.01 in H_2O)

文献
Bieber, H., Encycl. Chem. Process. Des., 1977, 3, 278, (レビュー)
Opdyke, D.L.J., Food Cosmet. Toxicol., 1978, 16, 785, (レビュー, 毒性)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, 2, 709, (レビュー)
De Rosa, S. et al., Phytochemistry, 1996, 42, 1031, (gentiobioside)

§ 4-Methylstigmast-7-en-3-ol; (3 β,4 α,5 α,24*R*)-form

[化学名・別名]24-Ethyllophenol
[CAS No.]36735-29-2
[化合物分類]ステロイド(Stigmastane steroid). (C29).
[構造式]



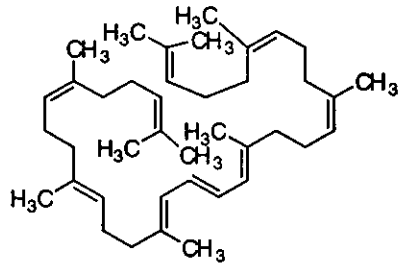
[基原]次の植物から分離: *Bryonia alba* の種子, *Lycopersicon esculentum*, 多くの植物(野菜)オイル
[性状]結晶(Me_2CO/MeOH)
[融点]Mp 175.5-176.5 ℃

----------文献----------

Panosyan, A.G. et al., Khim. Prir. Soedin., 1977, 13, 353; 1980, 16, 781; Chem. Nat. Compd. (Engl. Transl.), 1977, 13, 300; 1980, 16, 554, (分離)
Itoh, T. et al., Fette, Seifen, Anstrichm., 1978, 80, 382
Itoh, T. et al., Phytochemistry, 1980, 19, 2491
Itoh, T. et al., Yukagaku, 1981, 30, 586, (HPLC)

§ 7,7',8,8',11,11',12,12'-Octahydrolycopene; (15*Z*)-Isomer

[化学名・別名]15-*cis*-Pytoene. 15*Z*-Phytoene isomer
[CAS No.]13920-14-4
[化合物分類]テルペノイド(Tetraterpenoid)
[構造式]



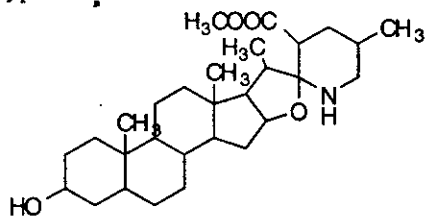
[基原]次の植物から分離: *Lycopersicon esculentum* var. `*Tangella*', *Dunaliella bardawil*
[性状]淡い橙色のオイル
[その他のデータ]λ_{max} 286, 296 nm (hexane)

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1817a, (生育)
Clough, J.M. et al., J.C.S. Perkin 1, 1983, 3011, (15Z-Phytoene, IR, H-NMR, C13-NMR)
Frecknell, E.A. et al., Phytochemistry, 1984, 23, 1707, (分離, 生育)
Straub, O. et al., Key to Carotenoids, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 44, (成書)

§ Spirosolane-3,23-diol; (3 β,5 α,22*R*,23*S*,25*R*)-form, 23-Ac

[化学名・別名]23-Acetoxysoladulcidine
[CAS No.]152128-85-3
[化合物分類]アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]



[分子式]$C_{29}H_{47}NO_4$
[分子量]473.695
[正確な分子量]473.350509
[基原]次の植物の根から得られるアルカロイド: *Lycopersicon esculentum* - *Lycopersicon hirsutum* hybrid
[性状]無定型
[比旋光度]:$[\alpha]_{D20}$ -46 (c, 0.37 in $CHCl_3$)

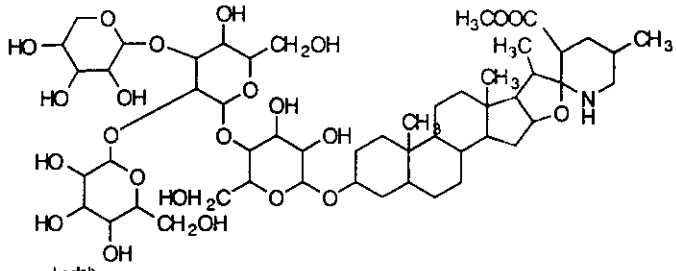
----------文献----------

Ripperger, H. et al., Phytochemistry, 1993, 32, 1607, (23-Hydroxysoladulcidine)
Nagaoka, T. et al., Phytochemistry, 1993, 34, 1153, (23-Acetoxysoladulcidines, 23-Acetoxytomatidine)
Yahara, S. et al., Phytochemistry, 1996, 42, 169, (Lycoperoside)

§ Spirosolane-3,23-diol; (3 β,5 α,22*R*,23*S*,25*R*)-form, 23-Ac, 3-*O*-[β-D-glucopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]

[化学名・別名]Lycoperoside B
[CAS No.]176300-86-0

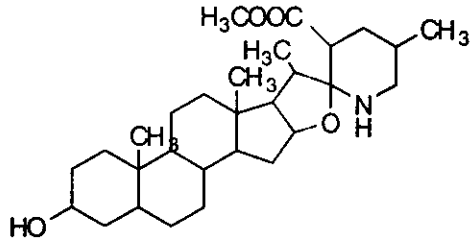
[化合物分類]アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]
[分子式]$C_{52}H_{85}NO_{23}$
[分子量]1092.236
[正確な分子量]1091.551244
[基原]次の植物から得られるアルカロイド:
Lycopersicon esculentum
[性状]無定型の粉末
[比旋光度]:[α]$_{D27}$ -40.3 (c, 0.56 in MeOH)



----------文献----------

Yahara, S. et al., Phytochemistry, 1996, 42, 169, (Lycoperoside)

§ Spirosolane-3,23-diol; (3 β,5 α,22*R*,23*S*,25)-form, 23-Ac
[化学名・別名]23-Acetoxy-25-episoladulcidine
[CAS No.]152128-86-4
[化合物分類]アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]
[分子式]$C_{29}H_{47}NO_4$
[分子量]473.695
[正確な分子量]473.350509

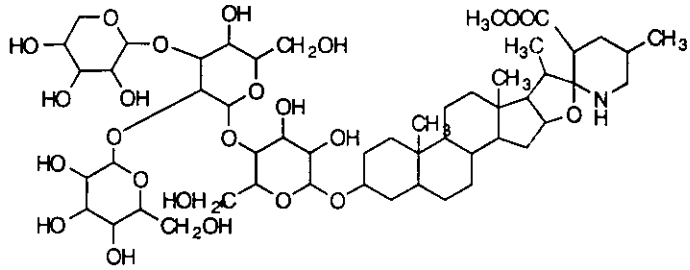


[基原]次の植物の根から得られるアルカロイド: *Lycopersicon esculentum* - *Lycopersicon hirsutum* hybrid
[性状]無定型
[比旋光度]:[α]$_{D20}$ -36.7 (c, 1.2 in $CHCl_3$)

----------文献----------

Ripperger, H. et al., Phytochemistry, 1993, 32, 1607, (23-Hydroxysoladulcidine)
Nagaoka, T. et al., Phytochemistry, 1993, 34, 1153, (23-Acetoxysoladulcidines, 23-Acetoxytomatidine)
Yahara, S. et al., Phytochemistry, 1996, 42, 169, (Lycoperoside)

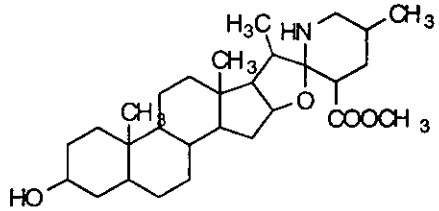
§ Spirosolane-3,23-diol; (3 β,5 α,22*R*,23*S*,25)-form, 23-Ac, 3-*O*-[β-D-glucopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]
[化学名・別名]Lycoperoside C
[CAS No.]176300-87-1
[化合物分類]アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]
[分子式]$C_{52}H_{85}NO_{23}$
[分子量]1092.236
[正確な分子量]1091.551244
[基原]次の植物から得られるアルカロイド: *Lycopersicon esculentum*
[性状]無定型の粉末
[比旋光度]:[α]$_{D27}$ -26.3 (c, 0.63 in MeOH)



----------文献----------

Ripperger, H. et al., Phytochemistry, 1993, 32, 1607, (23-Hydroxysoladulcidine)
Nagaoka, T. et al., Phytochemistry, 1993, 34, 1153, (23-Acetoxysoladulcidines, 23-Acetoxytomatidine)
Yahara, S. et al., Phytochemistry, 1996, 42, 169, (Lycoperoside)

§ Spirosolane-3,23-diol; (3 β,5 α,22*S*,23*R*,25)-form, 23-Ac
[化学名・別名]23 R -Acetoxytomatidine
[CAS No.]152128-84-2
[化合物分類]アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]
[分子式]$C_{29}H_{47}NO_4$

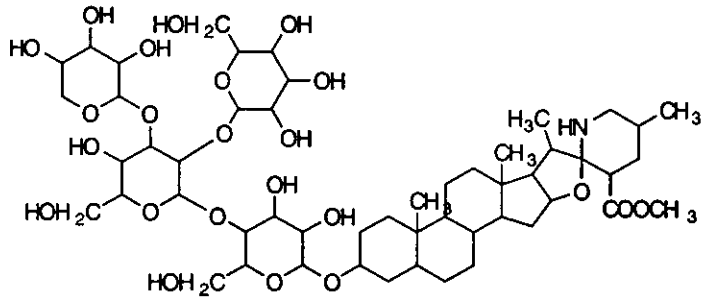


[分子量]473.695
[正確な分子量]473.350509
[基原]次の植物の根から得られるアルカロイド: *Lycopersicon esculentum* / *Lycopersicon hirsutum* hybrid
[性状]無定型
[比旋光度]:[α]$_{D20}$ -2.8 (c, 0.42 in $CHCl_3$)

----------文献----------

Ripperger, H. et al., Phytochemistry, 1993, 32, 1607, (23-Hydroxysoladulcidine)
Nagaoka, T. et al., Phytochemistry, 1993, 34, 1153, (23-Acetoxysoladulcidines, 23-Acetoxytomatidine)
Yahara, S. et al., Phytochemistry, 1996, 42, 169, (Lycoperoside)

§ Spirosolane-3,23-diol; (3 β,5 α,22*S*,23*R*,25*S*)-form, 23-Ac, 3-*O*-[β-D-glucopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]
[化学名・別名]23*R*-Acetoxytomatine. Lycoperoside A
[CAS No.]176181-33-2
[化合物分類]アルカロイド化合物 (Steroidal alkaloid) (spirosolane type)
[構造式]

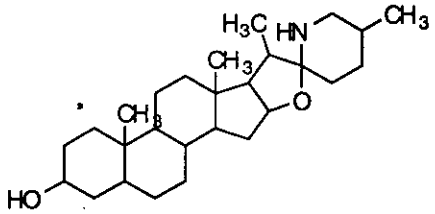


[分子式]$C_{52}H_{85}NO_{23}$
[分子量]1092.236
[正確な分子量]1091.551244
[基原]次の植物から得られるアルカロイド: *Lycopersicon esculentum*
[性状]無定型の粉末
[比旋光度]:[α]$_{D27}$ -31.6 (c, 0.8 in MeOH)

----------文献----------

Ripperger, H. et al., Phytochemistry, 1993, 32, 1607, (23-Hydroxysoladulcidine)
Nagaoka, T. et al., Phytochemistry, 1993, 34, 1153, (23-Acetoxysoladulcidines, 23-Acetoxytomatidine)
Yahara, S. et al., Phytochemistry, 1996, 42, 169, (Lycoperoside)

§ Spirosolan-3-ol; (3 β,5 α,22*S*,25*S*)-form
[化学名・別名]Tomatidine. 5 α-Tomatidan-3 β-ol(旧 CAS 名)
[CAS No.]77-59-8
[化合物分類]薬物: 抗コリンエステラーゼ(Anticholinesterase), 薬物: 抗カビ薬(Antifungal agent), 薬物: 抗炎症薬(Antiinflammatory agent), 薬物: 外皮用剤(Dermatological agent), アルカロイド化合物 (Steroidal alkaloid) (spirosolane type)
[構造式]



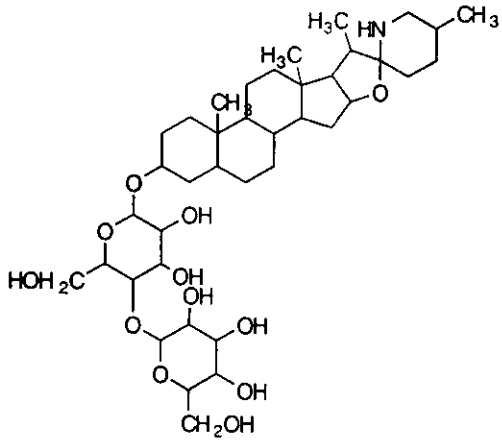
[基原]次の植物から得られるアルカロイド: *Lycopersicon esculentum*, *Solanum demissum*, その他多くの *Lycopersicon* や *Solanum* spp. (ナス科)の配糖体として得られる
[用途]抗カビ, 皮膚炎に対して治療に用いられる細胞増殖抑制活性を示す. コリンエステラーゼ抑制因子, 抗ヒスタミン作用.
[融点]Mp 210-211 ℃
[比旋光度]:[α]$_{D20}$ +5 (MeOH)
[Log P 計算値]Log P 6.08 (未確認値)(計算値)

----------文献----------

Brink, N.G. et al., J.A.C.S., 1951, 73, 4018, (分離, Tomatidine)
Sato, Y. et al., J.A.C.S., 1957, 79, 6089, (Tomatidine, 構造決定)
Budzikiewicz, H., Tetrahedron, 1964, 20, 2265, (Tomatidine, Mas)
Kennard, O. et al., J.C.S.(C), 1967, 956, (結晶構造, Tomatidine)
Weston, R.J. et al., Aust. J. Chem., 1977, 30, 917, (Tomatidine, C13-NMR)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, THG250

§ Spirosolan-3-ol; (3 β,5 α,22*S*,25*S*)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 4)-β-D-galactopyranoside]

[化学名・別名] γ-Tomatine. Lycoperoside D
[CAS No.] 81037-16-3
[化合物分類] アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]

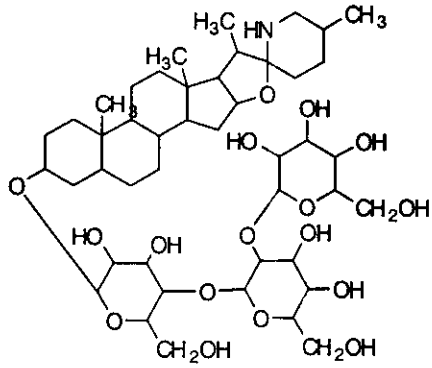


[分子式] $C_{39}H_{65}NO_{12}$
[分子量] 739.942
[正確な分子量] 739.450679
[基原] 次の植物から得られるアルカロイド: *Lycopersicon esculentum*
[性状] 無定型の粉末
[比旋光度]: [α]$_{D27}$ -10.8 (c, 0.6 in MeOH)

----------文献----------

Yahara, S. et al., Phytochemistry, 1996, 42, 169, (Lycoperoside)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, THG250

§ Spirosolan-3-ol; (3 β,5 α,22*S*,25*S*)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]
[化学名・別名] β$_1$-Tomatine
[CAS No.] 17406-46-1
[化合物分類] アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]



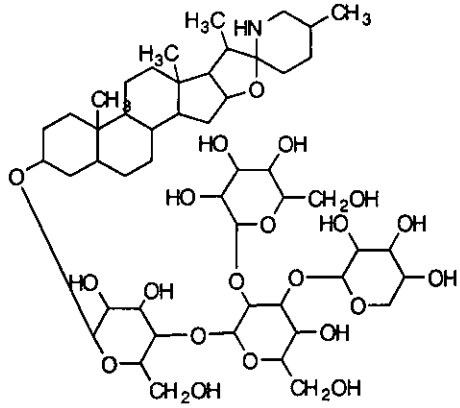
[分子式] $C_{45}H_{75}NO_{17}$
[分子量] 902.084
[正確な分子量] 901.503504
[基原] 次の植物から得られるアルカロイド: *Lycopersicon esculentum*, *Lycopersicon pimpinellifolium*, また Tomatine (ナス科) の部分的加水分解によっても得られる
[性状] 無定型の塊・一水和物
[融点] Mp 240-260 ℃で分解
[比旋光度]: [α]$_{D22}$ -28 (c, 1 in Py)
[その他のデータ] 完全な純品ではない.

----------文献----------

Kuhn, R. et al., Chem. Ber., 1957, 90, 203, (Tomatine)
Yahara, S. et al., Phytochemistry, 1996, 42, 169, (Lycoperoside)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, THG250

§ Spirosolan-3-ol; (3 β,5 α,22*S*,25*S*)-form, *O*-[β-D-Glucopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1

→ 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]
[化学名・別名]Tomatine. α-Tomatine. Lycopersicin
[CAS No.]17406-45-0
[化合物分類]薬物: 軟体動物(ナメクジ)駆除剤(Molluscicide) アルカロイド化合物(Steroidal alkaloid) (spirosolane type), 薬物: 抗菌性剤(Antibacterial agent), 薬物: 抗カビ薬(Antifungal agent), 薬物: 抗炎症薬(Antiinflammatory agent)
[構造式]



[分子式]$C_{50}H_{83}NO_{21}$
[分子量]1034.2
[正確な分子量]1033.545764
[基原]次の植物から得られるアルカロイド: *Lycopersicon esculentum*, *Lycopersicon cheesmanii*, *Lycopersicon chilense*, *Lycopersicon pruniforme*, *Solanum polyadenium*, *Solanum tomatillo*, *Solanum boerhaavii*, *Solanum demissum*, *Solanum acaule*, *Solanum kieseritzii*, *Solanum verbascifolium* (ナス科)
[用途]抗炎症薬. 抗菌, 抗カビ剤. 軟体動物(ナメクジ)駆除性を示す.
[融点]Mp 263-267 ℃で分解
[比旋光度]:[α]$_D$ -19(Py)
[溶解性] メタノール, エタノール, ヂオキサンに可溶; 水, エーテル, 酸, ヘキサンに易溶; クロロホルム, EtOAc, ベンゼンに難溶
[Log P 計算値]Log p -3.27 (未確認値)(計算値)
[UV]:[neutral] λ_{max} (EtOH)
[傷害・毒性]50 %致死量(LD_{50})(ラット, 経口) 900 mg/kg; BERDY HAZD : 50 %致死量(LD_{50})(マウス, 腹膜内) 25 mg/kg , 50 %致死量(LD_{50})(マウス, 皮下) 1000 mg/kg , 50 %致死量(LD_{50})(マウス, 経口) 500 mg/kg
[化学物質毒性データ総覧(RTEC)登録番号]XW1050000

----------文献----------

Kuhn, R. et al., Chem. Ber., 1957, 90, 203, (Tomatine)
Yahara, S. et al., Phytochemistry, 1996, 42, 169, (Lycoperoside)
THG250

*****RTECS (化学物質毒性データ) *****

生体影響物質　　: 変異原物質. 天然物.

*****健康障害に関するデータ*****

*****急性毒性に関するデータ*****

〈〈試験方法〉〉 LD50 試験(50%致死量試験).
曝露経路　　: 経口投与.
被験動物　　: げっ歯類-マウス
投与量・期間 : 500 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

FCTXAV Food and Cosmetics Toxicology. (London, UK) V.1-19, 1963-81. For publisher information, see FCTOD7. [Vol.,頁,年(19-)]17,61,1979

〈〈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 : 25 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

SZAPAC Schweizerische Zietschrift fuer Allgemeine Pathologie und Bakteriologie. (White Plains, NY) V.1-3, 1938-40; V.13-22, 1950-59. For publisher information, see ECEBDI. [Vol.,頁,年(19-)] 22,557,1959

〈〈試験方法〉〉 LD50 試験(50%致死量試験).
曝露経路　　: 皮下投与.
被験動物　　: げっ歯類-マウス
投与量・期間 : 1 gm/kg

毒性影響　　：致死量以外に毒性影響に関する報告はない.
参照文献

85GDA2 "CRC Handbook of Antibiotic Compounds," Vols.1- , Berdy, J., Boca Raton, FL, CRC Press, 1980- [Vol.,頁,年(19-)]8(2),218,1982

変異原性に関するデータ

〈〈試験方法〉〉 DNA 阻害.
試験系　　：微生物(種は未特定).
投与量・期間：25 ppm
参照文献

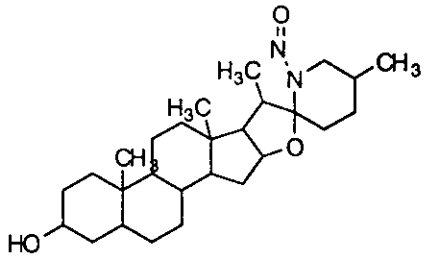
FCTXAV Food and Cosmetics Toxicology. (London, UK) V.1-19, 1963-81. For publisher information, see FCTOD7. [Vol.,頁,年(19-)]17,61,1979

〈〈試験方法〉〉 変異原試験-通常の試験法.
試験系　　：微生物(種は未特定).
投与量・期間：25 ppm
参照文献

FCTXAV Food and Cosmetics Toxicology. (London, UK) V.1-19, 1963-81. For publisher information, see FCTOD7. [Vol.,頁,年(19-)]17,61,1979

§ Spirosolan-3-ol; (3 β,5 α,22*S*,25)-form, *N*-Nitroso

[化学名・別名]*N*-Nitrosotomatidine
[CAS No.]4847-05-6
[化合物分類]アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]



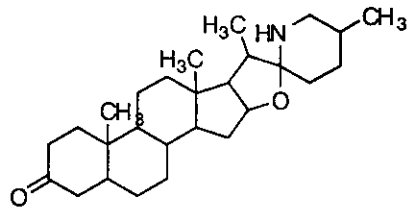
[分子式]$C_{27}H_{44}N_2O_3$
[分子量]444.656
[正確な分子量]444.335193
[基原]次の植物の葉と茎から得られるアルカロイド: *Lycopersicon esculentum* (ナス科)
[性状]六角形の結晶. 加熱により小枝状になる
[融点]Mp 234-237 ℃

----------文献----------

Garnero, J. et al., CA, 1982, 96, 148962t, (*N*-Nitrosotomatidine)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, THG250

§ Spirosolan-3-ol; (3 β,5 α,22*S*,25)-form, 3-Ketone

[化学名・別名]5 α-Tomatidan-3-one
[CAS No.]6870-84-4
[化合物分類]アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]

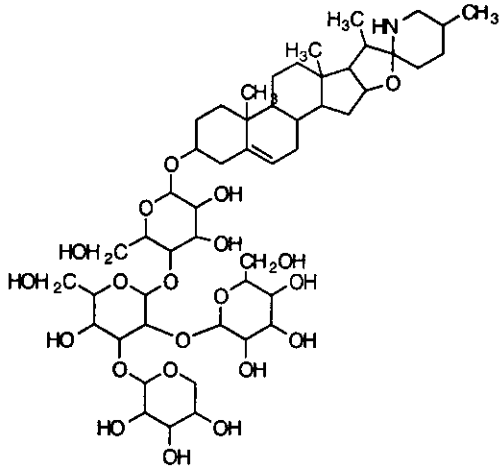


[分子式]$C_{27}H_{43}NO_2$
[分子量]413.642
[正確な分子量]413.329379
[基原]次の植物の根から得られるアルカロイド: *Lycopersicon esculentum* / *Lycopersicon hirsutum* hybrid
[性状]針状結晶(MeOH)
[融点]Mp 195-198 ℃
[比旋光度]:[α]$_{D20}$ +19 (c, 0.38 in $CHCl_3$)

----------文献----------

Nagaoka, T. et al., Phytochemistry, 1993, 34, 1153, (5 α-Tomatidan-3-one)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, THG250

§ Spirosol-5-en-3-ol; (3 β,22*S*,25*)*-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]

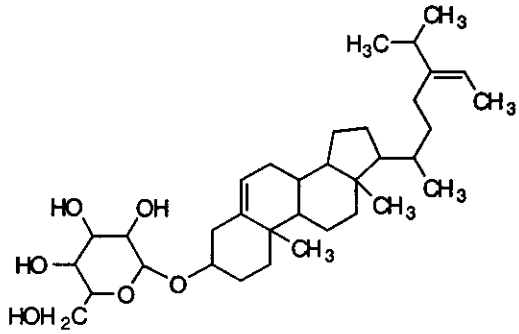


[化学名・別名]Dehydrotomatine. Tomatidenol 3-lycotetraoside
[CAS No.]157604-98-3
[化合物分類]アルカロイド化合物(Steroidal alkaloid) (spirosolane type)
[構造式]
[分子式]$C_{50}H_{81}NO_{21}$
[分子量]1032.184
[正確な分子量]1031.530114
[基原]次の植物から得られるアルカロイド: *Lycopersicon esculentum*（ナス科）

----------文献----------

Friedman, M. et al., J. Agric. Food Chem., 1997, 45, 1541,（Dehydrotomatine）
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, POJ000

§ Stigmasta-5,24(28)-dien-3-ol; (3 β,20*R*,24*Z*)-form, 3-*O*-β-D-Glucopyranoside



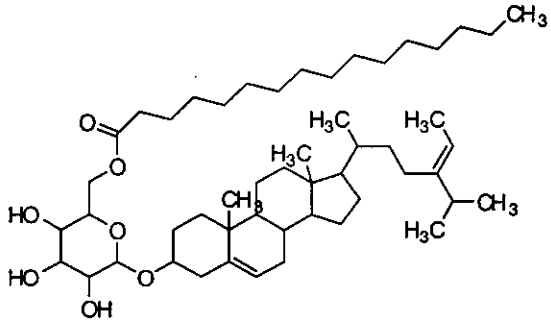
[化学名・別名]Isofucosterol glucoside
[CAS No.]87678-84-0
[化合物分類]ステロイド(Stigmastane steroid).(C29).
[構造式]
[分子式]$C_{35}H_{58}O_6$
[分子量]574.84
[正確な分子量]574.42334
[基原]*Lycopersicon esculentum*
[性状]結晶
[融点]Mp 266-268 ℃
[比旋光度]:[α]$_D$ -40.8 (c, 0.05 in $CHCl_3$)

----------文献----------

Dusza, J.P., J.O.C., 1960, 25, 93,（合成法, Isofucosterol）
De Rosa, S. et al., Phytochemistry, 1997, 44, 861; 1998, 48, 103,（Isofucosterol glucoside, acylglucosylisofucosterol）

§ Stigmasta-5,24(28)-dien-3-ol; (3 β,20*R*,24*Z*)-form, 3-*O*-[6-*O*-Hexadecanoyl-β-D-glucopyranoside]

[CAS No.]209903-43-5
[化合物分類]ステロイド(Stigmastane steroid).(C29).
[構造式]



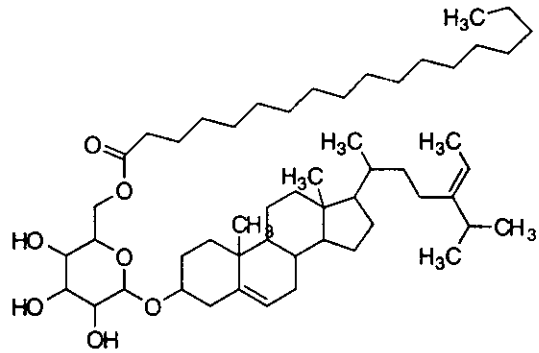
[分子式]$C_{51}H_{88}O_7$
[分子量]813.252
[正確な分子量]812.653005
[基原]*Lycopersicon esculentum*

----------文献----------

Heilbron, I. et al., J.C.S., 1934, 1572,（分離）
Idler, D.R. et al., J.A.C.S., 1953, 75, 1712,（分離）
C.Djerassi et al.,Dictionary of Natural Products, Chapman, Hall,2002

§ Stigmasta-5,24(28)-dien-3-ol; (3 β,20*R*,24*Z*)-form, 3-*O*-[6-*O*-Octadecanoyl-β-D-glucopyranoside]

[CAS No.]209903-44-6
[化合物分類]ステロイド(Stigmastane steroid). (C29).
[構造式]

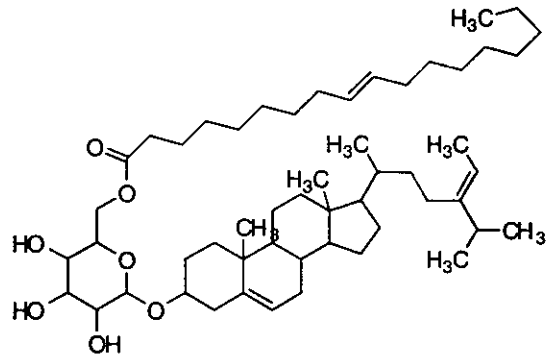


[分子式]$C_{53}H_{92}O_7$
[分子量]841.306
[正確な分子量]840.684305
[基原]*Lycopersicon esculentum*

----------文献----------

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

§ Stigmasta-5,24(28)-dien-3-ol; (3 β,20*R*,24*Z*)-form, 3-*O*-[6-*O*-(9-Octadecenoyl)-β-D-glucopyranoside]
[CAS No.]209903-45-7
[化合物分類]ステロイド(Stigmastane steroid). (C29).
[構造式]

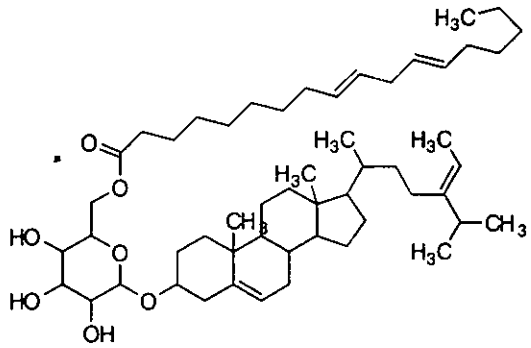


[分子式]$C_{53}H_{90}O_7$
[分子量]839.29
[正確な分子量]838.668655
[基原]*Lycopersicon esculentum*

----------文献----------

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

§ Stigmasta-5,24(28)-dien-3-ol; (3 β,20*R*,24*Z*)-form, 3-*O*-[6-*O*-(9,12-Octadecadienoyl)-β-D-glucopyranoside]
[CAS No.]209903-47-9
[化合物分類]ステロイド(Stigmastane steroid). (C29).
[構造式]



[分子式]$C_{53}H_{88}O_7$
[分子量]837.274
[正確な分子量]836.653005
[基原]*Lycopersicon esculentum*

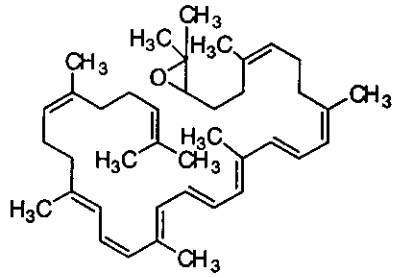
----------文献----------

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

§ Systemin
[CAS No.]137181-56-7
[化合物分類]アミノ酸とペプチド(Linear polypeptide)
[構造式] H-Ala-Val-Gln-Ser-Lys-Pro-Pro-Ser-Lys-Arg-Asp-Pro-Pro-Lys-Met-Gln-Thr-Asp-OH
[分子式]$C_{85}H_{144}N_{26}O_{28}S$
[分子量]2010.296
[正確な分子量]2009.036414
[基原]トマト(*Lycopersicon esculentum*)の葉

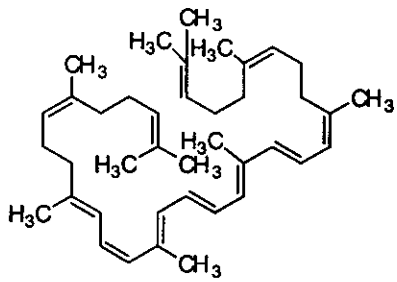
----------文献----------

Pearce, G. et al., Science (Washington, D.C.), 1991, 253, 895, (分離, 構造決定, 合成法, 性質)
Toumadje, A. et al., J.A.C.S., 1995, 117, 7023, (構造決定)
Schaller, A. et al., BioEssays, 1996, 18, 27, (レビュー)

§ 7,7',8,8'-Tetrahydrolycopene; 1 ξ,2 ξ-Epoxide
[化学名・別名]1,2-Epoxy-1,2-dihydro-ζ-carotene. ζ-Carotene epoxide
[CAS No.]93861-35-9
[化合物分類]テルペノイド(Tetraterpenoid)
[構造式]

[分子式]$C_{40}H_{60}O$
[分子量]556.913
[正確な分子量]556.464415
[基原]次の植物から分離: cherry tomato (*Lycopersicon esculentum*)
[性状]結晶(CH_2Cl_2/MeOH)
[UV]:[neutral] λ_{max} 232 (); 359 (); 378 (); 400 (); 425 () (hexane)

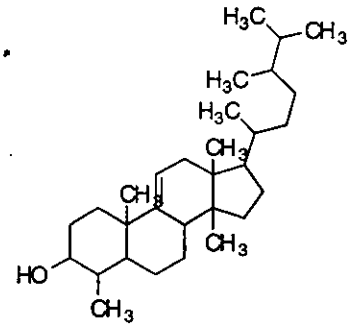
----------文献----------

Davis, J.B. et al., J.C.S.(C), 1966, 2154, (H-NMR, UV, IR, 成書)
Ben-Aziz, A. et al., Phytochemistry, 1973, 12, 2759, (分離, epoxide)
Arm, C. et al., Helv. Chim. Acta, 1984, 67, 1540, (合成法, epoxide)
Frecknell, E.A. et al., Phytochemistry, 1984, 23, 1707, (分離, 生育)
Straub, O. et al., Key to Carotenoids, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 38, (成書)

§ 7,7',8,8'-Tetrahydrolycopene; (9Z,9'Z)-form
[CAS No.]72746-33-9
[化合物分類]テルペノイド(Tetraterpenoid)
[構造式]

[基原]次の植物から分離: cherry tomato *Lycopersicon esculentum* var. *'Tangella'*
[性状]粘着性の橙色オイル
[UV]:[neutral] λ_{max} 284 (); 294 (); 361 (); 379 (); 401 (); 427 () (hexane)

----------文献----------

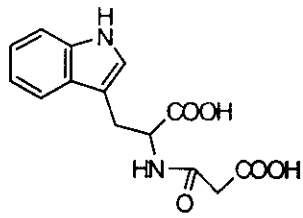
Frecknell, E.A. et al., Phytochemistry, 1984, 23, 1707, (分離, 生育)
Straub, O. et al., Key to Carotenoids, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 38, (成書)

§ 4,14,24-Trimethylcholest-9(11)-en-3-ol; (3 β,4 α,5 α,14 α,24 ξ)-form
[CAS No.]68520-27-4
[化合物分類]ステロイド(Neutral cholestane steroid). (C27).
[構造式]

[基原]*Lycopersicon esculentum* の種子

----------文献----------

Itoh, T. et al., Phytochemistry, 1978, 17, 971, (分離)
Naora, M. et al., Bull. Chem. Soc. Jpn., 1986, 59, 1767, (分離)
Yamashita, M. et al., Bull. Chem. Soc. Jpn., 1987, 60, 1383, (合成法)

§ **Tryptophan, *N*-(Carboxyacetyl)**



[化学名・別名]*N*-Malonyltryptophan
[CAS No.]29399-11-9
[化合物分類]アミノ酸とペプチド(Non-protein α-aminoacid)
[構造式]
[分子式]$C_{14}H_{14}N_2O_5$
[分子量]290.275
[正確な分子量]290.090273
[基原]次の植物を含む種々の植物: *Lycopersicon esculentum, Malus esculentum, Medicago sativa, Melilotus albus*

----------文献----------

Rzesztarska, B. et al., Org. Prep. Proced. Int., 1990, 22, 655, (レビュー, peptide)
Gamburg, K.Z. et al., Plant Sci. (Limerick, Irel.), 1991, 77, 149, (*N*-Malonyltryptophan)
Sakagami, Y. et al., Biosci., Biotechnol., Biochem., 1995, 59, 1362, (*N*-Malonyltryptophan, 絶対構造)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, ADE075; TNX000; TNW250; TNW500

**********ドラゴンブラット (Dragon's blood) **********

§§ヤシ科キリンケツ(*Daemonorhops ruber* Martius (*D. draco* Blume))の果実から得られる樹脂。
該当物質なし

**********ドリアン (Durian) **********

§§パンヤ科ドリアン(*Durio zibethinus* L.)の果実。

§ **Diethyl disulfide(CAS 名)**
[化学名・別名]Ethyl disulfide. 3,4-Dithiahexane
[CAS No.]110-81-6
[化合物分類]脂肪族化合物(Disulfides, trisulfide)
[構造式]Et-S-S-Et
[分子式]$C_4H_{10}S_2$
[分子量]122.255
[正確な分子量]122.02239
[基原]*Dipteryx odorata* の豆, *Durio zibethinus* の果実
[性状]ニンニク臭を持つオイル
[沸点]Bp 154 ℃. Bp_{11} 46 ℃
[溶解性]水にほとんど溶けない
[濃度]d^{20}_4 0.993
[屈折率]n^{20}_D 1.5063
[傷害・毒性]発火点:42 ℃. 皮膚と眼を刺激する. 50 %致死量(LD_{50})(ラット, 経口) 2030 mg/kg
[化学物質毒性データ総覧(RTEC)登録番号]JO1925000

----------文献----------

Haines, W.E. et al., J. Phys. Chem., 1954, 58, 270, (性質, IR, UV)
Baldry, J. et al., Phytochemistry, 1972, 11, 2081, (分離)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, DJC600

***RTECS (化学物質毒性データ) ***

生体影響物質　　: 一時刺激物質

健康障害に関するデータ

皮膚/眼の刺激に関するデータ

<<試験方法>> 標準ドライズ試験.
曝露経路　　: 皮膚への塗布