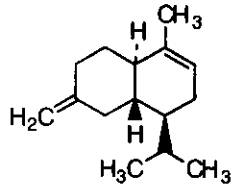
§ 4(15),9-Cadinadiene

[化学名・別名] γ-Cadinene



[CAS No.] 66141-11-5

[化合物分類] 脂肪族化合物(Simple heteroalicyclics (2 × O))

[構造式]

[分子式] $C_{15}H_{24}$

[分子量] 204.355

[基原] Malabar lemon grass oil (*Cymbopogon nardu*), *Hardwickia pinnata*, *Dictyopteris divaricata*

[沸点] Bp_9 120-121 ℃

[比旋光度]: $[\alpha]_D$ -19

[屈折率] $n^{26.5}{}_D$ 1.5155

----------文献----------

Dev, S. et al., J. Indian Chem. Soc., 1949, 26, 263, (分離)

Irie, T. et al., Bull. Chem. Soc. Jpn., 1964, 37, 1053, (分離)

Andersen, N.H. et al., Phytochemistry, 1977, 16, 1731, (構造決定)

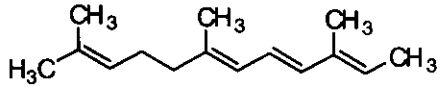
Vig, O.P. et al., Indian J. Chem., Sect. B, 1979, 17, 552, (合成法)

§ 2,4,6,10-Farnesatetraene

[化学名・別名] 3,7,11-Trimethyl-2,4,6,10-dodecatetraene. Allofarnesene

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

[構造式]



[分子式] $C_{15}H_{24}$

[分子量] 204.355

[正確な分子量] 204.1878

[基原] 次の植物のオイルから分離： *Cymbopogon nardus*, *Cananga odorata*, その他

[沸点] $Bp_{4.4}$ 121-122 ℃

----------文献----------

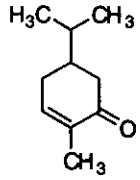
Naves, Y.R., Helv. Chim. Acta, 1966, 49, 1029, (合成法, UV, IR, H-NMR)

Sakai, T. et al., Bull. Chem. Soc. Jpn., 1969, 42, 3615, (分離)

Brieger, G. et al., J.O.C., 1969, 34, 3789, (合成法)

Miyaura, N. et al., Bull. Chem. Soc. Jpn., 1982, 55, 2221, (合成法)

§ *p*-Menth-1-en-6-one; (*R*)-form



[CAS No.] 33375-08-5

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

[構造式]

[基原] *Piper nigrum*. また *Tanacetum vulgare*, *Eucalyptus deglupta*, *Cymbopogon nardus*

[性状] オイル

[沸点] Bp 227-229 ℃

----------文献----------

Simonsen, J.L. et al., J.C.S., 1922, 876, (分離, 構造決定)

Sutherland, M.D. et al., Aust. J. Chem., 1960, 13, 357, (分離)

Org. Synth., 1973, 53, 63, (合成法)

Noma, Y. et al., Agric. Biol. Chem., 1974, 38, 1637, (合成法)

Debraumere, J. et al., Bull. Soc. Chim. Belg., 1975, 84, 167, (分離, 構造決定)

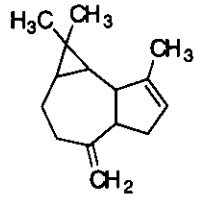
§§イネ科ジャワシトロネラソウ(*Cymbopogon winterianus* Jowitt (*C. nardus* var. *mahapengiri*))の葉または全草。

本調査研究では研究報告ない。

***********シヌス (Schinus molle) ***********

§ § ウルシ科コショウボク(*Schinus molle* L.)の果実。

§ 3,10(14)-Aromadendradiene; (1 α,5 β,6 α,7 α)-form



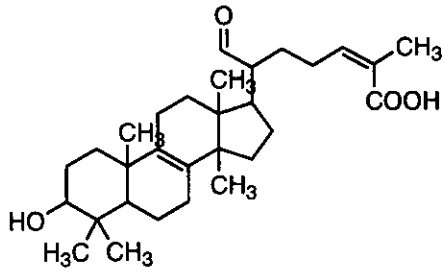
[化学名・別名] β-Spathulene
[CAS No.] 53526-64-0
[化合物分類] テルペノイド(Aromadendrane sesquiterpenoid)
[構造式]
[基原] *Schinus molle* のオイル

----------文献----------

Terhune, S.J. et al., Phytochemistry, 1974, 13, 865

§ 3-Hydroxy-21-oxoeupha-8,24-dien-26-oic acid; (3 α,20*R*,24*Z*)-form

[CAS No.] 195204-05-8
[化合物分類] テルペノイド(Tirucallane/euphane triterpenoid)
[構造式]



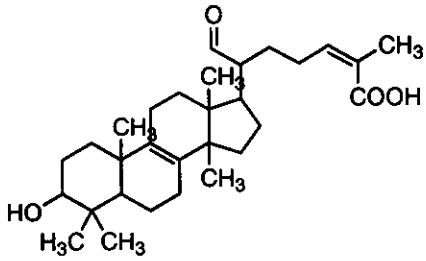
[基原] *Schinus molle*

----------文献----------

Olafsson, K. et al., Planta Med., 1997, 63, 352, (分離, H-NMR, C13-NMR)

§ 3-Hydroxy-21-oxoeupha-8,24-dien-26-oic acid; (3 α,20*S*,24*Z*)-form

[化学名・別名] 3-Hydroxy-21-oxotirucalla-8,24-dien-26-oic acid
[化合物分類] テルペノイド(Tirucallane/euphane triterpenoid)
[構造式]



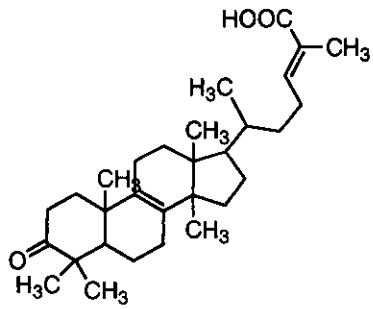
[基原] *Schinus molle*

----------文献----------

Olafsson, K. et al., Planta Med., 1997, 63, 352, (分離, H-NMR, C13-NMR)

§ 3-Hydroxytirucalla-8,24-dien-26-oic acid; (3 α,24*Z*)-form, 3-Ketone

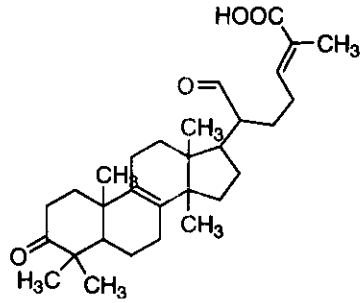
[化学名・別名] 3-Oxotirucalla-8,24-dien-26-oic acid. Isomasticadienonic acid
[CAS No.] 5956-26-3
[化合物分類] テルペノイド(Tirucallane/euphane triterpenoid)
[構造式]



[分子式] $C_{30}H_{46}O_3$
[分子量] 454.692
[正確な分子量] 454.344695
[基原] *Pistacia terebinthus*, *Schinus molle*
[性状] 結晶(petrol)
[融点] Mp 166-167 ℃
[比旋光度]: $[\alpha]_D$ +34 ($CHCl_3$)

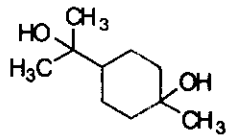
----------文献----------

Lanfredi, A.M.M. et al., Cryst. Struct. Commun., 1975, 4, 551, (結晶構造, Isomasticadienonic acid)

§ 3-Hydroxytirucalla-8,24-dien-26-oic acid; (3 α,24*Z*)-form, 3-Ketone, 21-oxo
[化学名・別名]3,21-Dioxotirucalla-8,24*E*-dien-26-oic acid. Isomasticadienonalic acid
[CAS No.]62499-11-0
[化合物分類]AJ1790, テルペノイド(Tirucallane/euphane triterpenoid)
[構造式]

[分子式]$C_{30}H_{44}O_4$
[分子量]468.675
[正確な分子量]468.32396
[基原]*Schinus molle*
[性状]結晶(hexane) (as Me ester)
[融点]Mp 136-138 ℃ (Me ester)
[比旋光度]:[α]$_D$ +40 (c, 0.65 in $CHCl_3$) (Me ester)
[その他のデータ]20-Config. は決定していない

----------文献----------

Seaone, E., J.C.S., 1956, 4158, (分離, 構造決定, 誘導体)
Caputo, R. et al., Gazz. Chim. Ital., 1970, 100, 317, (分離)
Lanfredi, A.M.M. et al., Cryst. Struct. Commun., 1975, 4, 551, (結晶構造, Isomasticadienonic acid)
Pozzo-Balbi, T. et al., Gazz. Chim. Ital., 1976, 106, 785, (分離)
Watson, W.H. et al., Rev. Latinoam. Quim., 1987, 18, 89, (Instipolinacic acid)
Olafsson, K. et al., Planta Med., 1997, 63, 352, (C13-NMR)

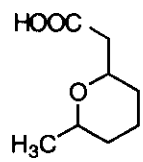
§ *p*-Menthane-1,8-diol; (1*RS*,4*RS*)-form
[化学名・別名]*cis*-form
[CAS No.]565-48-0
[化合物分類]テルペノイド(*p*-Menthane monoterpenoid)
[構造式]

[基原]次の植物から分離: *Cupressus torulosa* の葉, *Schinus molle* の果実
[用途]去痰薬
[性状]プリズム結晶もしくは板状結晶(EtOAc)
[融点]Mp 104-105 ℃
[沸点]Bp 263-265 ℃
[溶解性]水に難溶

----------文献----------

Barnes, C.S., Aust. J. Chem., 1958, 11, 134, (構造, 成書)
Peyron, L. et al., Bull. Soc. Chim. Fr., 1969, 339, (分離)
Pertoldi, M. et al., CA, 1970, 73, 91168, (分離)
Suga, T. et al., Bull. Chem. Soc. Jpn., 1982, 55, 914, (結晶構造)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 2029
Hassan, M.M.A. et al., Anal. Profiles Drug Subst., 1985, 14, 273, (レビュー, 合成法, 薬理, 分析)
Ho, T.-I. et al., Acta Cryst. C, 1986, 42, 1787, (結晶構造)

*********シベット (Civet) *********

§ § ジャコウネコ科アフリカジャコウネコ(*Viverra civetta* Schreber)の肛門腺分泌物。

§ Tetrahydro-6-methyl-2*H*-pyran-2-acetic acid; (2*S*,6*S*)-form
[化学名・別名](+)-*cis*-form
[CAS No.]69493-11-4
[化合物分類]脂肪族化合物(Simple heteroalicyclics (1 × O))
[構造式]

[基原]*Viverra civetta*
[性状]粘調性液体もしくは結晶 (Et_2O)
[融点]Mp 52-53 ℃

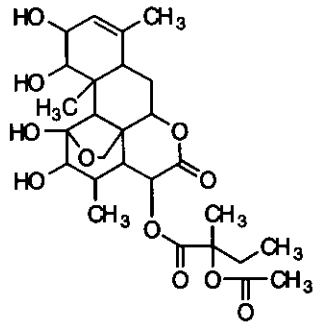
[沸点] $Bp_{0.004}$ 150 ℃
[比旋光度]:[α]$_D$ +32.86 (c, 1.05 in C_6H_6)
----------文献----------
Maurer, B. et al., Helv. Chim. Acta, 1979, 62, 44; 1096, (分離, 合成法, H-NMR, C13-NMR, IR, Mass, 絶対構造)
Seebach, D. et al., Helv. Chim. Acta, 1979, 62, 843, (合成法, H-NMR)
Kim, Y. et al., J.O.C., 1982, 47, 3556, (合成法)
Bates, H.A. et al., J.O.C., 1983, 48, 4479, (合成法)
Nussbaumer, C. et al., Helv. Chim. Acta, 1987, 70, 396, (合成法, H-NMR)
Ragoussis, V. et al., Synthesis, 1993, 84, (合成法, H-NMR, Mas)
Varelis, P. et al., Aust. J. Chem., 1994, 47, 1735, (合成法, H-NMR, C13-NMR, 結晶構造)
Muraoka, O. et al., Chem. Pharm. Bull., 1995, 43, 517, (合成法, 成書)

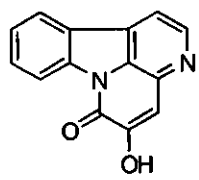
§§ ジャコウネコ科(*Viverra zibetha* Schreber)の肛門腺分泌物。
本調査研究では研究報告ない。

§§ ジャコウネコ科(*Viverricula indica* Desmarest)の肛門腺分泌物。
本調査研究では研究報告ない。

***********シマルーバ (Simarouba) ***********

§§ ニガキ科シマルバ(*Simarouba amara* Aublet)の樹皮。

§ Glaucarubol; 15-(2-Acetoxy-2-methylbutanoyl)
[化学名・別名]2'-Acetylglaucarubin
[CAS No.]68703-93-5
[化合物分類]テルペノイド(Quassinoid nortriterpenoid)
[構造式]

[分子式] $C_{27}H_{38}O_{11}$
[分子量]538.591
[正確な分子量]538.241415
[基原]*Simarouba amara*
[性状]結晶
[融点]Mp 243-246 ℃
[比旋光度]:[α]$_D$ +29.5 (c, 1.1 in Py)
[溶解性]メタノール, クロロホルムに可溶; 水に難溶
[UV]:[neutral] λ $_{max}$ 240 (ε 10700) (EtOH)
----------文献----------
Ham, A. et al., J.A.C.S., 1954, 76, 6066, (分離, IR, Glaucarubin)
Kartha, G. et al., J.A.C.S., 1964, 86, 3630, (結晶構造, Glaucarubin)
Gaudemer, A. et al., Phytochemistry, 1965, 4, 149, (Glaucarubinone)
Rodriguez Fo, E. et al., Phytochemistry, 1996, 43, 857, (Glaucarubolone, H-NMR, C13-NMR)
Vieira, I.J.C. et al., Fitoterapia, 1998, 69, 88, (Glaucarubol, Glaucarubolone, H-NMR, C13-NMR)

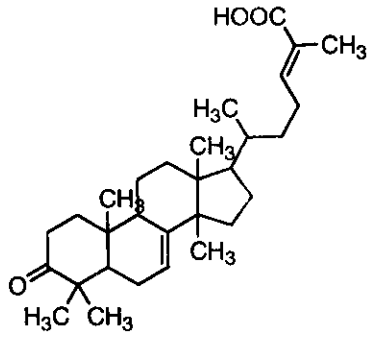
§ 5-Hydroxycanthin-6-one
[化学名・別名]5-Hydroxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one(CAS 名)
[CAS No.]64118-73-6
[化合物分類]アルカロイド化合物(Indolonaphthyridine alkaloid)
[構造式]

[分子式] $C_{14}H_8N_2O_2$
[分子量]236.229

[基原]次の植物の根皮から得られるアルカロイド: *Simarouba amara*（ニガキ科）
[性状]橙-黄色の板状結晶（MeOH）
[融点]Mp 259-261 ℃で分解
[溶解性]メタノール, クロロホルムに可溶

----------文献----------

Haynes, H.F. et al., Aust. J. Sci. Res., Ser. A, 1952, 5, 387,（分離）
Awad, A.T. et al., J. Pharm. Sci., 1967, 56, 279,（分離）
Della Casa, D. et al., J.C.S.(C), 1967, 2155,（分離, UV, IR, H-NMR）
Lassak, E.V. et al., Phytochemistry, 1977, 16, 1126,（分離, 合成法, UV, Mass, 構造決定）
Cordell, G.A. et al., J. Nat. Prod., 1978, 41, 166,（分離, UV, IR, H-NMR, Mas）
Wagner, H. et al., Planta Med., 1979, 36, 113,（分離）
Forgacs, P. et al., Planta Med., 1982, 46, 187,（分離）

§ 3-Hydroxytirucalla-7,24-dien-26-oic acid; 24*E*-form, 3-Ketone
[化学名・別名]Adenophoric acid
[CAS No.]66052-86-6
[化合物分類]テルペノイド(Tirucallane/euphane triterpenoid)
[構造式]

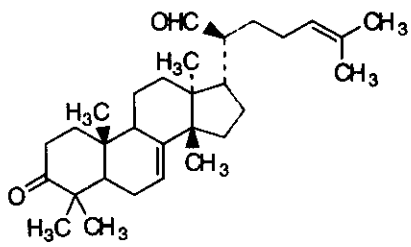


[基原]*Simarouba amara*, *Dysoxylum pettigrewianum*
[性状]結晶
[融点]Mp 170-174 ℃
[比旋光度]:[α]$_D^{22}$ -12.3 (c, 0.292 in $CHCl_3$)

----------文献----------

Kier, L.B. et al., Bull. Soc. Chim. Fr., 1963, 911,（分離）
Corsano, S. et al., Tet. Lett., 1965, 2377,（構造決定）
Monaca, P. et al., Phytochemistry, 1974, 13, 1992,（分離）
Polonsky, J. et al., Isr. J. Chem., 1977, 16, 16,（分離, H-NMR）
Mulholland, D.A. et al., Phytochemistry, 1994, 37, 1409,（分離, H-NMR, C13-NMR）

§ 3-Oxotirucalla-7,24-dien-21-al
[CAS No.]59781-40-7
[化合物分類]テルペノイド(Tirucallane/euphane triterpenoid)
[構造式]

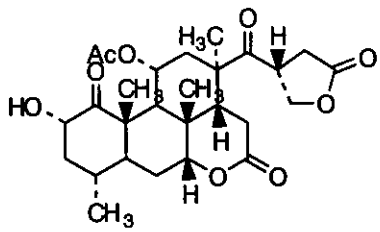


[分子式]$C_{30}H_{46}O_2$
[分子量]438.692
[正確な分子量]438.34978
[基原]*Simarouba amara*, *Owenia cepiodora*
[性状]結晶(MeOH/Et_2O)
[融点]Mp 154-155 ℃
[比旋光度]:[α]$_D$ -63 (c, 0.87 in $CHCl_3$)

----------文献----------

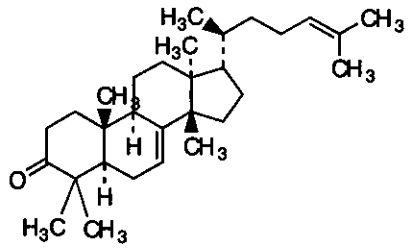
Polonsky, J. et al., Phytochemistry, 1976, 15, 337
Mulholland, D.A. et al., Phytochemistry, 1998, 49, 2457,（分離, H-NMR, C13-NMR）

§ Simarolide

[CAS No.]1260-58-8
[化合物分類]テルペノイド(C_{25} Quassinoid triterpenoid)
[構造式]

[分子式]$C_{27}H_{36}O_9$
[分子量]504.576
[正確な分子量]504.235935
[基原]*Simarouba amara* の苦味成分
[性状]結晶(EtOAc or EtOH)
[融点]Mp 264-270 ℃
[比旋光度]:[α]$_D$ +73.6 (c, 0.79 in $CHCl_3$)
[溶解性]ヘキサンに難溶

----------文献----------

Polonsky, J., Proc. Chem. Soc., London, 1964, 292, (分離, 構造決定)
Brown, W.A.C. et al., Proc. Chem. Soc., London, 1964, 293, (結晶構造)
Vanhaelen-Fastreacute, R. et al., Phytochemistry, 1987, 26, 317, (Klaineanolide B)

§ Tirucalla-7,24-dien-3-one
[CAS No.]59781-41-8
[化合物分類]テルペノイド(Tirucallane/euphane triterpenoid)
[構造式]
[分子式]$C_{30}H_{48}O$
[

[分子量]424.709
[正確な分子量]424.370515
[基原]*Simarouba amara*
[性状]結晶(MeOH/Et_2O)
[融点]Mp 115-116 ℃
[比旋光度]:[α]$_D$ -70 (c, 1.06 in $CHCl_3$)

----------文献----------

Polonsky, J. et al., Phytochemistry, 1976, 15, 337

***********シメジ (Shimeji) **********

§§キシメジ科ホンシメジ(*Lyophyllum aggregatum* (Secr.) Kuhner (*L. shimeji* Hongo ; *Tricholoma shimeji* Kawamura))の子実体。
本調査研究では研究報告ない。

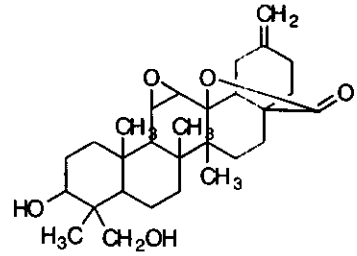
§§キシメジ科シャカシメジ(*Lyophyllum cinerascens* (Konr.) Konr. et Maubl. (*L. aggregatum* Khner var. fumosum ; *L. fumosom* Orton))の子実体。
本調査研究では研究報告ない。

***********シャクヤク (Shakuyaku, Chinese peony) **********

§§ボタン科シャクヤク(*Paeonia lactiflora* Palla)の根茎。

§ 11,12-Epoxy-3,13,23-trihydroxy-30-nor-20(29)-oleanen-28-oic acid; (3 β,11 α,12 α,13 β)-form, 28 → 13 Lactone
[化学名・別名]11,12-Epoxy-3,23-dihydroxy-30-nor-20(29)-oleanen-28,13-olide

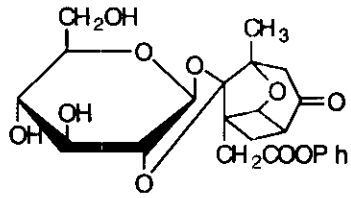
[CAS No.]186140-36-3
[構造式]
[分子式]$C_{29}H_{42}O_5$
[分子量]470.648
[正確な分子量]470.303225
[基原]*Paeonia lactiflora*
[性状]無定型の粉末
[比旋光度]:[α]$_D^{27}$ +78.4 (c, 0.89 in $CHCl_3$)



----------文献----------

Kamiya, K. et al., Phytochemistry, 1997, 44, 141, (分離, H-NMR, C13-NMR)

§ Lactiflorin
[化合物分類]テルペノイド(Miscellaneous bicyclic monoterpenoid)
[構造式]
[分子式]$C_{23}H_{26}O_{10}$
[分子量]462.452
[正確な分子量]462.1526
[基原]*Paeonia lactiflora*
[性状]結晶($CHCl_3$/MeOH)
[融点]Mp 207-209 ℃
[比旋光度]:[α]$_D^{23}$ +37.2 (c, 0.01 in EtOH)



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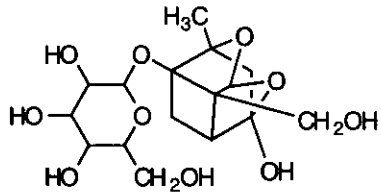
Yu, J. et al., Phytochemistry, 1990, 29, 3859, (分離, H-NMR, C13-NMR)
Lang, H.Y. et al., Tetrahedron, 1990, 46, 3123, (構造決定)

§ Paeoniflorin; Debenzoyl
[化学名・別名]8-Debenzoylpaeoniflorin
[化合物分類]テルペノイド(Pinane monoterpenoid)
[構造式]
[分子式]$C_{16}H_{24}O_{10}$
[分子量]376.36
[正確な分子量]376.13695
[基原]*Paeonia lactiflora*
[性状]無定型の粉末
[比旋光度]:[α]$_D$ -9.6 (c, 1 in MeOH)



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Hsu, F.-L. et al., Planta Med., 1997, 63, 323, (8-Debenzoylpaeoniflorin)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, PAC000

§ 1,2,3,4,6-Pentagalloylglucose; β-D-Pyranose-form, *O*-3,4,5-Trihydroxybenzoyl(4)
[化学名・別名]6-*O*-Digalloyl-1,2,3,4-tetra-*O*-galloyl-β-D-glucopyranose
[CAS No.]60768-30-1
[化合物分類]タンニン化合物(Simple gallate ester tannin)
[構造式]有効な構造式はない
[分子式]$C_{48}H_{36}O_{30}$
[分子量]1092.794
[正確な分子量]1092.12915
[基原]Gallotannin constit.of twig galls (*Quercus infectoria*) and of *Paeonia lactiflora*
[性状]淡褐色の無定型粉末
[比旋光度]:[α]$_D^{20}$ +43.4 (c, 0.53 in Me_2CO)

----------文献----------

Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515, (分離, 構造決定, H-NMR, C13-NMR)
Nishizawa, M. et al., J.C.S. Perkin 1, 1982, 2963; 1983, 961, (誘導体)
Nishizawa, M. et al., Chem. Pharm. Bull., 1983, 31, 2593, (誘導体)

Nishizawa, M. et al., Phytochemistry, 1985, 24, 2411,（誘導体）
Nonaka, G. et al., Chem. Pharm. Bull., 1987, 35, 3127,（構造決定, H-NMR, C13-NMR）
Ciufolini, M.A. et al., Tetrahedron, 1997, 53, 11049,（合成法, 成書）

§ 1,2,3,4,6-Pentagalloylglucose; β-D-Pyranose-form, Bis(3,4,5-trihydroxybenzoyl) (3)
[化学名・別名]2,6-Di-*O*-digalloyl-1,3,4-tri-*O*-galloyl-β-D-glucopyranose
[CAS No.]87861-32-3
[化合物分類]タンニン化合物(Simple gallate ester tannin)
[構造式]有効な構造式はない
[分子式]$C_{55}H_{40}O_{34}$
[分子量]1244.901
[正確な分子量]1244.14011
[基原]Gallotannin from *Paeonia lactiflora*
[性状]淡褐色の無定型粉末 ・二水和物
[比旋光度]:$[\alpha]_D^{20}$ +48.6 (c, 0.40 in Me_2CO)
----------文献----------
Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515,（分離, 構造決定, H-NMR, C13-NMR）
Nishizawa, M. et al., J.C.S. Perkin 1, 1982, 2963; 1983, 961,（誘導体）
Nishizawa, M. et al., Chem. Pharm. Bull., 1983, 31, 2593,（誘導体）
Nishizawa, M. et al., Phytochemistry, 1985, 24, 2411,（誘導体）
Nonaka, G. et al., Chem. Pharm. Bull., 1987, 35, 3127,（構造決定, H-NMR, C13-NMR）
Kandil, F.E. et al., Phytochemistry, 1996, 42, 1243,（2-Trigalloyl-1,3,4,6-tetragalloylglucose, UV, H-NMR, C13-NMR）
Ciufolini, M.A. et al., Tetrahedron, 1997, 53, 11049,（合成法, 成書）

§ 1,2,3,4,6-Pentagalloylglucose; β-D-Pyranose-form, Bis(3,4,5-trihydroxybenzoyl) (5)
[化学名・別名]3,6-Di-*O*-digalloyl-1,2,4-tri-*O*-galloyl-β-D-glucopyranose
[CAS No.]87860-74-0
[化合物分類]タンニン化合物(Simple gallate ester tannin)
[構造式]有効な構造式はない
[分子式]$C_{55}H_{40}O_{34}$
[分子量]1244.901
[正確な分子量]1244.14011
[基原]次の植物の根から分離: *Paeonia lactiflora*
[性状]淡褐色の無定型粉末 ・二水和物
[比旋光度]:$[\alpha]_D^{20}$ +33.6 (c, 0.54 in Me_2CO)
----------文献----------
Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515,（分離, 構造決定, H-NMR, C13-NMR）
Nishizawa, M. et al., J.C.S. Perkin 1, 1982, 2963; 1983, 961,（誘導体）
Nishizawa, M. et al., Chem. Pharm. Bull., 1983, 31, 2593,（誘導体）
Nishizawa, M. et al., Phytochemistry, 1985, 24, 2411,（誘導体）
Nonaka, G. et al., Chem. Pharm. Bull., 1987, 35, 3127,（構造決定, H-NMR, C13-NMR）
Kandil, F.E. et al., Phytochemistry, 1996, 42, 1243,（2-Trigalloyl-1,3,4,6-tetragalloylglucose, UV, H-NMR, C13-NMR）
Ciufolini, M.A. et al., Tetrahedron, 1997, 53, 11049,（合成法, 成書）

§ 1,2,3,4,6-Pentagalloylglucose; β-D-Pyranose-form, Bis(3,4,5-trihydroxybenzoyl) (6)
[化学名・別名]4,6-Di-*O*-digalloyl-1,2,3-tri-*O*-galloyl-β-D-glucopyranose
[CAS No.]87861-31-2
[化合物分類]タンニン化合物(Simple gallate ester tannin)
[構造式]有効な構造式はない
[分子式]$C_{55}H_{40}O_{34}$
[分子量]1244.901
[正確な分子量]1244.14011
[基原]Gallotannin of *Paeonia lactiflora*

[性状]淡褐色の無定型粉末

----------文献----------

Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515,（分離, 構造決定, H-NMR, C13-NMR）
Nishizawa, M. et al., J.C.S. Perkin 1, 1982, 2963; 1983, 961,（誘導体）
Nishizawa, M. et al., Chem. Pharm. Bull., 1983, 31, 2593,（誘導体）
Nishizawa, M. et al., Phytochemistry, 1985, 24, 2411,（誘導体）
Nonaka, G. et al., Chem. Pharm. Bull., 1987, 35, 3127,（構造決定, H-NMR, C13-NMR）
Kandil, F.E. et al., Phytochemistry, 1996, 42, 1243,（2-Trigalloyl-1,3,4,6-tetragalloylglucose, UV, H-NMR, C13-NMR）
Ciufolini, M.A. et al., Tetrahedron, 1997, 53, 11049,（合成法, 成書）

§ 1,2,3,4,6-Pentagalloylglucose; β-D-Pyranose-form, Tris(3,4,5-trihydroxybenzoyl)

[化学名・別名]2,3,6-Tri-*O*-digalloyl-1,4-di-*O*-galloyl-β-D-glucopyranose
[CAS No.]87823-32-3
[化合物分類]タンニン化合物(Simple gallate ester tannin)
[構造式]有効な構造式はない
[分子式]$C_{62}H_{44}O_{38}$
[分子量]1397.007
[正確な分子量]1396.15107
[基原]Gallotannin constit. of *Paeonia lactiflora*
[性状]淡褐色の無定型粉末・一水和物
[比旋光度]:$[\alpha]_D^{20}$ +39.3 (c, 0.82 in Me_2CO)

----------文献----------

Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515,（分離, 構造決定, H-NMR, C13-NMR）
Nishizawa, M. et al., J.C.S. Perkin 1, 1982, 2963; 1983, 961,（誘導体）
Nishizawa, M. et al., Chem. Pharm. Bull., 1983, 31, 2593,（誘導体）
Nishizawa, M. et al., Phytochemistry, 1985, 24, 2411,（誘導体）
Nonaka, G. et al., Chem. Pharm. Bull., 1987, 35, 3127,（構造決定, H-NMR, C13-NMR）
Kandil, F.E. et al., Phytochemistry, 1996, 42, 1243,（2-Trigalloyl-1,3,4,6-tetragalloylglucose, UV, H-NMR, C13-NMR）
Ciufolini, M.A. et al., Tetrahedron, 1997, 53, 11049,（合成法, 成書）

§ 1,2,3,4,6-Pentagalloylglucose; β-D-Pyranose-form, *O*-(Galloylgalloyl) (1)

[化学名・別名]3-*O*-Trigalloyl-1,2,4,6-tetra-*O*-galloyl-β-D-glucopyranose
[CAS No.]85249-60-1
[化合物分類]タンニン化合物(Simple gallate ester tannin)
[構造式]有効な構造式はない
[分子式]$C_{55}H_{40}O_{34}$
[分子量]1244.901
[正確な分子量]1244.14011
[基原]*Paeonia lactiflora* and Chinese gallotannin (twig galls of Rhus semialata)
[性状]淡褐色の無定型粉末
[比旋光度]:$[\alpha]_D^{20}$ +13.4 (c, 1.35 in Me_2CO)

----------文献----------

Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515,（分離, 構造決定, H-NMR, C13-NMR）
Nishizawa, M. et al., J.C.S. Perkin 1, 1982, 2963; 1983, 961,（誘導体）
Nishizawa, M. et al., Chem. Pharm. Bull., 1983, 31, 2593,（誘導体）
Nishizawa, M. et al., Phytochemistry, 1985, 24, 2411,（誘導体）
Nonaka, G. et al., Chem. Pharm. Bull., 1987, 35, 3127,（構造決定, H-NMR, C13-NMR）
Kandil, F.E. et al., Phytochemistry, 1996, 42, 1243,（2-Trigalloyl-1,3,4,6-tetragalloylglucose, UV, H-NMR, C13-NMR）
Ciufolini, M.A. et al., Tetrahedron, 1997, 53, 11049,（合成法, 成書）

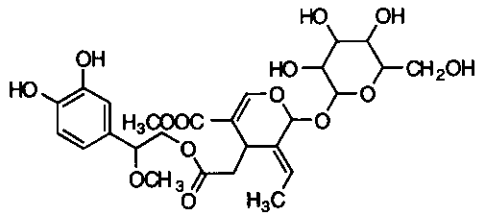
§§ ボタン科(*Paeonia veitchii* Lynch)の根茎。

本調査研究では研究報告ない。

**********ジャスミン（Jasmin）**********

§§モクセイ科ジャスミン(*Jasminum officinale* L.)

§ Oleuropein; β-Methoxy (*S*-)

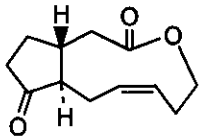
[CAS No.]256498-11-0
[化合物分類]テルペノイド(Secoiridoid monoterpenoid)
[構造式]

[分子式]$C_{26}H_{34}O_{14}$
[分子量]570.546
[正確な分子量]570.19486
[基原]*Jasminum officinale* var. *grandiflorum*
[性状]無定型の粉末
[比旋光度]:[α]$_D^{25}$ -121 (c, 0.98 in MeOH)
[UV]:[neutral] λ $_{max}$ 232 (log ε 4.15); 281 (log ε 3.4) (MeOH)

----------文献----------

Panizzi, L. et al., Gazz. Chim. Ital., 1965, 95, 1279, (分離)
Asaka, Y. et al., Chem. Lett., 1972, 141, (分離, 構造決定)
Inouye, H. et al., Tetrahedron, 1974, 30, 201, (絶対構造)
Kikuchi, M. et al., CA, 1985, 103, 147026, (分離, H-NMR, C13-NMR)
Kurkin, V.A. et al., Khim. Prir. Soedin., 1990, 695; Chem. Nat. Compd. (Engl. Transl.), 1990, 26, 592, (demethyl, 分離, UV)
Damtoft, S. et al., Phytochemistry, 1992, 31, 4197; 1993, 34, 1291; 1995, 40, 785, (生合成, Oleuropein, Ligustroside)
Tanahashi, T. et al., Chem. Pharm. Bull., 1999, 47, 1582, (β-methoxy deriv)

§§モクセイ科タイワンソケイ(*Jasminum grandiflorum* L.)の花。

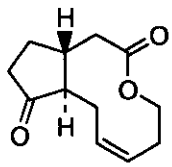
§ 5'-Hydroxyjasmonic acid lactone

[化合物分類]脂肪族化合物(Monocarbocyclic aldehydes and ketone), ポリケチド(Lactone polyketide)
[構造式]

[分子式]$C_{12}H_{16}O_3$
[分子量]208.257
[正確な分子量]208.109945
[基原]*Jasminum grandiflorum*
[性状]結晶
[融点]Mp 104 ℃
[比旋光度]:[α]$_D^{20}$ -260 (c, 3 in EtOH)

----------文献----------

Demole, E. et al., Helv. Chim. Acta, 1964, 47, 1152

§ Jasmine ketolactone

[化学名・別名]1,4,5,8,8*a*,10,11,11*a*-Octahydrocyclopent[*d*]oxecin-2,9-dione(CAS 名). Jasmine oil ketolactone
[CAS No.]70981-24-7
[化合物分類]ポリケチド(Lactone polyketide)
[構造式]

[分子式]$C_{12}H_{16}O_3$
[分子量]208.257
[正確な分子量]208.109945
[基原]イタリアンジャスミンオイル(*Jasminum grandiflorum*)

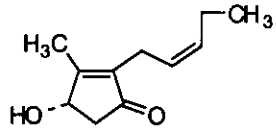
[性状]小針状結晶（petrol）
[融点]Mp 104 ℃
[比旋光度]:[α]$_D^{20}$ -260（c, 3.05 in MeOH）

----------文献----------

Demole, E. et al., Helv. Chim. Acta, 1964, 47, 1152,（分離, IR, H-NMR, Mass, 構造決定）
Inoue, M. et al., Biosci., Biotechnol., Biochem., 1999, 63, 1122,（合成法）

§ Jasmolone

[化学名・別名]4-Hydroxy-3-methyl-2-(2-pentenyl)-2-cyclopenten-1-one(CAS 名). Jasmololone
[CAS No.]54383-66-3
[化合物分類]脂肪族化合物(Monocarbocyclic aldehydes and ketone)
[構造式]
[分子式]$C_{11}H_{16}O_2$
[分子量]180.246
[正確な分子量]180.11503
[基原]*Jasminum grandiflorum* のオイル
[性状]オイル



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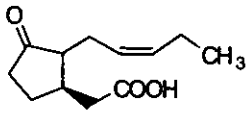
Pattenden, G. et al., J.C.S. Perkin 1, 1974, 1603,（合成法）
Ficini, P. et al., Bull. Soc. Chim. Fr., 1975, 1811,（合成法）
Crombie, L. et al., J.C.S. Perkin 1, 1975, 1500,（C13-NMR）
Sato, T. et al., Bull. Chem. Soc. Jpn., 1981, 54, 505,（合成法）
Takahashi, T. et al., Chem. Lett., 1981, 1189,（合成法）
Yamamura, S. et al., Phytochemistry, 1998, 48, 131,（分離, 配糖体）

§ Jasmonic acid

[化学名・別名]3-Oxo-2-(2-pentenyl) cyclopentaneacetic acid(CAS 名)(旧 CAS 名)
[CAS No.]6894-38-8
[関連 CAS No.]76968-33-7, 77026-92-7, 135911-63-6
[化合物分類]脂肪族化合物(Monocarbocyclic carboxylic acids and lactone)
[構造式]
[分子式]$C_{12}H_{18}O_3$
[分子量]210.272
[正確な分子量]210.125595
[基原]*Jasminum grandiflorum*
[用途]植物毒
[性状]粘調性のオイル
[沸点]$Bp_{0.001}$ 125 ℃
[比旋光度]:[α]$_D$ -83.5（c, 0.97 in $CHCl_3$）
[屈折率]n^{19}_D 1.4885
[UV]:[neutral] λ_{max} 0 (end)(ε)(MeOH)



Absolute configuration

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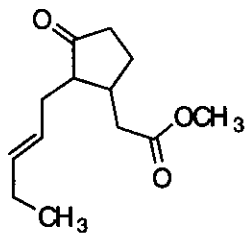
Hill, R.K. et al., Tetrahedron, 1965, 21, 1501,（絶対構造）
Kaiser, R. et al., Tet. Lett., 1974, 3413,（4,5-didehydro Me ester）
Miersch, O. et al., Phytochemistry, 1986, 26, 1037; 1989, 28, 339; 1303; 1992, 31, 3835,（分離, 誘導体）
Farmer, E.E. et al., Proc. Natl. Acad. Sci. U.S.A., 1990, 87, Ford, R.A. et al., Food Chem. Toxicol., 1992, 30, 85S,（レビュー, 毒性）
Sembdner, G. et al., Annu. Rev. Plant Physiol., 1993, 44, 569,（レビュー）
Matsuura, H. et al., Biosci., Biotechnol., Biochem., 1993, 57, 1253,（誘導体）
Husain, A. et al., J. Nat. Prod., 1993, 56, 2008,（分離, C13-NMR）
Wasternack, C. et al., Fett/Lipid, 1998, 100, 139,（レビュー）

§ Jasmonic acid; Me ester

[化学名・別名]Methyl jasmonate

[CAS No.]1211-29-6
[化合物分類]脂肪族化合物(Monocarbocyclic methyl ester)
[構造式]

[分子式]$C_{13}H_{20}O_3$
[分子量]224.299
[正確な分子量]224.141245
[基原]*Jasminum grandiflorum*
[用途]特異的なジャスミン臭気を有する; 香水に使われる.
[性状]オイル
[沸点]$Bp_{0.001}$ 81-84 ℃
[比旋光度]:$[\alpha]_D$ -76.5 (c, 3.4 in MeOH)
[屈折率]$n^{22}{}_D$ 1.473

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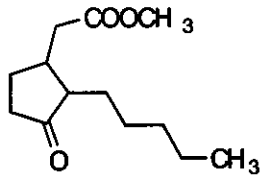
Hill, R.K. et al., Tetrahedron, 1965, 21, 1501, (絶対構造)
Kaiser, R. et al., Tet. Lett., 1974, 3413, (4,5-didehydro Me ester)
Kitahara, T. et al., Agric. Biol. Chem., 1982, 46, 1369; 1984, 48, 1731; 1987, 51, 1129; 1991, 55, 1013, (合成法)
Miersch, O. et al., Phytochemistry, 1986, 26, 1037; 1989, 28, 339; 1303; 1992, 31, 3835, (分離, 誘導体)
Farmer, E.E. et al., Proc. Natl. Acad. Sci. U.S.A., 1990, 87, Ford, R.A. et al., Food Chem. Toxicol., 1992, 30, 85S, (レビュー, 毒性)
Sembdner, G. et al., Annu. Rev. Plant Physiol., 1993, 44, 569, (レビュー)
Matsuura, H. et al., Biosci., Biotechnol., Biochem., 1993, 57, 1253, (誘導体)
Husain, A. et al., J. Nat. Prod., 1993, 56, 2008, (分離, C13-NMR)
Kiyota, H. et al., Phytochemistry, 1997, 46, 983, (誘導体, 合成法)
Wasternack, C. et al., Fett/Lipid, 1998, 100, 139, (レビュー)

§ 3-Oxo-2-pentylcyclopentaneacetic acid; (1*R*,2*R*)-form, Me ester
[化学名・別名]Methyl dihydrojasmonate. Hedione. FEMA 3408
[CAS No.]24851-98-7
[化合物分類]WE2000, 脂肪族化合物(Monocarbocyclic carboxylic acids and lactone)
[構造式]

[分子式]$C_{13}H_{22}O_3$
[分子量]226.315
[正確な分子量]226.156895
[基原]Odiferous component in jasmine oil (*Jasminum grandiflorum*)
[用途]香水原料として重要
[性状]液体
[沸点]Bp_3 102-108 ℃ (Bp_4 118-119 ℃)
[化学物質毒性データ総覧(RTECS)登録番号]GY2453800

----------文献----------

Torii, S. et al., J.O.C., 1975, 40, 2221, (合成法, IR, H-NMR, Mas)
Matsuda, I. et al., J.O.C., 1980, 45, 237, (IR, H-NMR)
Miersch, O. et al., Phytochemistry, 1987, 26, 1037-1039; 1989, 28, 339-340, (分離)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 496, (Me ester)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1753-1754, (Me ester)

***RTECS (化学物質毒性データ) ***

生体影響物質　　: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-ラット.
投与量・期間:>5 gm/kg
毒性影響　　:致死量以外に毒性影響に関する報告はない.

参照文献

FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- [Vol.,頁,年(19-)]30,85S,1992

〈〈試験方法〉〉認知されている最小致死量(LDLo)試験.

曝露経路 ：皮膚への塗布

被験動物 ：げっ歯類-ウサギ.

投与量・期間：5 gm/kg

毒性影響 ：致死量以外に毒性影響に関する報告はない.

参照文献

FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- [Vol.,頁,年(19-)]30,85S,1992

米国ＮＩＯＳＨ基準の発展とサーベランス

米国ＮＩＯＳＨ職業暴露調査データ

全米職業曝露調査(NOES)-米国全国職業ばく露調査(1983)

全米職業曝露調査(NOES) Hazard Code - X2419

No. of Facilities: 884 (評価)

No. of Industries: 2

No. of Occupations: 6

No. of Employees: 9641 (評価)

No. of Female Employees: 4689 (評価)

米国に於ける状況

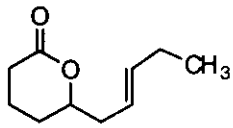
EPA TSCA Section 8(b) CHEMICAL INVENTORY

§ Tetrahydro-6-(2-pentenyl)-2*H*-pyran-2-one; (-)-(Z)-form

[CAS No.]25524-95-2

[化合物分類]含酸素複素環式化合物(Pentanolide)

[構造式]



[基原] jasmine (*Jasminum grandiflorum*)

[沸点]$Bp_{0.3}$ 95-96.5 ℃

[比旋光度]:$[\alpha]_D^{16}$ -30.4 (neat)

[屈折率]$n^{14.9}{}_D$ 1.4773

----------文献----------

Winter, M. et al., Helv. Chim. Acta, 1962, 45, 1250, (分離)

Dubs, P. et al., Helv. Chim. Acta, 1978, 61, 998, (分離)

Yamanishi, T. et al., Agric. Biol. Chem., 1980, 44, 2139, (分離)

Haffner, T. et al., Helv. Chim. Acta, 1996, 79, 2088, (生合成, Mas)

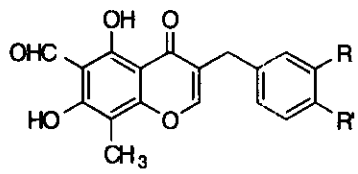
**********ジャノヒゲ (Janohige) **********

§§ユリ科ジャノヒゲ(*Ophiopogon japonicus* Ker-Gawl)の塊根。

§ 6-Aldehydoisoophiopogone A

[化合物分類]フラボノイド(Homoisoflavonoid)

[構造式]



RR' = -OCH_2O-

[分子式]$C_{19}H_{14}O_7$

[分子量]354.315

[正確な分子量]354.073955

[基原]*Ophiopogon japonicus*

[性状]橙色の針状結晶 (MeOH/$CHCl_3$)

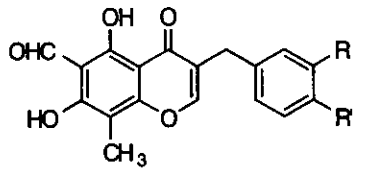
[融点]Mp 170-172 ℃

----------文献----------

Zhu, Y. et al., Phytochemistry, 1987, 26, 2873

§ 6-Aldehydoisoophiopogone B

[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]
[分子式]$C_{19}H_{16}O_6$
[分子量]340.322
[正確な分子量]340.09469
[基原]*Ophiopogon japonicus*
[性状]結晶(MeOH/$CHCl_3$)
[融点]Mp 144-145 ℃

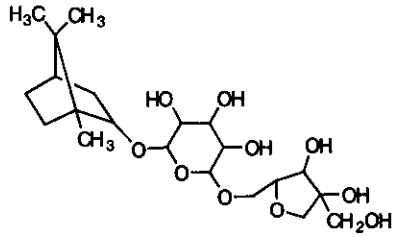


R = H, R' = OMe

----------文献----------

Zhu, Y. et al., Phytochemistry, 1987, 26, 2873

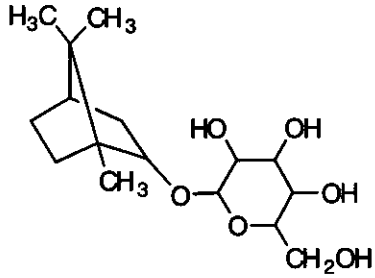
§ 2-Bornanol; (1*R*,2*S*)-form, *O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside]
[CAS No.]88700-35-0
[化合物分類]テルペノイド(Camphane monoterpenoid)
[構造式]
[分子式]$C_{21}H_{36}O_{10}$
[分子量]448.509
[正確な分子量]448.23085
[基原]*Ophiopogon japonicus*



----------文献----------

Kadyrov, A.S. et al., Khim. Prir. Soedin., 1972, 8, 59; 808; Chem. Nat. Compd. (Engl. Transl.), 1972, 8, 53; 796, (Tschimgin)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, nos. 312; 313, (生育)
Vernon, G.S.B. et al., Phytochemistry, 1975, 14, 583, (ferulate)
Tadesa, K. et al., Agric. Biol. Chem., 1976, 40, 1069, (生合成)
Suire, C. et al., Phytochemistry, 1982, 21, 349, (ferulate)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 68; 69; 70; 71; 384; 385; 386, (レビュー)

§ 2-Bornanol; (1*S*,2*R*)-form, *O*-β-D-Glucopyranoside
[CAS No.]88763-93-3
[構造式]
[分子式]$C_{16}H_{28}O_6$
[分子量]316.394
[正確な分子量]316.18859
[基原]*Ophiopogon japonicus*

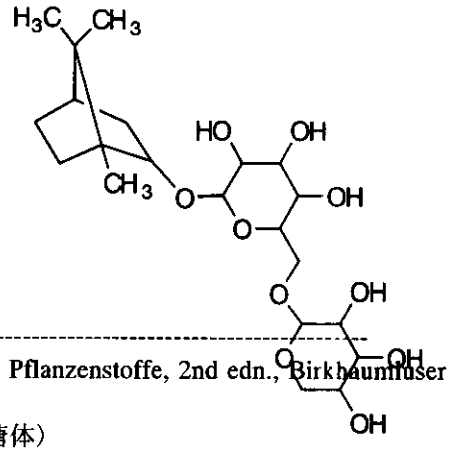


----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, nos. 312; 313, (生育)
Adinolfi, M. et al., Phytochemistry, 1990, 29, 1696, (分離, 配糖体)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 68; 69; 70; 71; 384; 385; 386, (レビュー)

§ 2-Bornanol; (1*S*,2*R*)-form, *O*-[α-L-Arabinofuranosyl-(1 → 6)-β-D-glucopyranoside]

[CAS No.] 128529-77-1
[化合物分類] テルペノイド (Camphane monoterpenoid)
[構造式]

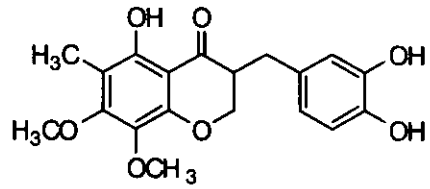


[分子式] $C_{21}H_{36}O_{10}$
[分子量] 448.509
[正確な分子量] 448.23085
[基原] *Ophiopogon japonicus*

----------文献----------

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhauser Verlag, Basel, 1972, nos. 312; 313, (生育)
Adinolfi, M. et al., Phytochemistry, 1990, 29, 1696, (分離, 配糖体)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 2, 68; 69; 70; 71; 384; 385; 386, (レビュー)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, BMD000; IHY000; NCQ820

§ 3-(3,4-Dihydroxybenzyl)-5,7,8-trihydroxy-6-methyl-4-chromanone; (±)-form, 7,8-Di-Me ether
[化学名・別名] 3-(3,4-Dihydroxybenzyl)-5-hydroxy-7,8-dimethoxy-6-methyl-4-chromanone
[CAS No.] 149180-48-3
[化合物分類] フラボノイド (Homoisoflavonoid)
[構造式]

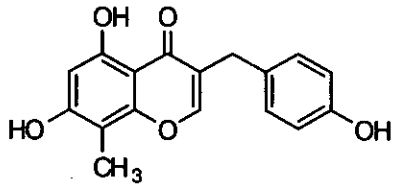


[分子式] $C_{19}H_{20}O_7$
[分子量] 360.363
[正確な分子量] 360.120905
[基原] *Ophiopogon japonicus*
[性状] 黄色のシロップ
[UV]: [neutral] λ_{max} 216 ; 286 (MeOH)

----------文献----------

Asano, T. et al., Chem. Pharm. Bull., 1993, 41, 391, (分離, UV, H-NMR, C13-NMR)

§ 5,7-Dihydroxy-3-(4-methoxybenzyl)-8-methyl-4-chromone
[化学名・別名] 5,7-Dihydroxy-3-[(4-hydroxyphenyl)methyl]-8-methyl-4*H*-1-benzopyran-4-one (CAS 名).
Desmethylisoophiopogonone B
[CAS No.] 75239-64-4
[化合物分類] フラボノイド (Homoisoflavonoid)
[構造式]

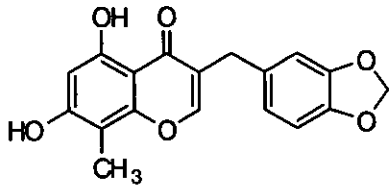


[分子式] $C_{17}H_{14}O_5$
[分子量] 298.295
[正確な分子量] 298.084125
[基原] *Ophiopogon japonicus*
[性状] 青白い黄色の粉末 (EtOH)
[融点] Mp 208-210 ℃

----------文献----------

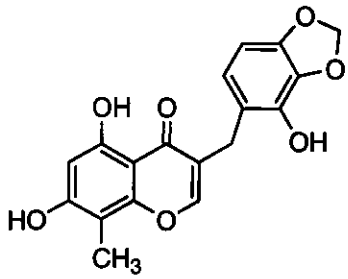
Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 2039; 2487, (分離)

§ Isoophiopogonone A
[化学名・別名] 3-(1,3-Benzodioxol-5-ylmethyl)-5,7-dihydroxy-8-methyl-4*H*-1-benzopyran-4-one.
5,7-Dihydroxy-8-methyl-3-(3,4-methylenedioxybenzyl)-4-chromenone

[CAS No.]75239-61-1
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]

[分子式]$C_{18}H_{14}O_6$
[分子量]326.305
[正確な分子量]326.07904
[基原]*Ophiopogon japonicus*
[性状]黄色の針状結晶(EtOH)
[融点]Mp 202-203 ℃

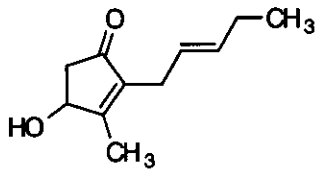
----------文献----------

Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 2039, (分離)
Asano, T. et al., Chem. Pharm. Bull., 1993, 41, 391, (2'-Hydroxyoxyisoophiopogonone A)

§ Isoophiopogonone A; 2'-Hydroxy
[化学名・別名]2'-Hydroxyisoophiopogonone A
[CAS No.]149155-31-7
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]

[分子式]$C_{18}H_{14}O_7$
[分子量]342.304
[正確な分子量]342.073955
[基原]*Ophiopogon japonicus*
[性状]青白い黄色の針状結晶(MeOH)
[融点]Mp 226-227 ℃

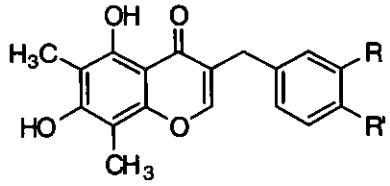
----------文献----------

Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 2039, (分離)
Asano, T. et al., Chem. Pharm. Bull., 1993, 41, 391, (2'-Hydroxyoxyisoophiopogonone A)

§ Jasmololone; (Z)-form
[化合物分類]脂肪族化合物(Monocarbocyclic aldehydes and ketone)
[構造式]

[基原]*Chrysanthemum cinerariaefolium*, *Ophiopogon japonicus*

----------文献---------- ------

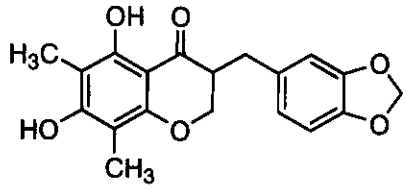
Takahashi, T. et al., Chem. Lett., 1981, 1189, (合成法, H-NMR, C13-NMR)
Ando, T. et al., J. Agric. Food Chem., 1983, 31, 151, (合成法)
Ballini, R. et al., Synthesis, 1986, 849, (合成法)
Zhu, Y. et al., CA, 1991, 115, 99055z, (生育)

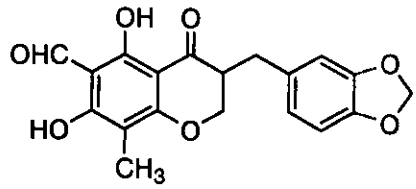
§ Methylophiopogonone A
[化学名・別名]3-(1,3-Benzodioxol-5-ylmethyl)-5,7-dihydroxy-6,8-dimethyl-4*H*-1-benzopyran-4-one(CAS名). 5,7-Dihydroxy-6,8-dimethyl-3-(3,4-methylenedioxybenzyl)-4-chromenone
[CAS No.]74805-90-6
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]

R, R' = $-OCH_2O-$
[分子式]$C_{19}H_{16}O_6$
[分子量]340.322
[正確な分子量]340.09469
[基原]*Ophiopogon japonicus*
[性状]青白い黄色の針状結晶(EtOH)
[融点]Mp 210-211 ℃

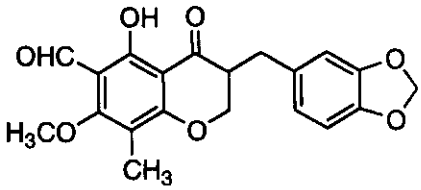
----------文献----------

Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 1477

Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (誘導体)
Watanabe, Y. et al., Chem. Pharm. Bull., 1985, 33, 5358, (誘導体)

§ Methylophiopogonone A; 2,3-Dihydro
[化学名・別名]Methylophiopogonanone A
[CAS No.]74805-92-8
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]

[分子式]$C_{19}H_{18}O_6$
[分子量]342.348
[正確な分子量]342.11034
[基原]*Ophiopogon japonicus*
[性状]針状結晶(CCl_4)
[融点]Mp 166-167 ℃
[比旋光度]:$[\alpha]_D^{19}$ -72 (c, 1 in $CHCl_3$)
[その他のデータ]絶対構造は決定してない
----------文献----------
Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 1477
Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (誘導体)
Watanabe, Y. et al., Chem. Pharm. Bull., 1985, 33, 5358, (誘導体)

§ Methylophiopogonone A; 2,3-Dihydro, 1''-oxo
[化学名・別名]6-Formylisoophiopogonanone A
[CAS No.]88700-29-2
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]

[分子式]$C_{19}H_{16}O_7$
[分子量]356.331
[正確な分子量]356.089605
[基原]*Ophiopogon japonicus*, *Ophiopogon ohwii*
[性状]針状結晶(MeOH/$CHCl_3$)
[融点]Mp 176 ℃
[比旋光度]:$[\alpha]_D^{21}$ -11.2 (c, 0.41 in $CHCl_3$)
----------文献----------
Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 1477
Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (誘導体)
Watanabe, Y. et al., Chem. Pharm. Bull., 1985, 33, 5358, (誘導体)

§ Methylophiopogonone A; 2,3-Dihydro, 1''-oxo, 7-Me ether
[化学名・別名]7-*O*-Methyl-6-formylisoophiopogonanone A
[CAS No.]88700-31-6
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]

[分子式]$C_{20}H_{18}O_7$
[分子量]370.358
[正確な分子量]370.105255
[基原]*Ophiopogon japonicus*
[融点]Mp 113 ℃
[比旋光度]:$[\alpha]_D$ -43.4
----------文献----------
Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 1477
Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (誘導体)
Watanabe, Y. et al., Chem. Pharm. Bull., 1985, 33, 5358, (誘導体)

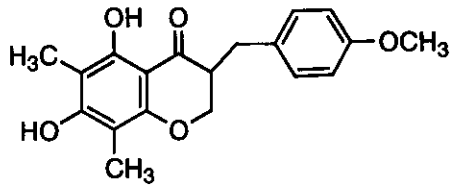
§ Methylophiopogonone B

[化学名・別名]5,7-Dihydroxy-3-[(4-methoxyphenyl) methyl]-6,8-dimethyl-4*H*-1-benzopyran-4-one(CAS名). 5,7-Dihydroxy-3-(4-methoxybenzyl)-6,8-dimethyl-4-chromenone
[CAS No.]74805-89-3
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]As Methylophiopogonone A with R = H, R' = OMe
[分子式]$C_{19}H_{18}O_5$
[分子量]326.348
[正確な分子量]326.115425
[基原]*Ophiopogon japonicus*, *Ophiopogon ohwii*
[性状]青白い黄色の針状結晶(EtOH)
[融点]Mp 219-220 ℃

----------文献----------

Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 1477
Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (誘導体)
Watanabe, Y. et al., Chem. Pharm. Bull., 1985, 33, 5358, (誘導体)

§ Methylophiopogonone B; 2,3-Dihydro
[化学名・別名]Methylophiopogonanone B
[CAS No.]74805-91-7
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]

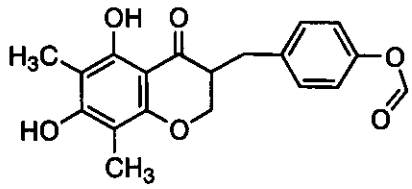


[分子式]$C_{19}H_{20}O_5$
[分子量]328.364
[正確な分子量]328.131075
[基原]*Ophiopogon japonicus*
[性状]針状結晶(CCl_4)
[融点]Mp 159-160 ℃
[比旋光度]:$[\alpha]_D^{17}$ -53 (c, 1 in dioxan)

----------文献----------

Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 1477
Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (誘導体)
Watanabe, Y. et al., Chem. Pharm. Bull., 1985, 33, 5358, (誘導体)

§ Methylophiopogonone B; 2,3-Dihydro, 1''-oxo
[化学名・別名]6-Formylisoophiopogonanone B
[CAS No.]88700-30-5
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]



[分子式]$C_{19}H_{18}O_6$
[分子量]342.348
[正確な分子量]342.11034
[基原]*Ophiopogon japonicus*, *Ophiopogon ohwii*
[性状]針状結晶($MeOH/CHCl_3$)
[融点]Mp 141 ℃
[比旋光度]:$[\alpha]_D^{21}$ -10.4 (c, 0.24 in $CHCl_3$)

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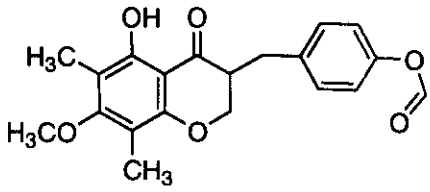
Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 1477
Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (誘導体)
Watanabe, Y. et al., Chem. Pharm. Bull., 1985, 33, 5358, (誘導体)

§ Methylophiopogonone B; 2,3-Dihydro, 1''-oxo, 7-Me ether
[化学名・別名]7-*O*-Methyl-6-formylisoophiopogonanone B
[CAS No.]88700-32-7
[化合物分類]フラボノイド(Homoisoflavonoid)

[構造式]
[分子式] $C_{20}H_{20}O_6$
[分子量] 356.374
[正確な分子量] 356.12599
[基原] *Ophiopogon japonicus*
[融点] Mp 93 ℃
[比旋光度]: $[\alpha]_D$ -47.4 (c, 0.5 in $CHCl_3$)



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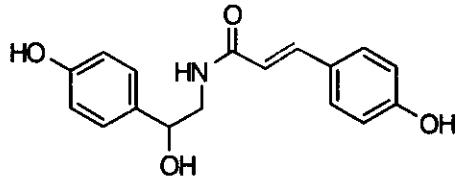
Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 1477
Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (誘導体)
Watanabe, Y. et al., Chem. Pharm. Bull., 1985, 33, 5358, (誘導体)

§ Octopamine; (ξ)-form, *N*-(4-Hydroxy-*E*-cinnamoyl)
[化学名・別名] *N-trans-p*-Coumaroyloctopamine
[CAS No.] 66648-45-1
[化合物分類] アルカロイド化合物 (Cinnamic acid amide)
[構造式]
[分子式] $C_{17}H_{17}NO_4$
[分子量] 299.326
[正確な分子量] 299.115759
[基原] 次の植物から得られるアルカロイド: *Capsicum annuum* var. *grossum*, *Ophiopogon japonicus*, *Solanum khasianum*
[性状] 結晶
[融点] Mp 214-215 ℃



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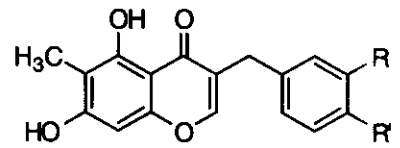
Negwer, M., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag, 1987, 945
Midgley, J.M. et al., J.C.S. Perkin 2, 1989, 963, (結晶構造, 絶対構造, 成書)
Matsuda, F. et al., Biosci., Biotechnol., Biochem., 2000, 64, 625, (*N*-Coumaroyloctopamine)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, AKT250

§ Ophiopogonone A
[化学名・別名] 3-(1,3-Benzodioxol-5-ylmethyl)-5,7-dihydroxy-6-methyl-4*H*-1-benzopyran-4-one (CAS 名). 5,7-Dihydroxy-6-methyl-3-(3,4-methylenedioxybenzyl)-4-chromenone
[CAS No.] 75239-62-2
[化合物分類] フラボノイド (Homoisoflavonoid)
[構造式]
[分子式] $C_{18}H_{14}O_6$
[分子量] 326.305
[正確な分子量] 326.07904
[基原] *Ophiopogon japonicus*
[性状] 青白い黄色の針状結晶 (EtOH)
[融点] Mp 235-236 ℃



R, R' = $-OCH_2O-$

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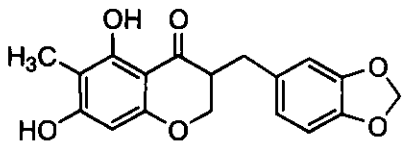
Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 2039, (分離, H-NMR)
Asano, T. et al., Chem. Pharm. Bull., 1993, 41, 391, (2'-Hydroxyophiopogonone A)

§ Ophiopogonone A; 2,3-Dihydro
[化学名・別名] Ophiopogonanone A
[CAS No.] 75239-63-3
[化合物分類] フラボノイド (Homoisoflavonoid)
[構造式]
[分子式] $C_{18}H_{16}O_6$
[分子量] 328.321
[正確な分子量] 328.09469



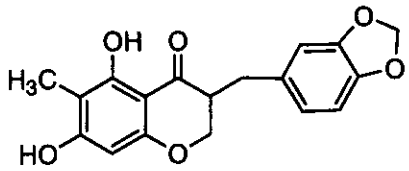
[基原]次の植物から分離:*Ophiopogon japonicus*
[性状]針状結晶(EtOH)
[融点]Mp 175-176 ℃
[比旋光度]:[α]$_D$ -13 (c, 1 in dioxan)

----------文献----------

Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 2039, (分離, H-NMR)
Asano, T. et al., Chem. Pharm. Bull., 1993, 41, 391, (2'-Hydroxyophiopogonone A)

§ Ophiopogonone A; 2'-Hydroxy

[化学名・別名]2',5,7-Trihydroxy-6-methyl-3-(3',4'-methylenedioxybenzyl)-4-chromenone.
2'-Hydroxyophiopogonone A
[CAS No.]149155-30-6
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]



[分子式]$C_{18}H_{14}O_7$
[分子量]342.304
[正確な分子量]342.073955
[基原]*Ophiopogon japonicus*
[性状]青白い黄色の針状結晶(MeOH)
[融点]Mp 275-276 ℃で分解

----------文献----------

Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 2039, (分離, H-NMR)
Asano, T. et al., Chem. Pharm. Bull., 1993, 41, 391, (2'-Hydroxyophiopogonone A)

§ Ophiopogonone B

[化学名・別名]5,7-Dihydroxy-3-[(4-methoxyphenyl)methyl]-6-methyl-4*H*-1-benzopyran-4-one.
5,7-Dihydroxy-3-(4-methoxybenzyl)-4-chromenone
[CAS No.]75239-60-0
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式] As Ophiopogonone A with R = H, R' = OMe
[分子式]$C_{18}H_{16}O_5$
[分子量]312.321
[正確な分子量]312.099775
[基原]*Ophiopogon japonicus*
[性状]青白い黄色の針状結晶(EtOH)
[融点]Mp 235-237 ℃

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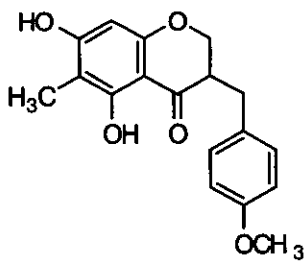
Tada, A. et al., Chem. Pharm. Bull., 1980, 28, 2039, (分離)
Camarda, L. et al., Heterocycles, 1983, 20, 39, (分離)
Kaneda, N. et al., Yakugaku Zasshi, 1983, 103, 1133, (Ophiopogonanone)
Mezey-Vandor, G. et al., Annalen, 1987, 447, (合成法)
Jain, A.C. et al., Indian J. Chem., Sect. B, 1990, 29, 338, (合成法)

§ Ophiopogonone B; 2,3-Dihydro

[化学名・別名]Ophiopogonanone
[CAS No.]88700-33-8
[化合物分類]フラボノイド(Homoisoflavonoid)
[構造式]



[分子式]$C_{18}H_{18}O_5$
[分子量]314.337
[正確な分子量]314.115425
[基原]*Ophiopogon japonicus*
[融点]Mp 176 ℃
[比旋光度]:[α]$_D$ -9.9

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