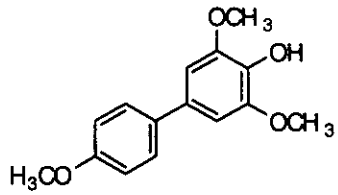
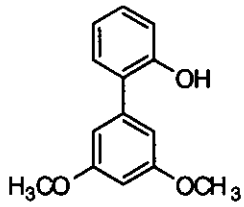
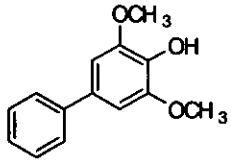
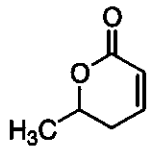
Nilsson, M. et al., Acta Chem. Scand., 1963, 17, 1157, (Methoxyaucuparin)
Borejsza-Wysocki, W. et al., Phytochemistry, 1999, 50, 231, (分離, H-NMR, C13-NMR, Mas)

§ 3,4,4',5-Biphenyltetrol; 3,4',5-Tri-Me ether
[化学名・別名]4-Hydroxy-3,4',5-trimethoxybiphenyl. 4'-Methoxyaucuparin
[CAS No.]54961-04-5
[化合物分類]単環芳香族(Biphenyl)
[構造式]

[分子式]$C_{15}H_{16}O_4$
[分子量]260.289
[正確な分子量]260.10486
[基原]*Photinia glabra*, *Rhaphiolepsis umbellata*, *Sorbus aucuparia*, *Aronia arbutifolia*, *Chaenomeles* spp.
[用途]ファイトアレキシン. 抗カビ剤.
[融点]Mp 99 ℃ (synthetic)
[UV]:[base] λ max (溶媒の報告はない) [neutral] λ max 268 (ε 13500) (EtOH) [neutral] λ max 267 (ε 13800) (MeOH) [neutral] λ max 268 (ε 13700) (EtOH) [base] λ max 298 () (MeOH-NAOH)
----------文献----------
Cotterill, P.J. et al., J.C.S. Perkin 1, 1974, 2423, (4'-Methoxyaucuparin)
Watanabe, K. et al., Agric. Biol. Chem., 1990, 54, 1861, (4'-Methoxyaucuparin, Rhaphiolepsin)
Kokubun, T. et al., Phytochemistry, 1995, 40, 57, (4'-Methoxyaucuparin)

§ 2,3',5'-Biphenyltriol; 3',5'-Di-Me ether
[化学名・別名]2-(3,5-Dimethoxyphenyl) phenol. 2-Hydroxy-3',5'-dimethoxybiphenyl. Isoaucuparin
[CAS No.]168301-25-5
[化合物分類]単環芳香族(Biphenyl)
[構造式]

[分子式]$C_{14}H_{14}O_3$
[分子量]230.263
[正確な分子量]230.094295
[基原]*Sorbus aucuparia*
[用途]ファイトアレキシン
[UV]:[neutral] λ max 291 (ε 3500) (MeOH)
----------文献----------
Kokubun, T. et al., Phytochemistry, 1995, 40, 57, (分離, UV, H-NMR)

§ 3,4,5-Biphenyltriol; 3,5-Di-Me ether
[化学名・別名]3,5-Dimethoxy-4-biphenylol. 4-Hydroxy-3,5-dimethoxybiphenyl. Aucuparin
[化合物分類]単環芳香族(Biphenyl)
[構造式]

[分子式]$C_{14}H_{14}O_3$
[分子量]230.263
[正確な分子量]230.094295
[基原]次の植物の幹から分離: *Sorbus aucuparia*
[性状]結晶
[融点]Mp 101-101.5 ℃
[溶解性]BERDY SOL: アセトン, ヘキサンに可溶; 水, ヘキサンに難溶
[UV]:[neutral] λ max 228 (ε 38900); 274 (ε 15135) (MeOH) [neutral] λ max 273 (ε 15135) (EtOH) [base] λ max 314 () (MeOH-NAOH)
----------文献----------
Narasimhachari, N. et al., Can. J. Chem., 1962, 40, 1118, (分離, 誘導体)
Erdtman, H. et al., Acta Chem. Scand., 1963, 17, 1151, (UV, H-NMR)
Nilsson, M. et al., Acta Chem. Scand., 1963, 17, 1157, (合成法)

§ 5,6-Dihydro-6-methyl-2*H*-pyran-2-one (*S*-form)



[CAS No.] 10048-32-5
[化合物分類] 含酸素複素環式化合物 (Pentanolide)
[構造式]
[基原] ナナカマドの液果 (*Sorbus aucuparia*)
[性状] オイル
[沸点] Bp_{14} 104-105 ℃
[比旋光度]: $[\alpha]_D^{24}$ +206 (c, 1 in EtOH)
[UV]: [neutral] λ_{max} 205 (ε 10700) (MeOH) [neutral] λ_{max} 213 (ε 10000); 221 (ε 8100) (EtOH)
[傷害・毒性] 50 %致死量 (LD_{50}) (マウス, 腹腔内投与) 250 mg/kg. 催腫瘍性; BERDY HAZD : 50 %致死量 (LD_{50}) (マウス, 腹腔内投与) 250 mg/kg
[化学物質毒性データ総覧 (RTEC) 登録番号] UQ0525000

----------文献----------

Hofmann, A.W., Annalen, 1859, 110, 129, (分離)
Kuhn, R. et al., Chem. Ber., 1962, 95, 2009, (絶対構造)
Crombie, L. et al., J.C.S.(C), 1968, 2852, (生合成)
IARC Monog., 1976, 10, 199; Suppl. 7, 1987, 42, 69; 255, (レビュー, 毒性)
Yamagiwa, S. et al., J.C.S. Perkin 1, 1978, 214, (合成法, IR, H-NMR)
Lichtenthaler, F.W. et al., Carbohydr. Res., 1984, 132, C1, (合成法, *S*-form)
Dupont, J. et al., Tetrahedron: Asymmetry, 1998, 9, 949, (*S*-form, 合成法)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, PAJ500

*****RTECS (化学物質毒性データ) *****

生体影響物質　　: 催腫瘍物質. 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　　: 腹腔内投与
被験動物　　: げっ歯類-マウス
投与量・期間 : 250 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

85GDA2 "CRC Handbook of Antibiotic Compounds," Vols.1- , Berdy, J., Boca Raton, FL, CRC Press, 1980- [Vol.,頁,年 (19-)] 8 (1),253,1982

〈〈試験方法〉〉 LD50 試験 (50%致死量試験).
曝露経路　　: 静脈注射
被験動物　　: げっ歯類-マウス
投与量・期間 : 195 mg/kg
毒性影響　　: 〔行動〕痙攣または発作閾値への影響.
〔行動〕活動度の変化 (特定の試験).

参照文献

ARZNAD Arzneimittel-Forschung. 医薬品. Research. (Editio Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep. Ger.) V.1- 1951- [Vol.,頁,年 (19-)] 19,617,1969

〈〈試験方法〉〉 LD50 試験 (50%致死量試験).
曝露経路　　: 皮膚への塗布
被験動物　　: げっ歯類-ウサギ.
投与量・期間 : 5040 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

AIHAAP American Industrial Hygiene Association Journal. (AIHA, 475 Wolf Ledges Pkwy., Akron, OH 44311) V.19- 1958- [Vol.,頁,年 (19-)] 30,470,1969

*****催腫瘍性に関するデータ*****

〈〈試験方法〉〉 最小毒性量 (TDLo) 試験.
曝露経路　　: 皮下投与.
被験動物　　: げっ歯類-ラット.

投与量・期間：1280 mg/kg/32W-I
毒性影響　　：〔催腫瘍性〕RTECS 基準による催腫瘍性.
〔催腫瘍性〕適用部位の腫瘍

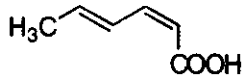
参照文献

BJCAAI British Journal of Cancer. (Macmillan Press Ltd., Houndmills, Basingstoke, Hants. RG21 2XS, UK) V.1- 1947- [Vol.,頁,年(19-)]17,100,1963

§ 2,4-Hexadienoic acid; (*E, E*)-form

[化学名・別名]Panasorb

[CAS No.]110-44-1



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

[構造式]

[基原]次の植物から分離: ベリー類の *Sorbus aucuparia* (ナナカマド), おそらく非天然物

[用途]Preservative for many foodstuffs, cosmetic and pharmaceutical products (K and Ca salts used similarly)

[性状]針状結晶(EtOH 溶液)

[融点]Mp 134.5 ℃

[沸点]Bp 228 ℃で分解

[溶解性]温水に適度に溶ける

[PKa 値]pK_a 4.51 (25 ℃, 0.1*M* NaCl)

[傷害・毒性]皮膚, 眼を刺激する, contact sensitizer. 50 %致死量(LD_{50})(ラット, 経口) 7360 mg/kg

[化学物質毒性データ総覧(RTEC)登録番号]WG2100000

----------文献----------

Eisner, U. et al., J.C.S., 1953, 1372, (合成法, UV, EE-form, ZE-form)
Woodford, R. et al., CA, 1970, 72, 136 312x, (レビュー)
Frighetto, N. et al., Chem. Phys. Lipids, 1978, 22, 115, (C13-NMR, EE-form)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, 21, 402, (レビュー)
Lewis, R.J., Food Additives Handbook, Van Nostrand Reinhold International, New York, 1989, SKU000
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1990, 15, 296, (用途)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1146
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 100, (2-Propenyl ester)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, SKU000

*****RTECS (化学物質毒性データ) *****

生体影響物質　　：農芸化学. 催腫瘍物質. 変異原物質. 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
被験動物　　：ヒト-男性
投与量・期間：150 mg/1 時間
反応の症度　：重度

参照文献

JPPMAB Journal of Pharmacy and Pharmacology. (Pharmaceutical Soc. of Great Britain, 1 Lambeth High St., London SEI 7JN, UK) V.1- 1949- [Vol.,頁,年(19-)]10,719,1958

〈〈試験方法〉〉標準ドライズ試験.
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：1 mg
反応の症度　：重度

参照文献

UCDS** Union Carbide Data Sheet. (Union Carbide Corp., 39 Old Ridgebury Rd., Danbury, CT 06817) [Vol.,頁,年(19-)]7/14/1965

*****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：7360 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
JIHTAB Journal of Industrial Hygiene and Toxicology. (Cambridge, MA) V.18-31, 1936-49. For publisher information, [Vol.,頁,年(19-)]30,63,1948
〈〈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-ラット.
投与量・期間：800 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
38MKAJ "Patty's Industrial Hygiene and Toxicology," 3rd rev. ed., Clayton, G.D., and F.E. Clayton, eds., New York, John Wiley & Sons, Inc., 1978-82. Vol. 3 originally pub. in 1979; pub. as 2nd rev. ed. in 1985. [Vol.,頁,年(19-)]2C,4953,1982
〈〈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：3200 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
38MKAJ "Patty's Industrial Hygiene and Toxicology," 3rd rev. ed., Clayton, G.D., and F.E. Clayton, eds., New York, John Wiley & Sons, Inc., 1978-82. Vol. 3 originally pub. in 1979; pub. as 2nd rev. ed. in 1985. [Vol.,頁,年(19-)]2C,4953,1982
〈〈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：2820 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
JPPMAB Journal of Pharmacy and Pharmacology. (Pharmaceutical Soc. of Great Britain, 1 Lambeth High St., London SEI 7JN, UK) V.1- 1949- [Vol.,頁,年(19-)]21,85,1969
〈〈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：2820 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
JPPMAB Journal of Pharmacy and Pharmacology. (Pharmaceutical Soc. of Great Britain, 1 Lambeth High St., London SEI 7JN, UK) V.1- 1949- [Vol.,頁,年(19-)]21,85,1969
〈〈試験方法〉〉 致死量試験
曝露経路　　：皮膚への塗布
被験動物　　：げっ歯類-ウサギ.
投与量・期間：>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
UCDS** Union Carbide Data Sheet. (Union Carbide Corp., 39 Old Ridgebury Rd., Danbury, CT 06817) [Vol.,頁,年(19-)]7/14/1965

*****催腫瘍性に関するデータ*****

〈〈試験方法〉〉 最小毒性量(TDLo)試験.
曝露経路　　：皮下投与.
被験動物　　：げっ歯類-ラット.
投与量・期間：1040 mg/kg/65 週間間欠投与
毒性影響　　：〔催腫瘍性〕 RTECS 基準による, 不確実な催腫瘍性物質

〔催腫瘍性〕適用部位の腫瘍

参照文献

BJCAAI British Journal of Cancer. (Macmillan Press Ltd., Houndmills, Basingstoke, Hants. RG21 2XS, UK) V.1- 1947- [Vol.,頁,年(19-)]20,134,1966

*****変異原性に関するデータ*****

<<試験方法>> 細胞遺伝学分析試験

試験系 : げっ類-ハムスター肺

投与量・期間 : 1050 mg/L

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-)]22,501,1984

<<試験方法>> 姉妹染色分体交換試験

試験系 : げっ類-ハムスター肺

投与量・期間 : 1050 mg/L

参照文献

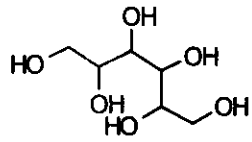
FCTOD7 Food and Chemical Toxicology. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.20- 1982- [Vol.,頁,年(19-)]22,501,1984

§ Iditol; L-form

[CAS No.]488-45-9

[化合物分類]炭水化物(Hexitol)

[構造式]



[基原]Occurs with D-glucitol in the berry of mountain ash (*Sorbus aucuparia*) and in other plants

[融点]Mp 73.5 ℃

[比旋光度]:[α]$_D^{20}$ -3.5 (c, 1.0 in H_2O)

----------文献----------

Bourne, E.J. et al., J.C.S., 1952, 2542, (L-isopropylidene, L-hexa-Ac, L-hexabenzoyl)

Jeffrey, G.A. et al., Carbohydr. Res., 1970, 14, 207, (conformn)

Azarnia, N. et al., Acta Cryst. B, 1972, 28, 1007, (結晶構造)

Angyal, S.J. et al., Carbohydr. Res., 1980, 84, 201, (C13-NMR)

Kopf, J. et al., Acta Cryst. C, 1992, 48, 339, (結晶構造)

Kopf, J. et al., Carbohydr. Res., 1992, 229, 17, (結晶構造, hexa-Ac)

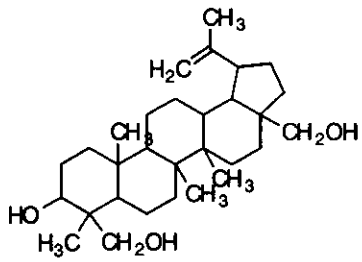
§ 20(29)-Lupene-3,23,28-triol; 3 β-form

[化学名・別名]Sorbikortal II

[CAS No.]76260-92-9

[化合物分類]テルペノイド(Lupane triterpenoid)

[構造式]



[基原]*Elaeodendron glaucum*, *Sorbus aucuparia*

[性状]結晶

[融点]Mp 256-258 ℃

[比旋光度]:[α]$_D$ +24.6 ($CHCl_3$). [α]$_D$ -28.9 ($CHCl_3$)

----------文献----------

Lawrie, W. et al., J.C.S., 1960, 4303, (分離)

Joshi, K.C. et al., J. Indian Chem. Soc., 1980, 57, 1042, (分離)

Adam, G. et al., Phytochemistry, 1982, 21, 1385, (誘導体)

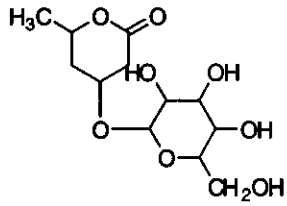
Ikuta, A. et al., Phytochemistry, 1988, 27, 2813, (分離)

Ye, W.C. et al., Chin. Chem. Lett., 1991, 2, 375, (分離, H-NMR, C13-NMR)

Miao, Z. et al., Youji Huaxue, 1992, 12, 610; CA, 118, 209389h, (分離)

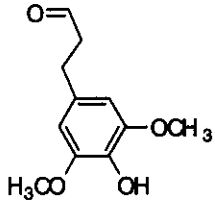
§ 3,4,5,6-Tetrahydro-4-hydroxy-6-methyl-2*H*-pyran-2-one; (4*S*,6*)*-form, *O*-β-D-Glucopyranoside

[化学名・別名]Parasorboside

[CAS No.]33276-04-9
[化合物分類]含酸素複素環式化合物(Pentanolide)
[構造式]

[分子式]$C_{12}H_{20}O_8$
[分子量]292.285
[正確な分子量]292.11582
[基原]*Sorbus aucuparia*
[性状]針状結晶(Me_2CO)
[融点]Mp 68.9 ℃. Mp 143.4 ℃ (double Mp)

----------文献----------

Fujii, M. et al., Nat. Med. (Tokyo), 1996, 50, 404; CA, 126, 347184, (Hydroxybenzoylparasorboside)
Weinges, K. et al., Eur. J. Org. Chem., 1998, 189, (結晶構造, Parasorboside)
Chandrareddy, U.D. et al., Phytochemistry, 1998, 47, 907, (Paashaanolactone)

§ 3-(3,4,5-Trihydroxyphenyl) propanal; 3,5-Di-Me ether
[化学名・別名]3-(4-Hydroxy-3,5-dimethoxyphenyl) propanal. Dihydrosinapic aldehyde
[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]

[分子式]$C_{11}H_{14}O_4$
[分子量]210.229
[正確な分子量]210.08921
[基原]*Sorbus aucuparia*
[性状]オイル

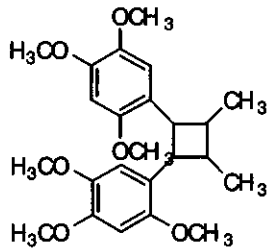
----------文献----------

Malterud, K.E. et al., Phytochemistry, 1989, 28, 1548

§§ バラ科ナナカマド(*Sorbus commixta* Hedel.)の葉及び果実。
該当物質なし

***********セキショウ (Sekisho) ***********

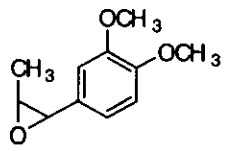
§§ サトイモ科セキショウ(*Acorus gramineus* Solander)の根茎。

§ 1,2-Dimethyl-3,4-bis(2,4,5-trimethoxyphenyl) cyclobutane; (1 ξ,2 ξ,3 ξ,4 ξ)-form
[化学名・別名]Acoradin. Bisasaricin
[CAS No.]73036-51-8
[化合物分類]リグナン化合物(7',7'-Cyclolignans (cyclobutane))
[構造式]

[基原]*Acorus calamus*, *Acorus gramineus*, *Cupressus dupreziana*, *Cupressus sempervirens*
[性状]プリズム結晶(Et_2O/petrol)
[融点]Mp 101 ℃
[比旋光度]:$[\alpha]_D$ 0 ($CHCl_3$)

----------文献----------

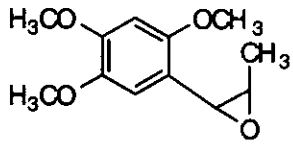
Niwa, M. et al., Tet. Lett., 1978, 4891, (分離, 構造決定, 合成法)
Patra, A. et al., Indian J. Chem., Sect. B, 1979, 17, 412, (Acoradin)
Mahindru, R.N. et al., Phytochemistry, 1993, 32, 1073, (結晶構造)

§ 4-(1-Propenyl)-1,2-benzenediol; (*E*)-form, Di-Me ether, 1'*R,2'*R**-epoxide**
[化学名・別名]2-(3,4-Dimethoxyphenyl)-3-methyloxirane(CAS 名). 1-(1,2-Epoxypropyl)-3,4-dimethoxybenzene. 1,2-Dimethoxy-4-(3-methyloxiranyl) benzene. 1-(3,4-Dimethoxyphenyl)-1,2-epoxypropane

[CAS No.] 124878-07-5
[その他の CAS No.] 40626-39-9
[化合物分類] 単環芳香族 (Simple phenylpropanoid)
[構造式]

[分子式] $C_{11}H_{14}O_3$
[分子量] 194.23
[正確な分子量] 194.094295
[基原] 次の植物から分離: *Acorus gramineus*
[性状] オイル
[比旋光度]: $[\alpha]_D$ +24 ($CHCl_3$)

----------文献----------

Briner, E. et al., Helv. Chim. Acta, 1963, 46, 2249, (IR, Raman)
Vajda, M. et al., Org. Magn. Reson., 1976, 8, 324, (C13-NMR, 誘導体)
Bohlmann, F. et al., Phytochemistry, 1980, 19, 2655, (分離)
Klungsoeyr, J. et al., Biomed. Mass Spectrom., 1982, 9, 323, (代謝物, ガスクロマト)
Della Greca, M. et al., Phytochemistry, 1989, 28, 2319, (di-Me ether epoxide)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, IRY000

§ 1,2,4-Trimethoxy-5-(1-propenyl) benzene; (*E*)-form, 1'*R,2'*R**-Epoxide**
[化学名・別名] 2-Methyl-3-(2,4,5-trimethoxyphenyl) oxirane. 1-(1,2-Epoxypropyl)-2,4,5-trimethoxybenzene. 1,2-Epoxy-1-(2,4,5-trimethoxyphenyl) propane. *trans*-Epoxyasarone
[CAS No.] 124878-08-6
[化合物分類] 単環芳香族 (Simple phenylpropanoid)
[構造式]

[分子式] $C_{12}H_{16}O_4$
[分子量] 224.256
[正確な分子量] 224.10486
[基原] *Acorus gramineus*
[性状] オイル
[比旋光度]: $[\alpha]_D$ +32 ($CHCl_3$)

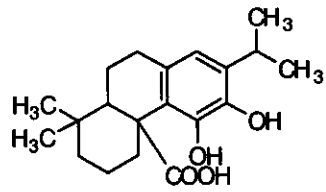
----------文献----------

Baxter, R.M., Can. J. Chem., 1962, 40, 154, (構造)
Patra, A. et al., J. Nat. Prod., 1981, 44, 668, (C13-NMR)
Della Greca, M. et al., Phytochemistry, 1989, 28, 2319, (epoxide)
Diaz, F. et al., Org. Prep. Proced. Int., 1991, 23, 133, (合成法, 成書)
Nawamaki, K. et al., Phytochemistry, 1996, 43, 1175, (分離, H-NMR)
Gonzalez, M.C. et al., Phytochemistry, 1996, 43, 1361, (分離, UV, IR, H-NMR, C13-NMR, Mas)
Siergiejczyk, L. et al., Magn. Reson. Chem., 2000, 38, 1037, (H-NMR, C13-NMR)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, IHX400

*********セージ (Sage) *********

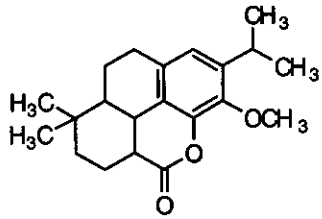
§§ シソ科セージ (*Salvia officinalis* L.) の茎葉または全草。

§ 8,11,13-Abietatriene-11,12,20-triol; 20-Carboxylic acid
[化学名・別名] 11,12-Dihydroxy-8,11,13-abietatrien-20-oic acid. Carnosic acid. Deoxypicrosalvinic acid. Salvin

[CAS No.]3650-09-7
[化合物分類]テルペノイド(Abietane diterpenoid)
[構造式]

[分子式]$C_{20}H_{28}O_4$
[分子量]332.439
[正確な分子量]332.19876
[基原]次の植物から分離: *Salvia officinalis*, *Salvia canariensis*, *Salvia apiana*, *Rosmarinus officinalis*
[性状]結晶(hexane)
[融点]Mp 185-190 ℃で分解
[比旋光度]:$[\alpha]_D^{23}$ +191 (c, 1.07 in MeOH)
Solubility: BERDY SOL: エーテル, メタノール, 塩基, クロロホルムに可溶; 水に難溶
[UV]:[neutral] λ_{max} 212 (ε 21500); 233 (ε 9650); 284 (ε 1690) (EtOH)

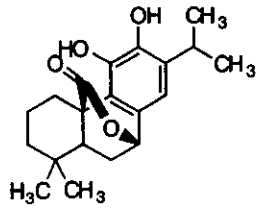
----------文献----------

Linde, H. et al., Helv. Chim. Acta, 1964, 47, 1234, (分離, UV, IR, H-NMR)
Wenkert, E. et al., J.O.C., 1965, 30, 2931, (分離. IR, H-NMR, 構造)
Narayanan, C.R. et al., Tet. Lett., 1965, 3647, (構造決定)
Dentali, S.J. et al., Phytochemistry, 1990, 29, 993, (分離)
Gonzaacutelez, A.G. et al., Phytochemistry, 1991, 30, 4067, (分離, H-NMR, C13-NMR)
Djarmati, Z. et al., Phytochemistry, 1992, 31, 1307, (分離, H-NMR, C13-NMR, 結晶構造)

§ 8,11,13-Abietatriene-11,12,20-triol; 20 → 11 Lactone, 12-Me ether
[化学名・別名]12-Methoxy-8,11,13-abietatrien-20,11-olide
[化合物分類]テルペノイド(Abietane diterpenoid)
[構造式]

[分子式]$C_{21}H_{28}O_3$
[分子量]328.45
[正確な分子量]328.203845
[基原]*Salvia officinalis*
[性状]結晶(petrol)
[融点]Mp 112-114 ℃

----------文献----------

Linde, H. et al., Helv. Chim. Acta, 1964, 47, 1234, (分離, UV, IR, H-NMR)
Wenkert, E. et al., J.O.C., 1965, 30, 2931, (分離. IR, H-NMR, 構造)
Narayanan, C.R. et al., Tet. Lett., 1965, 3647, (構造決定)
Meyer, W.L. et al., Tet. Lett., 1966, 4261, (合成法)
Dentali, S.J. et al., Phytochemistry, 1990, 29, 993, (分離)
Gonzaacutelez, A.G. et al., Phytochemistry, 1991, 30, 4067, (分離, H-NMR, C13-NMR)
Djarmati, Z. et al., Phytochemistry, 1992, 31, 1307, (分離, H-NMR, C13-NMR, 結晶構造)

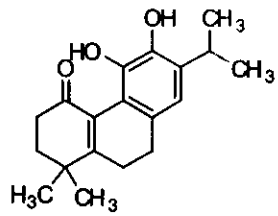
§ Carnosol
[化学名・別名]11,12-Dihydroxy-8,11,13-abietatrien-20,7 β -olide. Picrosalvin
[CAS No.]5957-80-2
[化合物分類]テルペノイド(Abietane diterpenoid)
[構造式]

[分子式]$C_{20}H_{26}O_4$
[分子量]330.423
[正確な分子量]330.18311
[基原]*Salvia carnosa* の苦味成分, *Salvia officinalis*, *Salvia triloba*, *Rosmarinus officinalis*
[性状]結晶(EtOH)
[融点]Mp 221-226 ℃
[比旋光度]:$[\alpha]_D$ -66 (EtOH)
[UV]:[neutral] λ_{max} 210 (ε 26300); 283 (ε 2510) (EtOH)

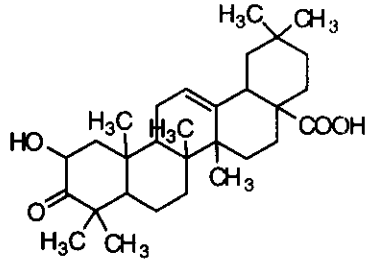
----------文献----------

Brieskorn, C.H. et al., J.O.C., 1964, 29, 2293, (構造決定, 生合成)
Nakatani, N. et al., Agric. Biol. Chem., 1984, 48, 2081, (Isorosmanol)

Al-Hazimi, H.M.G. et al., Phytochemistry, 1984, 23, 919, (Isocarnosol)
Kelecom, A. et al., Phytochemistry, 1984, 23, 1677, (Deoxocarnosol)
Fraga, B.M. et al., Phytochemistry, 1986, 25, 269, (誘導体)
Luis, J.G. et al., Phytochemistry, 1991, 31, 3272, (16-Acetoxycarnosol)
Luis, J.G. et al., Phytochemistry, 1994, 35, 1373, (di-Me ether)

§ 6-*O*-(3,4-Dihydroxycinnamoyl) glucose; β-D-Pyranose-form, 3'-Me ether, 2,3,4-trihydroxybutyl glycoside
[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]構造式はまだ有効ではない
[分子式]$C_{21}H_{30}O_{12}$
[分子量]474.461
[正確な分子量]474.17373
[基原]セージ, *Salvia officinalis*
[性状]粉末
----------文献----------
Shimomura, H. et al., Phytochemistry, 1987, 26, 249; 1988, 27, 641, (分離, H-NMR)
Machida, K. et al., CA, 1994, 120, 4693x, (分離, 配糖体)
Wang, M. et al., J. Agric. Food Chem., 2000, 48, 235, (Me ether feruloyltrihydroxybutyl)

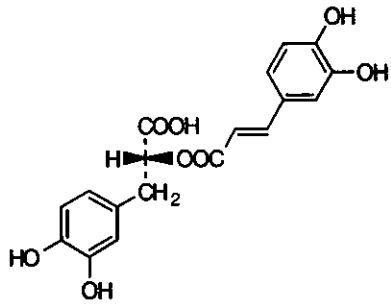
§ 11,12-Dihydroxy-20-nor-5(10),8,11,13-abietatetraen-1-one
[化学名・別名]Sageone
[CAS No.]142546-15-4
[化合物分類]テルペノイド(Nor- and homoabietane diterpenoid)
[構造式]

[分子式]$C_{19}H_{24}O_3$
[分子量]300.397
[正確な分子量]300.172545
[基原]*Salvia mellifera, Salvia officinalis*
[性状]無定型の黄色の塊もしくはオイル
----------文献----------
Gonzaacutelez, A.G. et al., Phytochemistry, 1992, 31, 1297, (分離, H-NMR, C13-NMR)
Tada, M. et al., Phytochemistry, 1994, 35, 539, (分離, H-NMR, C13-NMR)
Majetich, G. et al., J.O.C., 1997, 62, 6928, (合成法)

§ 2,3-Dihydroxy-12-oleanen-28-oic acid; (2α,3α)-form, 3-Ketone
[化学名・別名]2-Hydroxy-3-oxo-12-oleanen-28-oic acid
[CAS No.]73584-62-0
[化合物分類]テルペノイド(Oleanane triterpenoid)
[構造式]

[分子式]$C_{30}H_{46}O_4$
[分子量]470.691
[正確な分子量]470.33961
[基原]*Salvia officinalis*
[性状]結晶(MeOH) (as Me ester, Ac)
[融点]Mp 226-227℃ (Me ester, Ac)
[比旋光度]:$[\alpha]_D^{20}$ +63 (c, 1.8 in $CHCl_3$) (Me ester, Ac)
----------文献----------
Caglioti, L. et al., Gazz. Chim. Ital., 1961, 91, 1387, (分離, 構造決定)
Glen, A.T. et al., J.C.S.(C), 1967, 510, (分離)
Cheung, H.T. et al., Aust. J. Chem., 1972, 25, 2003, (分離)
Yagi, A. et al., Chem. Pharm. Bull., 1978, 26, 3075, (分離)
Brieskorn, C.H. et al., Planta Med., 1980, 38, 86, (3-ketone)
Kumar, N.S. et al., Phytochemistry, 1985, 24, 2454, (分離)
Kojimo, H. et al., Phytochemistry, 1986, 25, 729, (分離, C13-NMR)

Alam, M.S. et al., Phytochemistry, 1996, 41, 1197, (Augustic acid)
Monte, F.J.Q. et al., Magn. Reson. Chem., 1997, 35, 802, (H-NMR, C13-NMR)
Siddiqui, B.S. et al., Planta Med., 1997, 63, 47, (Eucalyptolic acid)
Zhao, Q.-S. et al., Phytochemistry, 1998, 48, 1025, (Maslinic acid, H-NMR, C13-NMR)

§ 3-(3,4-Dihydroxyphenyl)-2-hydroxypropanoic acid; (*R*)-form, 2-*O*-(3,4-Dihydroxy-*E*-cinnamoyl)

[化学名・別名]Rosmarinic acid. Labiatenic acid. Rosemarinic acid
[CAS No.]537-15-5
[関連 CAS No.]20283-92-5
[化合物分類]薬物: 抗 HIV 薬(Anti-HIV agent), 単環芳香族(Simple phenylpropanoid), 薬物: 抗炎症薬(Antiinflammatory agent), 薬物: (Antithrombotic agent), 薬物: 抗ウイルス物質(Antiviral agent), 薬物: 血小板凝集阻害薬(Platelet aggregation inhibiting agent)
[構造式]



[分子式]$C_{18}H_{16}O_8$
[分子量]360.32
[正確な分子量]360.08452
[基原]*Rosmarinus officinalis*, *Melissa officinalis*, *Momordica balsamina*, *Mentha piperita*, *Salvia officinalis*, *Teucrium scorodonia*, *Sanicula europaea*, *Coleus blumei*, *Thymus* spp., その他の植物属
[用途]Exhibits antithrombotic and antiplatelet effects. 抗炎症薬. 抗 HIV 活性, 抗菌, 抗カビ作用を示す; 鎮吐作用, 抗遺伝子毒性活性, 等. 植物成長抑制活性を示す.
[性状]結晶・二水和物
[融点]Mp 204 ℃で分解
[比旋光度]:$[\alpha]_D^{20}$ +145
[Log P 計算値]Log P 1.01 (計算値)
[UV]:[neutral] λ_{max} 230 (); 329 () (MeOH)
[傷害・毒性]50 %致死量(LD_{50})(マウス, 静脈内投与) 561 mg/kg
[化学物質毒性データ総覧(RTEC)登録番号]GD8990000

----------文献----------
Parnham, M.J. et al., Drugs of the Future, 1985, 10, 756, (レビュー)
Englberger, W. et al., Int. J. Immunopharmacol., 1988, 10, 729, (薬理)
Peake, P.W. et al., Int. J. Immunopharmacol., 1991, 13, 853, (薬理)
Mahmood, N., Antiviral Chem. Chemother., 1993, 4, 235, (anti-HIV activity, NMR, Mas)
Zou, Z.W. et al., Yaoxue Xuebao, 1993, 28, 241, (薬理)
Zhao, L.M. et al., Chin. Chem. Lett., 1996, 7, 449, (Salviaflaside)
Abraham, S.K., Food Chem. Toxicol., 1996, 34, 15, (活性)
Binutu, O.A. et al., Planta Med., 1996, 62, 352, (活性)
Robinson, W.E.Jr. et al., Proc. Natl. Acad. Sci. U.S.A., 1996, 93, 6326, (活性)
Huang, H. et al., Planta Med., 1999, 65, 92, (butyl ester)
Kuo, Y.-H. et al., J. Chin. Chem. Soc. (Taipei), 2000, 47, 241, (Me ester)

*****RTECS (化学物質毒性データ) *****

生体影響物質　　: 医薬品.

*****健康障害に関するデータ*****
*****急性毒性に関するデータ*****

〈〈試験方法〉〉 LD50 試験(50%致死量試験).
曝露経路　　: 静脈注射
被験動物　　: げっ歯類-マウス
投与量・期間 : 561 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

DRFUD4 Drugs of the Future. (J.R. Prous, S.A., Apartado de Correos 540, 08080 Barcelona, Spain) V.1- 1975/76- [Vol.,頁,年(19-)]10,756,1985

§ GD9095000

RTECS（化学物質毒性データ）
健康障害に関するデータ
急性毒性に関するデータ

〈〈試験方法〉〉 LD50 試験(50%致死量試験).
曝露経路　：経口投与.
被験動物　：げっ歯類-マウス
投与量・期間：2850 mg/kg
毒性影響　：〔行動〕傾眠(全身活動度の低下).
〔肺,胸郭,または呼吸〕呼吸抑制.

参照文献

GNRIDX Gendai no Rinsho. (Tokyo, Japan) V.1-10, 1967-76(?). [Vol.,頁,年(19-)]3,675,1969

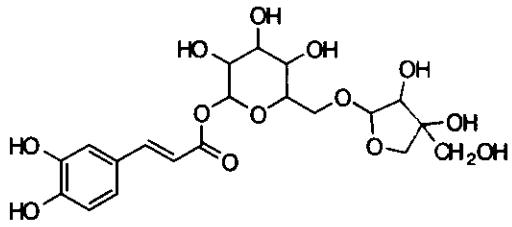
〈〈試験方法〉〉 LD50 試験(50%致死量試験).
曝露経路　：腹腔内投与
被験動物　：げっ歯類-マウス
投与量・期間：1160 mg/kg
毒性影響　：〔行動〕傾眠(全身活動度の低下).
〔肺,胸郭,または呼吸〕呼吸抑制.

参照文献

GNRIDX Gendai no Rinsho. (Tokyo, Japan) V.1-10, 1967-76(?). [Vol.,頁,年(19-)]3,675,1969

§ 3-(3,4-Dihydroxyphenyl)-2-propenoic acid; (*E*)-form, [β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranosyl] ester

[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]
[分子式]$C_{20}H_{26}O_{13}$
[分子量]474.418
[正確な分子量]474.137345
[基原]*Salvia officinalis*
[性状]結晶(MeOH)
[融点]Mp 69-71 ℃
[比旋光度]:[α]$_D^{23}$ -21.8 (c, 0.15 in MeOH)



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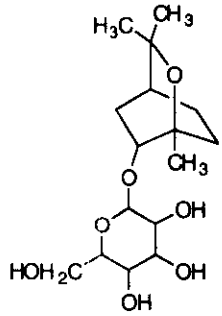
Hermann, F.X., Pharmazie, 1956, 11, 433, (レビュー)
Achenbach, H. et al., Chem. Ber., 1971, 104, 1468, (分離, 誘導体)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 957
Bowden, B.F. et al., Aust. J. Chem., 1975, 28, 91, (誘導体)
Saha, M.M. et al., Phytochemistry, 1991, 30, 3834, (分離, エステル)
Iriye, R. et al., Biosci., Biotechnol., Biochem., 1992, 56, 1773, (Petasiphenol)
IARC Monog., 1993, 56, 115, (Caffeic acid, レビュー, 毒性)
Mellidis, A.S. et al., J. Nat. Prod., 1993, 56, 949, (分離, エステル)

§ 1,8-Epoxy-*p*-menthan-2-ol; (1*S*,2*R*,4*R*)-form, *O*-β-D-Glucopyranoside

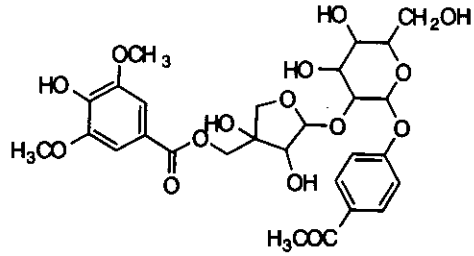
[CAS No.]168038-89-9
[化合物分類]テルペノイド(*p*-Menthane monoterpenoid)
[構造式]
[分子量]332.393
[正確な分子量]332.183505
[基原]*Foeniculum vulgare*, *Cunila spicata*, Dalmation sage (*Salvia officinali*)の葉
[性状]無定型の塊
[融点]Mp 92-94 ℃
[比旋光度]:[α]$_D^{21}$ -46.3 (c, 1.5 in MeOH)



----------文献----------

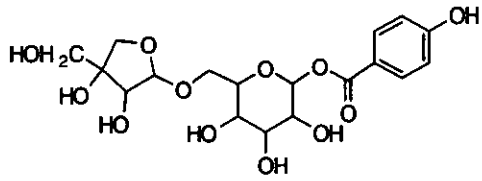
Manns, D., Phytochemistry, 1995, 39, 1115, (*Cunila spicata* glucoside)
Yoshikawa, Y. et al., Nat. Med. (Tokyo), 1996, 50, 176, (*Citrus unshiu* glucoside)

Kitajima, J. et al., Chem. Pharm. Bull., 1998, 46, 1583, (apiosylglucoside)
Ishikawa, T. et al., Chem. Pharm. Bull., 1998, 46, 1738, (*Foeniculum vulgare* glucoside)
Wang, M., J. Agric. Food Chem., 1998, 46, 2509, (1*S*,2*R*,4*R*-glucopyranoside, 分離, NMR)

§ 4'-Hydroxyacetophenone; *O*-[4-Hydroxy-3,5-dimethoxybenzoyl-(→ 5)-β-D-apiofuranosyl-(1 → 2)-β-D-glucopyranoside]
[CAS No.] 228405-06-9
[化合物分類] 炭水化物(Disaccharide), 単環芳香族(Simple aryl ketone)
[構造式]

[分子式] $C_{28}H_{34}O_{15}$
[分子量] 610.568
[正確な分子量] 610.189775
[基原] *Salvia officinalis*, *Thymus vulgaris*
[性状] 粉末

----------文献----------

Montgomery, H. et al., J.A.C.S., 1947, 64, 693, (配糖体)
Edwards, O.E. et al., Can. J. Chem., 1962, 40, 256, (isol)
Tsuzuki, Y. et al., Bull. Chem. Soc. Jpn., 1971, 44, 526, (配糖体)
Opdyke, D.L.J., Food Cosmet. Toxicol., Suppl., 1974, 927, (レビュー, 誘導体)
Selikson, S.J. et al., Tet. Lett., 1974, 3029, (合成法, 誘導体)
Wang, M. et al., J. Agric. Food Chem., 1999, 47, 1911-1914; 2000, 48, 235-238, (benzoylapiosylglucoside)
Miyase, T. et al., J. Nat. Prod., 1999, 62, 993-996, (Sibiricaphenone)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, HIO000; MDW750

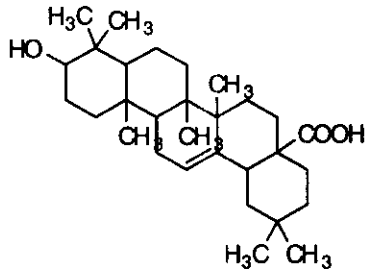
§ 4-Hydroxybenzoic acid; [β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranosyl] ester
[化合物分類] 単環芳香族(Simple benzoic acid and ester)
[構造式]

[分子式] $C_{18}H_{24}O_{12}$
[分子量] 432.38
[正確な分子量] 432.12678
[基原] *Salvia officinalis*
[性状] オイル
[比旋光度]: $[\alpha]_D^{23}$ -32.7 (c, 0.04 in MeOH)

----------文献----------

Cavallito, C.J. et al., J.A.C.S., 1943, 65, 2140, (benzyl ether, benzyl ether chloride)
Cavill, G.W.K. et al., J. Soc. Chem. Ind., London, 1947, 66, 175, (エステル)
Koichi, N. et al., Yakugaku Zasshi, 1954, 74, 498; CA, 49, 8182h, (Ph ester)
Org. Synth., Coll. Vol., 4, 1963, 178, (Ph ester)
Strohl, M.J. et al., Phytochemistry, 1965, 4, 383, (配糖体)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 889, (生育)
Baggaley, K.H. et al., J. Med. Chem., 1977, 20, 1388, (benzyl ether)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, 7, 812; 20, 500, (レビュー)
Perkins, M.V. et al., J.C.S. Perkin 1, 1990, 1111, (エステル)
Davidson, P.M., Antimicrobials in Foods, 2nd edn., (Eds. Davidson, P.M. et al), M. Dekker, 1993, 263, (parabens, レビュー)
Bairati, C. et al., Clin. Chim. Acta, 1994, 224, 147, (parabens, 薬理)
Wang, M. et al., J. Nat. Prod., 1999, 62, 454, (apiosylglucosyl ester)

§ 3-Hydroxy-12-oleanen-28-oic acid; 3 α-form
[化学名・別名] 3-Epioleanolic acid. 3-*epi*-Oleanolic acid

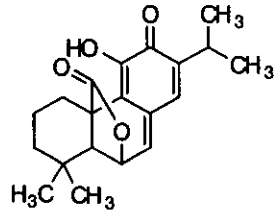
[CAS No.]25499-90-5
[化合物分類]テルペノイド(Oleanane triterpenoid)
[構造式]
[基原]次の植物から分離: sagel *Salvia officinalis*, *Boschniakia rossica*, *Liquidamber orientalis*, その他の植物
[性状]針状結晶(MeOH)
[融点]Mp 297-299 ℃
[比旋光度]:[α]$_D^{20}$ +68 (c, 1.66 in $CHCl_3$)



----------文献----------

Filczewski, M et al., Pol. J. Pharmacol. Pharm., 1988, 40, 233, (薬理, Succinoyloleanolic acid)
Maillard, M. et al., Phytochemistry, 1992, 31, 1321, (Oleanolic acid, C13-NMR)

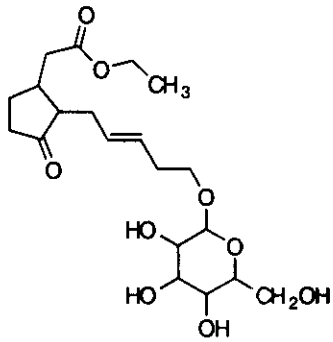
§ 11-Hydroxy-12-oxo-7,9(11),13-abietatrien-20,6-olide; 6 β-form
[化学名・別名]Sagequinone methide A
[CAS No.]194472-90-7
[化合物分類]テルペノイド(Abietane diterpenoid)
[構造式]
[基原]*Salvia officinalis*
[性状]黄色の結晶
[融点]Mp 145-147 ℃
[比旋光度]:[α]$_D^{25}$ -80.7 (c, 0.29 in $CHCl_3$)



----------文献----------

Tada, M. et al., Phytochemistry, 1997, 45, 1475, (分離, H-NMR, C13-NMR)

§ 2-(5-Hydroxy-2-pentenyl)-3-oxocyclopentaneacetic acid; (3 ξ,7 ξ)-form, *O*-β-D-Glucopyranoside, Et ester
[化合物分類]脂肪族化合物(Other monocarbocyclic ester)

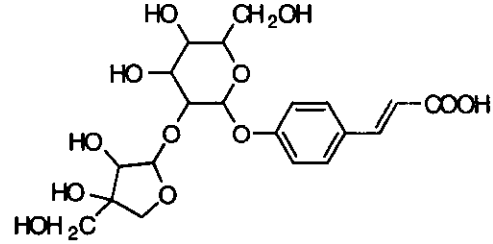


[構造式]
[分子式]$C_{20}H_{32}O_9$
[分子量]416.467
[正確な分子量]416.204635
[基原]セージ(*Salvia officinali*)
[性状]オイル
[その他のデータ]構造式は確定していない

----------文献----------

Yoshihara, T. et al., Agric. Biol. Chem., 1989, 53, 2835, (分離)
Miersch, O. et al., Phytochemistry, 1991, 30, 4049, (分離)
Cui, B. et al., Chem. Pharm. Bull., 1993, 41, 178, (配糖体)
Wang, M. et al., J. Agric. Food Chem., 2000, 48, 235-238, (配糖体, Et ester)
Ueda, M. et al., Tetrahedron, 2000, 56, 8101-8105, (分離, 配糖体)

§ 3-(4-Hydroxyphenyl)-2-propenoic acid; (*E*)-form, *O*-[β-D-Apiofuranosyl-(1 → 2)-β-D-glucopyranoside]
[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]
[分子式]$C_{20}H_{26}O_{12}$
[分子量]458.418
[正確な分子量]458.14243
[基原]*Salvia officinalis*
[UV]:[neutral] λ $_{max}$ 296 ()(溶媒の報告はない)

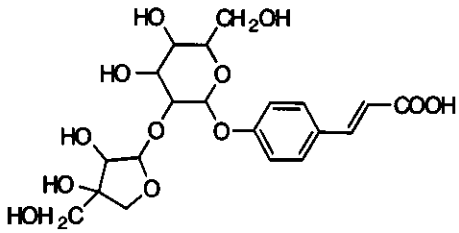


----------文献----------

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)
Ueda, M. et al., Phytochemistry, 1998, 49, 633, (配糖体)
Tazawa, S. et al., Chem. Pharm. Bull., 1999, 47, 1388, (4-Dihydrocinnamoyloxycinnamic acid)
Dai, W.-M. et al., J.O.C., 1999, 64, 5062, (Me ether, Me ester, 合成法, IR, H-NMR, C13-NMR)
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, CNU825

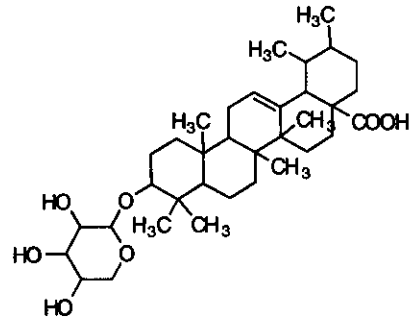
§ 3-(4-Hydroxyphenyl)-2-propenoic acid; (*Z*)-form, *O*-[β-D-Apiofuranosyl-(1 → 2)-β-D-glucopyranoside]



[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]
[分子式]$C_{20}H_{26}O_{12}$
[分子量]458.418
[正確な分子量]458.14243
[基原]*Salvia officinalis*
[UV]:[neutral] λ max 282 ()(溶媒の報告はない)

----------文献----------
Zincke, T., Annalen, 1902, 322, 224, (分離)
Ogawa, S., Bull. Chem. Soc. Jpn., 1927, 2, 25, (分離)
Bate-Smith, E.C., Sci. Proc. R. Dublin Soc., 1956, 27, 165, (生育)
Prager, R.H. et al., Aust. J. Chem., 1966, 19, 451, (Methyl *p*-geranyloxycinnamate)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 951; 953; 955, (生育)
Durkee, A.B. et al., Carbohydr. Res., 1979, 77, 252, (配糖体)
Winter, M. et al., J. Agric. Food Chem., 1986, 34, 616, (配糖体)
Cui, C.-B. et al., Chem. Pharm. Bull., 1990, 38, 3218, (配糖体)
Sashida, Y. et al., Chem. Pharm. Bull., 1991, 39, 709, (coumaroylglucoside, acetylcoumaroylglucoside)
Lemmich, J., Phytochemistry, 1995, 38, 427, (配糖体)
Rasmussen, S. et al., Phytochemistry, 1996, 42, 81, (*cis*-glucoside)
Ueda, M. et al., Phytochemistry, 1998, 49, 633, (配糖体)
1992, CNU825

§ 3-Hydroxy-12-ursen-28-oic acid; 3 β-form, 3-*O*-β-L-Arabinopyranoside

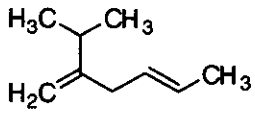


[化学名・別名]Sanguisorbin B
[CAS No.]32180-34-0
[化合物分類]テルペノイド(Ursane triterpenoid)
[構造式]
[分子式]$C_{35}H_{56}O_7$
[分子量]588.823
[正確な分子量]588.402605
[基原]*Salvia officinalis*
[性状]結晶
[融点]Mp 266-267 ℃

----------文献----------
Bukharov, V.G. et al., Izv. Akad. Nauk Kaz. SSR, Ser. Khim., 1970, 171; 2402, (Sanguisorbins, Empetroside C)

§ 2-Isopropyl-1,4-hexadiene(旧 CAS 名)
[化学名・別名]6-Methyl-5-methylene-2-heptene(CAS 名). Salvene
[関連 CAS No.]33746-69-9, 33746-70-2
[化合物分類]テルペノイド(Irregular acyclic monoterpenoid)

[構造式]
[分子式]C_9H_{16}
[分子量]124.225
[正確な分子量]124.1252


(*E*)-form

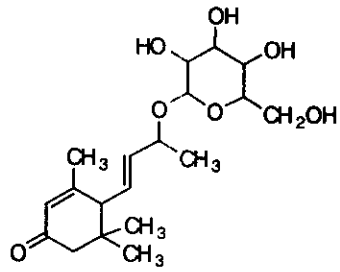
[基原]セージオイル(*Salvia officinali*)に存在, おそらく thujanes の脱炭酸した非天然物

----------文献----------

Brieskorn, C.H. et al., Annalen, 1964, 676, 171, (分離)
Laurence, B.M. et al., Parfums, Cosmet. Savons Fr., 1971, 1, 256; CA, 75, 80186b, (分離)
Dillenberger, Z. et al., Helv. Chim. Acta, 1978, 61, 1856, (合成法, H-NMR)
Cooke, R.J. et al., J.A.C.S., 1981, 103, 7317, (合成法, 成書)

§ 4,7-Megastigmadiene-3,9-diol; (3*S*,7*E*,9*R*)-form, 3-Ketone, 9-*O*-β-D-glucopyranoside

[化合物分類]テルペノイド(Megastigmane norterpenoid)
[構造式]



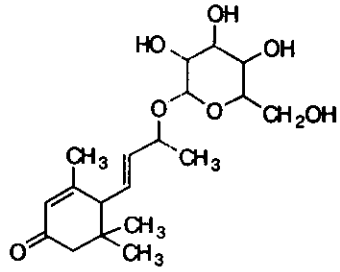
[分子式]$C_{19}H_{30}O_7$
[分子量]370.442
[正確な分子量]370.199155
[基原]次の植物から分離: *Polystichum tripteron*, *Dennstaedtia wilfordii*, ブラックベリー(*Rubus idaeu*), Dalmation sage (*Salvia officinali*)の葉
[性状]オイル
[比旋光度]:$[\alpha]_D^{20}$ +58.6 (c, 1.5 in MeOH)

----------文献----------

Murakami, T. et al., Chem. Pharm. Bull., 1981, 29, 866, (3-ketone 9-glucoside)
Wang, M. et al., J. Agric. Food Chem., 1998, 46, 2509, (3-ketone glucoside, 分離, NMR)

§ 4,7-Megastigmadiene-3,9-diol; (3*S*,7*E*,9)-form, 3-Ketone, 9-*O*-β-D-glucopyranoside

[化合物分類]テルペノイド(Megastigmane norterpenoid)
[構造式]

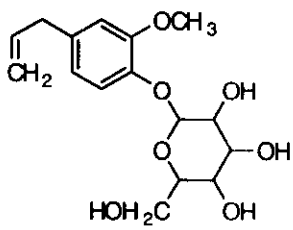


[分子量]370.442
[基原]ブラックベリー(*Rubus idaeu*), Dalmation sage (*Salvia officinali*)の葉
[性状]無定型の粉末

----------文献----------

Murakami, T. et al., Chem. Pharm. Bull., 1981, 29, 866, (3-ketone 9-glucoside)
Wang, M. et al., J. Agric. Food Chem., 1998, 46, 2509, (3-ketone glucoside, 分離, NMR)

§ 2-Methoxy-4-(2-propenyl) phenol; *O*-β-D-Glucopyranoside



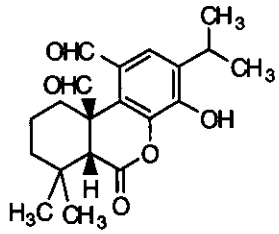
[化学名・別名]Citrusin C
[CAS No.]18604-50-7
[化合物分類]単環芳香族(Simple phenylpropanoid)
[構造式]
[分子式]$C_{16}H_{22}O_7$
[分子量]326.346
[正確な分子量]326.136555
[基原]白い花が咲く perilla *Perilla frutescens* var. *forma viridis* の葉, Dalmation sage (*Salvia officinali*)の葉
[性状]粉末
[融点]Mp 130-131 ℃
[比旋光度]:$[\alpha]_D^{22}$ -50.7 (c, 0.13 in MeOH)

----------文献----------

Fujita, T. et al., Phytochemistry, 1992, 31, 3265, (Citrusin C)

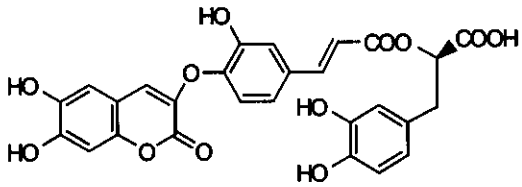
§ Safficinolide

[CAS No.]153660-18-5
[化合物分類]テルペノイド(Secoabietane and secofriedoabietane diterpenoid)
[構造式]
[分子式]$C_{20}H_{24}O_5$
[分子量]344.407
[正確な分子量]344.162375
[基原]*Salvia officinalis*
[性状]結晶
[融点]Mp 223-224 ℃で分解
[比旋光度]:[α]$_D^{26}$ -165 (c, 0.41 in EtOH)
[UV]:[neutral] λ $_{max}$ 235 (ε 25118); 290 (ε 25703) (EtOH)



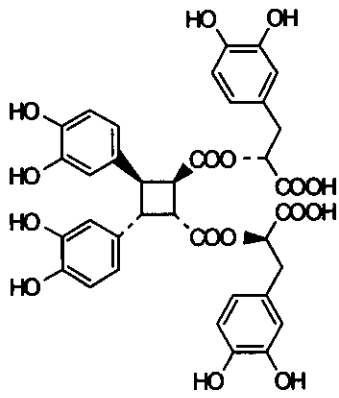
----------文献----------
Tada, M. et al., Phytochemistry, 1994, 35, 539, (分離, H-NMR, C13-NMR)

§ Sagecoumarin
[化合物分類]ベンゾピラノイド(3,6,7-Trioxygenated coumarin), リグナン化合物(Neolignan)
[構造式]
[分子式]$C_{27}H_{20}O_{12}$
[分子量]536.448
[正確な分子量]536.09548
[一般的性質]化学構造は Melitric acid A と似ている
[基原]*Salvia officinalis* (Sage)
[性状]淡褐色の粉末
[比旋光度]:[α]$_D^{20}$ +52 (c, 0.2 in MeOH)
[UV]:[neutral] λ $_{max}$ 288 (log ε 4.3); 332 (log ε 4.27) (MeOH)



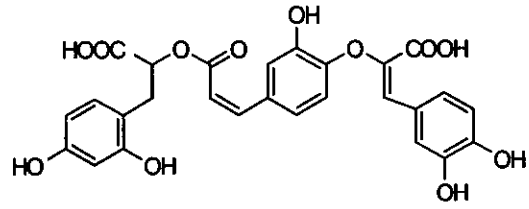
----------文献----------
Lu, Y. et al., Phytochemistry, 1999, 52, 1149

§ Sagerinic acid
[化合物分類]脂肪族化合物(Other monocarbocyclic ester), 単環芳香族(Simple phenylpropanoid)
[構造式]



[分子式]$C_{36}H_{32}O_{16}$
[分子量]720.639
[正確な分子量]720.16904
[一般的性質]Rosmarinic acid から誘導された
[基原]*Salvia officinalis*
[比旋光度]:[α]$_D^{20}$ +4 (c, 0.2 in MeOH)
[UV]:[neutral] λ $_{max}$ 232 (log ε 4.08); 286 (log ε 4.09) (MeOH)
----------文献----------
Lu, Y. et al., Phytochemistry, 1999, 51, 91, (分離, UV, H-NMR, C13-NMR, Mas)

§ Salvianolic acid I; 8''Z-Isomer
[化学名・別名]Melitric acid A. Schizotenuin E
[CAS No.]153765-45-8
[化合物分類]単環芳香族(Dimeric unchlorinated depside), リグナン化合物(Neolignan)
[構造式]
[分子式]$C_{27}H_{22}O_{12}$
[分子量]538.464
[正確な分子量]538.11113
[基原]*Melissa officinalis*, *Salvia officinalis*, *Schizonepeta tenuifolia*
[性状]淡褐色の粉末 + 1/2H_2O
[融点]Mp 135-138 ℃

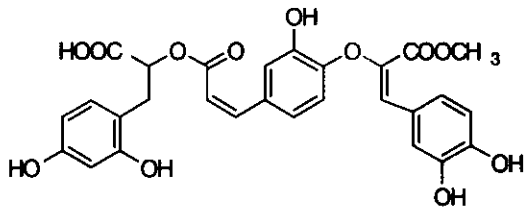


[比旋光度]:[α]$_D^{23}$ +45 (c, 0.2 in MeOH)
[UV]:[neutral] λ $_{max}$ 290 (log ε 4.32); 328 (log ε 4.34) (MeOH)
[その他のデータ]化学構造は Rosmarinic acid と似ている

----------文献----------

Agata, I. et al., Chem. Pharm. Bull., 1993, 41, 1608, (Melitric acid A)
Matsuta, M. et al., Nat. Med. (Tokyo), 1996, 50, 204, (Schizotenuin)
Lu, Y. et al., Phytochemistry, 1999, 52, 1149, (Melitric acid A)

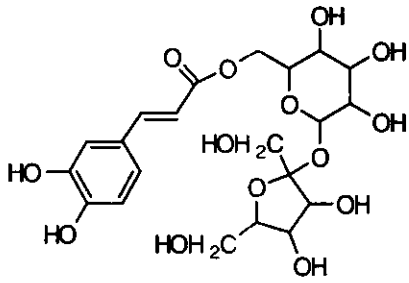
§ Salvianolic acid I; 8''Z-Isomer, 8''-Me ester
[化学名・別名]Schizotenuin F. Methyl melitrate A
[CAS No.]127498-36-6
[化合物分類]単環芳香族(Simple phenylpropanoid), リグナン化合物(Neolignan)
[構造式]
[分子式]$C_{28}H_{24}O_{12}$
[分子量]552.49
[正確な分子量]552.12678
[基原]*Salvia officinalis, Schizonepeta tenuifolia*
[用途]抗炎症薬
[性状]淡褐色の粉末
[UV]:[neutral] λ $_{max}$ 292 (log ε 4.33); 330 (log ε 4.36) (MeOH)



----------文献----------

Agata, I. et al., Chem. Pharm. Bull., 1993, 41, 1608, (Melitric acid A)
Matsuta, M. et al., Nat. Med. (Tokyo), 1996, 50, 204, (Schizotenuin)
Lu, Y. et al., Phytochemistry, 1999, 52, 1149, (Melitric acid A)

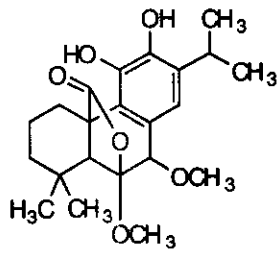
§ Sucrose; 6-*O*-(3,4-Dihydroxycinnamoyl) (*E*-)
[化学名・別名]6-Caffeoylsucrose
[化合物分類]炭水化物(Disaccharide), 単環芳香族(Simple phenylpropanoid)
[構造式]
[分子式]$C_{21}H_{28}O_{14}$
[分子量]504.444
[正確な分子量]504.14791
[基原]*Salvia officinalis*
[性状]結晶(MeOH)
[融点]Mp 210-212 ℃
[比旋光度]:[α]$_D^{23}$ +27.2 (c, 0.13 in MeOH)



----------文献----------

Wang, M. et al., J. Nat. Prod., 1999, 62, 454, (6-Caffeoylsucrose)

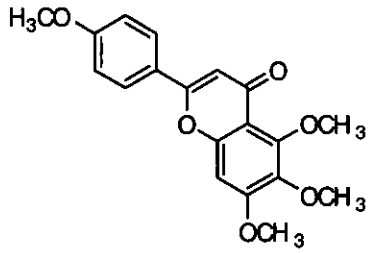
§ 6,7,11,12-Tetrahydroxy-8,11,13-abietatrien-20,6-olide; (6 α *OH*,7 β)-form, 6,7-Di-Me ether
[化学名・別名]6,7-Dimethoxy-7-epirosmanol
[CAS No.]194425-48-4
[化合物分類]テルペノイド(Abietane diterpenoid)
[構造式]
[分子式]$C_{22}H_{30}O_6$
[分子量]390.475
[正確な分子量]390.20424
[基原]*Salvia officinalis*
[性状]黄色の結晶
[融点]Mp 183-188 ℃
[比旋光度]:[α]$_D^{25}$ -30 (c, 0.02 in $CHCl_3$)



----------文献----------

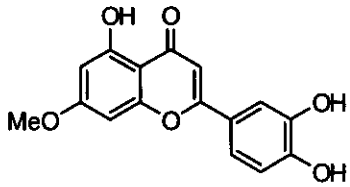
Tada, M. et al., Phytochemistry, 1997, 45, 1475, (分離, H-NMR, C13-NMR)

§ 4',5,6,7-Tetrahydroxyflavone; Tetra-Me ether
[化学名・別名]4',5,6,7-Tetramethoxyflavone. Tetra-*O*-methylscutellarein
[CAS No.]1168-42-9
[化合物分類]フラボノイド(Flavone; 4 × O-置換基)
[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]次の植物から分離: *Salvia officinalis* の葉, また *Callicarpa japonica*, *Orthosiphon stamineus*, *Marrubium peregrinum*, *Citrus*, *Chromolaena*, *Kickxia*, その他の植物からも得られる
[性状]結晶(EtOH) in 2 forms
[融点]Mp 142 ℃. Mp 166-167 ℃ (dimorph.)



----------文献----------
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

§ 3',4',5-Trihydroxy-7-methoxyflavone
[化学名・別名]2-(3,4-Dihydroxyphenyl)-5-hydroxy-7-methoxy-4*H*-1-benzopyran-4-one(CAS 名). Luteolin 7-methyl ether
[CAS No.]20243-59-8
[化合物分類]フラボノイド(Flavone; 4 × O-置換基)
[構造式]
[分子式]$C_{16}H_{12}O_6$
[分子量]300.267
[正確な分子量]300.06339
[基原]次の植物から分離: *Baccharis* spp., *Eremanthus* sp., *Hazardia* sp., *Salvia officinalis*, *Thymus membranaceus*, その他の植物
[性状]黄色のプリズム結晶 (EtOH)
[融点]Mp 266-268 ℃. Mp 306-308 ℃

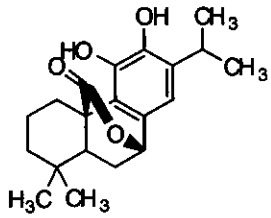


----------文献----------
Chumbalev, T.K. et al., Khim. Prir. Soedin., 1970, 6, 626; 1971, 7, 525; Chem. Nat. Compd. (Engl. Transl.), 1970, 6, 639; 1971, 7, 504, (Spinoside, glucofuranosylglucopyranoside)
Brieskorn, C.H. et al., Arch. Pharm. (Weinheim, Ger.), 1971, 304, 557, (分離)
Nunez-Alarcon, J. et al., Phytochemistry, 1973, 12, 1451, (5-xylosylglucoside)
Ulubelen, A. et al., Phytochemistry, 1982, 21, 801, (Yuanhuanin)
Wada, H. et al., Yakugaku Zasshi, 1986, 106, 989, (3'-glucoside)
Rettig, J.H. et al., Biochem. Syst. Ecol., 1990, 18, 393, (4'-diglucoside)

§§ シソ科(*Salvia lavandulaefolia* Vahl)の茎葉または全草。
該当物質なし

§§ シソ科(*Salvia triloba* Linne)の茎葉または全草。

§ Carnosol
[化学名・別名]11,12-Dihydroxy-8,11,13-abietatrien-20,7 β -olide. Picrosalvin
[CAS No.]5957-80-2
[化合物分類]テルペノイド(Abietane diterpenoid)
[構造式]
[分子式]$C_{20}H_{26}O_4$
[分子量]330.423
[正確な分子量]330.18311
[基原]次の植物の苦味成分: *Salvia carnosa*, *Salvia officinalis*, *Salvia triloba*, *Rosmarinus officinalis*



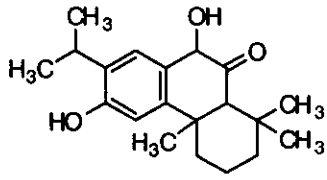
[性状]結晶(EtOH)
[融点]Mp 221-226 ℃
[比旋光度]:[α]$_D$ -66 (EtOH)
[UV]:[neutral] λ $_{max}$ 210 (ε 26300); 283 (ε 2510) (EtOH)

----------文献----------

Brieskorn, C.H. et al., J.O.C., 1964, 29, 2293, (構造決定, 生合成)
Narayanan, C.R. et al., Tet. Lett., 1965, 3647, (stereochem)
Nakatani, N. et al., Agric. Biol. Chem., 1984, 48, 2081, (Isorosmanol)
Al-Hazimi, H.M.G. et al., Phytochemistry, 1984, 23, 919, (Isocarnosol)
Kelecom, A. et al., Phytochemistry, 1984, 23, 1677, (Deoxocarnosol)
Fraga, B.M. et al., Phytochemistry, 1986, 25, 269, (誘導体)

§ 7,12-Dihydroxy-8,11,13-abietatrien-6-one; (7 ξ)-form

[化学名・別名]Trilobinone
[CAS No.]128741-29-7
[化合物分類]テルペノイド(Abietane diterpenoid)
[構造式]



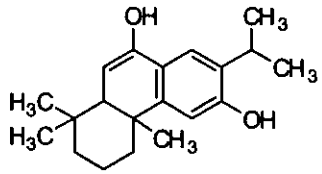
[基原]*Salvia triloba*
[性状]淡黄色の粉末

----------文献----------

Ulubelen, A., Planta Med., 1990, 56, 82, (分離, H-NMR, C13-NMR)

§ 12-Hydroxy-8,11,13-abietatrien-7-one; *enol*-form

[化学名・別名]6,8,11,13-Abietatetraene-7,12-diol. Trilobinol
[CAS No.]128741-28-6
[化合物分類]テルペノイド(Abietane diterpenoid)
[構造式]



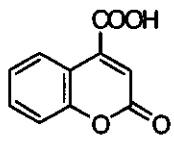
[分子式]$C_{20}H_{28}O_2$
[分子量]300.44
[正確な分子量]300.20893
[基原]次の植物から分離: *Salvia triloba*
[性状]黄色の無定型粉末

----------文献----------

Meyer, W.L. et al., J.O.C., 1975, 40, 3686, (合成法, 成書)
Matsumoto, T. et al., Bull. Chem. Soc. Jpn., 1977, 50, 1575, (成書)
Chang, H.M. et al., J.O.C., 1990, 55, 3537, (分離, H-NMR, C13-NMR)
Ulubelen, A. et al., Planta Med., 1990, 56, 82, (Trilobinol)

§ 2-Oxo-2*H*-1-benzopyran-4-carboxylic acid (CAS 名)

[化学名・別名]Coumarin-4-carboxylic acid
[CAS No.]27393-46-0
[化合物分類]ベンゾピラノイド(Non-oxygenated coumarin)
[構造式]

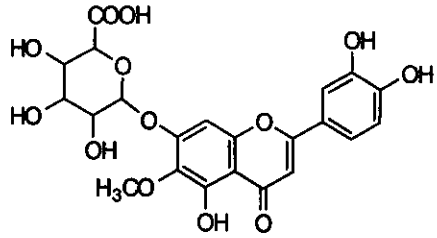


[分子式]$C_{10}H_6O_4$
[分子量]190.155
[正確な分子量]190.02661
[基原]*Salvia triloba*, *Salvia calycina* に存在
[性状]針状結晶(Me_2CO/petrol)
[融点]Mp 198-200 ℃
[その他のデータ]昇華する. アルカリで黄色を示す

----------文献----------

v. Pechmann, H. et al., Ber., 1901, 34, 421, (合成法, 誘導体)
Doganis, B., CA, 1973, 78, 33856x, (分離)
Joshi, S.D. et al., Indian J. Chem., Sect. B, 1982, 21, 399, (合成法)

§ 3',4',5,7-Tetrahydroxy-6-methoxyflavone; 7-*O*-β-D-Glucuronopyranoside
[CAS No.]82657-12-3
[化合物分類]フラボノイド(Flavone; 5 × O-置換基)
[構造式]

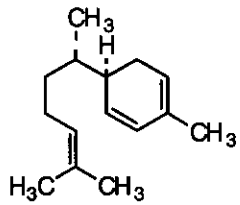


[分子式]$C_{22}H_{20}O_{13}$
[分子量]492.392
[正確な分子量]492.090395
[基原]次の植物から分離: *Digitalis lanata*, *Salvia triloba*
----------文献----------
Hiermann, A. et al., Planta Med., 1982, 45, 59, (7-glucuronoside)

***********ゼドアリー (Zedoary) ***********

§§ ショウガ科ガジュツ(*Curcuma zedoaria* Roscoe)の根茎。

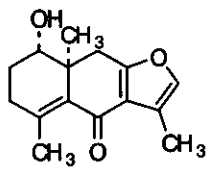
§ 1,3,10-Bisabolatriene
[化学名・別名]Zingiberene
[CAS No.]495-60-3
[化合物分類]テルペノイド(Bisabolane sesquiterpenoid)
[構造式]



Absolute configuration

[分子式]$C_{15}H_{24}$
[分子量]204.355
[正確な分子量]204.1878
[基原]ジンジャーオイル. また *Thymus serpyllum*, *Piper longum*, *Curcuma zedoaria* からも得られる
[性状]オイル
[沸点]Bp_{11} 128-130 ℃
[比旋光度]:$[\alpha]_D^{27}$ -61.7 ($CHCl_3$)
----------文献----------
Eschenmoser, A. et al., Helv. Chim. Acta, 1950, 33, 171, (分離, 構造決定)
Arigoni, D. et al., Helv. Chim. Acta, 1954, 37, 881, (絶対構造)
Soffer, M.D. et al., Tet. Lett., 1985, 26, 3543, (結晶構造)
Bhonsle, J.B. et al., Indian J. Chem., Sect. B, 1994, 33, 313, (合成法, 成書)
Breedon, D.C. et al., Tetrahedron, 1994, 50, 11123, (分離, C13-NMR, H-NMR)
Millar, J.G. et al., J. Nat. Prod., 1998, 61, 1025, (分離)

§ Curcolone
[化学名・別名]1 α-Hydroxyfuranoeudesm-4-en-6-one. Nehiptetol
[CAS No.]17015-43-9
[化合物分類]テルペノイド(12,8-Eudesmanolide and furanoeudesmane sesquiterpenoid)
[構造式]



[分子式]$C_{15}H_{18}O_3$
[分子量]246.305
[正確な分子量]246.125595
[基原]*Curcuma zedoaria*, *Nepeta hindostana*
[性状]結晶(MeOH)
[融点]Mp 139-139.5 ℃ (152-154 ℃)
[比旋光度]:$[\alpha]_D$ +13.7 (c, 3.8 in $CHCl_3$)
[UV]:[neutral] λ_{max} 261 (log ε 3.92); 290 (log ε 3.85) (EtOH)
----------文献----------