

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 : 10 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.  
参考文献

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-)]15,1227,1965

\*\*\*変異原性に関するデータ\*\*\*

<<試験方法>> 微生物を用いた突然変異試験.

試験系 : 大腸菌 *Salmonella typhimurium*.

投与量・期間 : 20 nmol/plate

参考文献

MUREAV Mutation Research. (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherland) V.1- 1964- [Vol.,頁,年(19-)]347,37,1995

\*\*\*米国に於ける状況\*\*\*

EPA TSCA Section 8(b) CHEMICAL INVENTORY

### § 8,11,13-Totaratriene-3,13-diol; 3 $\beta$ -form, 3-Ketone

[化学名・別名] 13-Hydroxy-8,11,13-totaratrien-3-one. Totarolone

[CAS No.] 6755-93-7

[化合物分類] テルペノイド (Totarane diterpenoid)

[構造式]

[分子式]  $C_{20}H_{28}O_2$

[分子量] 300.44

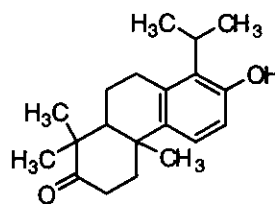
[正確な分子量] 300.20893

[基原] *Tetraclinis articulata*, *Juniperus conferta*

[性状] 結晶

[融点] Mp 188-189 °C

[比旋光度]:  $[\alpha]_D +102$  (EtOH)



-----文献-----

Chow, Y.-L. et al., Acta Chem. Scand., 1962, 16, 1305, (Totarolone)

Campello, J. de P. et al., Phytochemistry, 1975, 14, 243, (3-Hydroxytotarol)

Ying, B.-P. et al., Phytochemistry, 1991, 30, 1951, (H-NMR, C13-NMR)

### § 8,11,13-Totaratrien-13-ol

[化学名・別名] Totarol. 14-Isopropyl-8,11,13-podocarpatrien-13-ol

[CAS No.] 511-15-9

[化合物分類] テルペノイド (Totarane diterpenoid)

[構造式]

[分子式]  $C_{20}H_{30}O$

[分子量] 286.456

[正確な分子量] 286.229665

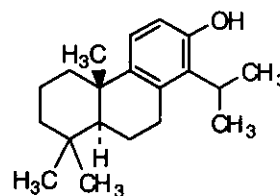
[基原] *Podocarpus* spp. また, *Dacrydium cupressinum*, *Tetraclinis articulata*, *Thujopsis dolabrata*

[性状] 結晶 (petrol)

[融点] Mp 132 °C

[比旋光度]:  $[\alpha]_D^{20} +42.5$  (EtOH)

[UV]: [neutral]  $\lambda_{max}$  278 ( $\epsilon$  1980) (EtOH)



-----文献-----

Bartrop, J.A. et al., J.C.S., 1958, 2566, (合成法)

Chow, Y.-L. et al., Acta Chem. Scand., 1962, 16, 1305, (構造決定)

Enzell, C.R., Tet. Lett., 1966, 2135, (Mas)

Nishida, T. et al., Org. Magn. Reson., 1977, 9, 203, (C13-NMR)

Matsumoto, T. et al., Bull. Chem. Soc. Jpn., 1979, 52, 1450, (合成法)

Ying, B.P. et al., Phytochemistry, 1991, 30, 1951, (H-NMR, C13-NMR)

Das, S. et al., Tetrahedron, 1992, 48, 9101, (合成法)

Bendall, J.G. et al., Aust. J. Chem., 1995, 48, 883, (レビュー)

§ 8,11,13-Totaratrien-13-ol; 1,2-Didehydro

[化学名・別名] 1,8,11,13-Totaratetraen-13-ol. Totarolenone

[化合物分類] テルペノイド (Totarane diterpenoid)

[構造式]

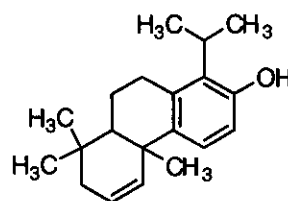
[分子式]  $C_{20}H_{28}O$

[分子量] 284.441

[正確な分子量] 284.214015

[基原] 次の植物から分離: *Tetraclinis articulata*

[その他のデータ] 次の物資との混合物として得られる: Totarolone



-----文献-----

Barltrop, J.A. et al., J.C.S., 1958, 2566, (合成法)

Chow, Y.-L. et al., Acta Chem. Scand., 1962, 16, 1305, (構造決定)

Enzell, C.R., Tet. Lett., 1966, 2135, (Mas)

Nishida, T. et al., Org. Magn. Reson., 1977, 9, 203, (C13-NMR)

Matsumoto, T. et al., Bull. Chem. Soc. Jpn., 1979, 52, 1450, (合成法)

Ying, B.P. et al., Phytochemistry, 1991, 30, 1951, (H-NMR, C13-NMR)

Das, S. et al., Tetrahedron, 1992, 48, 9101, (合成法)

Bendall, J.G. et al., Aust. J. Chem., 1995, 48, 883, (レビュー)

§ § マツ科マオウヒバ (*Callitris quadsivalvis* Ventenat) の樹脂。

本調査研究では研究報告ない。

\*\*\*\*\*サンダルウッド (Sandalwood) \*\*\*\*\*

§ § ピャクダン科ピャクダン (*Santalum album* L.) の材。

§ 4-Acetyl-1-methylcyclohexene

[化学名・別名] 1-(4-Methyl-3-cyclohexen-1-yl) ethanone (CAS 名).

1',2',3',6'-Tetrahydro-4'-methylacetophenone. Tetrahydro-*p*-acetyltoluene

[CAS No.] 6090-09-1

[関連 CAS No.] 70286-20-3

[化合物分類] 脂肪族化合物 (Monocarbocyclic aldehydes and ketone), テルペノイド (*p*-Menthane monoterpene) テルペノイド (Other cyclohexane monoterpene)

[構造式]

[分子式]  $C_9H_{14}O$

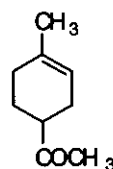
[分子量] 138.209

[正確な分子量] 138.104465

[基原] 次の植物から分離: *Santalum album* のオイル, *Cedrus* spp.

[性状] オイル

[沸点] Bp 205-206 °C



-----文献-----

Aldrich Library of FT-IR Spectra, 1st edn., 1985, 3, 530D, (IR)

Thomas, A.F., Helv. Chim. Acta, 1973, 56, 1800, (合成法, 構造決定)

Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (合成法)

§  $\alpha$ -Bergamotenol

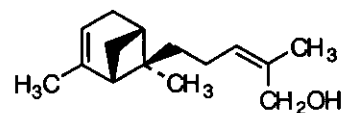
[CAS No.] 88034-74-6

[関連 CAS No.] 65336-63-2, 176777-61-0

[化合物分類] テルペノイド (Miscellaneous bicyclic sesquiterpenoid)

[構造式]

[分子式]  $C_{15}H_{24}O$



[分子量] 220.354

[正確な分子量] 220.182715

[基原] *Hyptis suaveolens*, *Santalum album*, *Santalum spicatum*. 次を示す物質の成分 : Guo Chan Tan Xiang Mu

[性状] オイル

[比旋光度]:  $[\alpha]_D -55.6$  (c, 0.39 in  $\text{CHCl}_3$ )

-----文献-----

Brunke, E.J. et al., *Dev. Food Sci.*, 1988, 18, 819-831, (レビュー)

Pant, A.K. et al., *J. Essent. Oil Res.*, 1992, 4, 9-13, (分離)

Yu, J.G. et al., *Yaoxue Xuebao*, 1993, 28, 840-844, (分離)

#### § 4,4'-Diaminodibutylamine (旧 CAS 名)

[化学名・別名] *N*-(4-Aminobutyl)-1,4-butanediamine (CAS 名). *sym*-Homospermidine.

1,9-Diamino-5-azanonane

[CAS No.] 4427-76-3

[関連 CAS No.] 138656-54-9

[化合物分類] アルカロイド化合物 (Homospermidine alkaloid)

[構造式]  $\text{H}_2\text{NCH}_2(\text{CH}_2)_3\text{NH}(\text{CH}_2)_3\text{CH}_2\text{NH}_2$

[分子式]  $\text{C}_8\text{H}_{21}\text{N}_3$

[分子量] 159.274

[正確な分子量] 159.173547

[基原] *Santalum album* (sandalwood) and present in legume root nodules. Also isol. from organs of the Japanese newt and from roots of water hyacinth *Eichhornia crassipes*

-----文献-----

Kuttan, R. et al., *Biochemistry*, 1971, 10, 361, (分離, 合成法)

Yamamoto, S. et al., *Chem. Pharm. Bull.*, 1983, 31, 3315, (分離)

Samejima, K. et al., *Chem. Pharm. Bull.*, 1984, 32, 3428, (Aminopropylhomospermidine)

Hamana, K. et al., *Can. J. Microbiol.*, 1990, 36, 567; 1991, 37, 350, (Aminopropylhomospermidine)

Ramaswamy, S. et al., *CA*, 1992, 116, 55605v, (結晶構造)

#### § 2,3-Dimethylbicyclo[2.2.1]heptan-2-ol

[化学名・別名] Santene hydrate

[CAS No.] 59432-92-7

[化合物分類] テルペノイド (Miscellaneous bicyclic monoterpene)

[構造式]

[分子式]  $\text{C}_9\text{H}_{16}\text{O}$

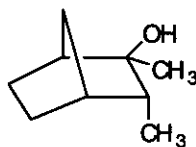
[分子量] 140.225

[正確な分子量] 140.120115

[基原] *Santalum album*

[性状] 結晶

[融点] Mp 102-103 °C



-----文献-----

Beckman, S. et al., *Chem. Ber.*, 1961, 94, 1905, (合成法)

Demole, E. et al., *Helv. Chim. Acta*, 1976, 59, 737, (分離)

#### § 5,6-Dimethylbicyclo[2.2.1]hept-5-en-2-ol; (1*R*\*,2*S*\*)-form

[化学名・別名] *exo*-form

[化合物分類] WE9999, テルペノイド (Miscellaneous bicyclic monoterpene)

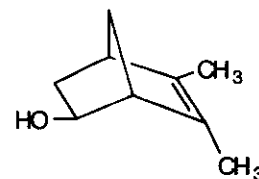
[構造式]

[基原] the oil of East Indian sandalwood (*Santalum album*)

[用途] タバコと食品の香料として使われる

[性状] 液体

[沸点] Bp<sub>10</sub> 87 °C



-----文献-----

Demole, E. et al., *Helv. Chim. Acta*, 1976, 59, 737, (分離, 合成法)

Swiss Pat., 1978, 600 799; CA, 89, 414992m, (合成法)

§ 1-(2-Furanylmethyl)-1H-pyrrole (CAS 名)

[化学名・別名] *N*-(2-Furfuryl) pyrrole. FEMA 3284

[CAS No.] 1438-94-4

[化合物分類] 含酸素複素環式化合物 (Furan), アルカロイド化合物 (Pyrrole alkaloid)

[構造式]

[分子式] C<sub>6</sub>H<sub>7</sub>NO

[分子量] 147.176

[正確な分子量] 147.068414

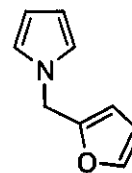
[基原] コーヒーの香気成分の一つ, また他のいくつかの基原, 例えばバン, ローストアーモンド, sandalwood oil (*Santalum album*), ポップコーン, モルト, ローストチキン, ビールに存在する

[用途] 香気成分

[沸点] Bp: 77-79 °C

[傷害・毒性] 50%致死量 (LD50) (マウス, 経口) 380 mg/kg

[化学物質毒性データ総覧 (RTECS) 登録番号] UX9631000



-----文献-----

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, 3, 42B, (NMR)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, 3, 1466A, (IR)

Gianturco, M.A. et al., Tetrahedron, 1964, 20, 1763; 2951, (分離, IR, H-NMR, 合成法)

\*\*\*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 : 380 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

DCTODJ Drug and Chemical Toxicology. (Marcel Dekker, 270 Madison Ave., New York, NY 10016)

V.1- 1977/78- [Vol.,頁,年(19-)] 3,249,1980

\*\*\*米国に於ける状況\*\*\*

EPA TSCA Section 8(b) CHEMICAL INVENTORY

§ 10-Hydroxy-16-hentriacontanone

[化学名・別名] 10-Hydroxypalmitone

[CAS No.] 87264-34-4

[化合物分類] 脂肪族化合物 (Saturated unbranched aldehydes and ketone)

[構造式] H<sub>3</sub>C(CH<sub>2</sub>)<sub>8</sub>CH(OH)(CH<sub>2</sub>)<sub>3</sub>CO(CH<sub>2</sub>)<sub>14</sub>CH<sub>3</sub>

[分子式] C<sub>31</sub>H<sub>62</sub>O<sub>2</sub>

[分子量] 466.83

[正確な分子量] 466.47498

[基原] 次の植物から分離: *Santalum album* の葉より得られるワックス, *Machilus glaucescens*

[性状] 板状結晶 (Me:CO)

[融点] Mp 96-97 °C

-----文献-----

Chibnall, A.C. et al., Biochem. J., 1937, 31, 1981, (分離, 構造決定, 合成法)

Talapatra, B. et al., J. Indian Chem. Soc., 1982, 59, 1364, (分離)

§ 2-Methyl-3-methylenebicyclo[2.2.1]heptan-2-ol; (1R\*,2S\*,4S\*)-form

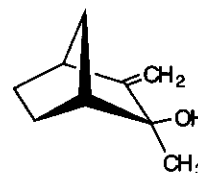
[化学名・別名] *exo*-form

[CAS No.] 59300-40-2

[化合物分類] テルペノイド (Miscellaneous bicyclic monoterpenoid)

[構造式]

[基原] *Santalum album* のオイル



[沸点] Bp<sub>10</sub> 70 °C  
[屈折率] n<sub>D</sub><sup>20</sup> 1.4975

-----文献-----

Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (合成法)

§ 11-Methyl-7-oxatetracyclo[6.3.1.0<sup>1,4</sup>.0<sup>4,11</sup>] dodecane

[化学名・別名] Hexahydro-5a-methyl-3H-1,6:3,8a-dimethano-1H-cyclopent[c]oxepin (旧 CAS 名)

[CAS No.] 28344-11-8

[化合物分類] テルペノイド (Miscellaneous tricyclic sesquiterpenoid)

[構造式]

[分子式] C<sub>12</sub>H<sub>18</sub>O

[分子量] 178.274

[正確な分子量] 178.135765

[基原] 次の植物から分離: ピャクダンオイル; *Santalum album*

[融点] Mp 178-180 °C



-----文献-----

Kretschmar, H.C. et al., Tet. Lett., 1970, 37, (分離, H-NMR, 構造決定, 合成法)

Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (分離)

§ Norbicycloekasantalal

[化学名・別名] 10,11,12,13-Tetranor-β-santal-3(15)-en-9-al

[CAS No.] 37720-84-6

[化合物分類] テルペノイド (β-Santalane sesquiterpenoid)

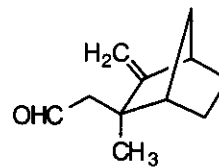
[構造式]

[分子式] C<sub>11</sub>H<sub>16</sub>O

[分子量] 164.247

[正確な分子量] 164.120115

[基原] *Santalum album*



-----文献-----

Gibson, T. et al., Tet. Lett., 1972, 2207

§ Norecasantalol

[化学名・別名] 10,11,12,13-Tetranor-α-santal-9-ol. Nortricycloekasantalol

[CAS No.] 59460-65-0

[化合物分類] テルペノイド (α-Santalane sesquiterpenoid)

[構造式]

[分子式] C<sub>11</sub>H<sub>18</sub>O

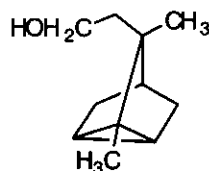
[分子量] 166.263

[正確な分子量] 166.135765

[基原] *Santalum album* のオイル

[性状] オイル

[沸点] Bp<sub>10</sub> 114-117 °C



-----文献-----

Demole, E. et al., Helv. Chim. Acta, 1976, 59, 237

Ngo, K.-S. et al., Phytochemistry, 1999, 50, 1213, (H-NMR, C13-NMR)

§ Norecasantalol; Aldehyde

[化学名・別名] Norecasantalal. 10,11,12,13-Tetranor-α-santal-9-al. Nortricycloekasantalal

[CAS No.] 59300-38-8

[化合物分類] テルペノイド (α-Santalane sesquiterpenoid)

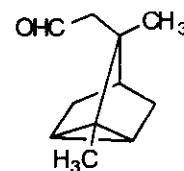
[構造式]

[分子式] C<sub>11</sub>H<sub>16</sub>O

[分子量] 164.247

[正確な分子量] 164.120115

[基原] *Santalum album* のオイル



[性状] オイル  
[沸点] Bp 222-224 °C

-----文献-----

Demole, E. et al., *Helv. Chim. Acta*, 1976, 59, 237  
Ngo, K.-S. et al., *Phytochemistry*, 1999, 50, 1213, (H-NMR, C13-NMR)

### § Norecasantalol; Carboxylic acid

[化学名・別名] Norecasantallic acid. 10,11,12,13-Tetranor- $\alpha$ -santalane-9-oic acid. Nortricycloekasantalic acid  
[CAS No.] 59300-52-6

[化合物分類] テルペノイド ( $\alpha$ -Santalane sesquiterpenoid)

[構造式]

[分子式] C<sub>11</sub>H<sub>16</sub>O<sub>2</sub>

[分子量] 180.246

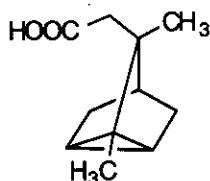
[正確な分子量] 180.11503

[基原] *Santalum album* のオイル

[性状] 結晶 (EtOH)

[融点] Mp 93 °C

[比旋光度]: [ $\alpha$ ]<sub>D</sub> -33.3 (EtOH)



-----文献-----

Demole, E. et al., *Helv. Chim. Acta*, 1976, 59, 237  
Ngo, K.-S. et al., *Phytochemistry*, 1999, 50, 1213, (H-NMR, C13-NMR)

### § $\beta$ -Santala-3(15),10-diene

[構造式]

[分子式] C<sub>15</sub>H<sub>24</sub>

[分子量] 204.355

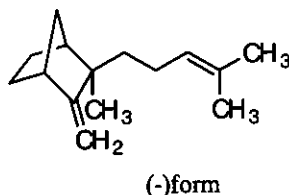
[正確な分子量] 204.1878

[基原] ビャクダンオイル (*Santalum album*)

[性状] スギのような香りを持つオイル

[沸点] Bp, 125-127 °C

[比旋光度]: [ $\alpha$ ]<sub>D</sub> -35



-----文献-----

C.Djerassi et al., *Dictionary of Natural Products*, Chapman, Hall, 2002  
Hodgson, G.L. et al., *J.C.S. Perkin 1*, 1973, 2113, (合成法, 絶対構造)

### § $\beta$ -Santala-3(15),10-diene; (1R,2R)-form

[化学名・別名] Epi- $\beta$ -santalene

[CAS No.] 25532-78-9

[化合物分類] テルペノイド ( $\beta$ -Santalane sesquiterpenoid)

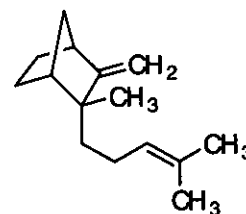
[構造式]

[基原] *Santalum album*, *Santalum spicatum*, その他の植物. 次に示す物質の成分:

Tan Xiang

[沸点] Bp: 105-107 °C

[比旋光度]: [ $\alpha$ ]<sub>D</sub><sup>20</sup> -26.6 (c, 1 in CHCl<sub>3</sub>)



-----文献-----

C.Djerassi et al., *Dictionary of Natural Products*, Chapman, Hall, 2002  
Hodgson, G.L. et al., *J.C.S. Perkin 1*, 1973, 2113, (合成法, 絶対構造)  
Kamikubo, T. et al., *Chem. Lett.*, 1995, 95, (合成法)

### § $\beta$ -Santala-3(15),10-diene; (1S,2R)-form

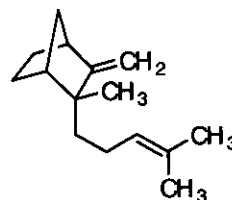
[化学名・別名]  $\beta$ -Santalene

[CAS No.] 511-59-1

[化合物分類] テルペノイド ( $\beta$ -Santalane sesquiterpenoid)

[構造式]

[基原] ビャクダンオイル (*Santalum album*), その他の植物属



[性状] ヒマラヤスギの香りを持つオイル

[沸点] Bp<sub>9</sub> 125-127 °C

[比旋光度]: [α]<sub>D</sub> -35

-----文献-----

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

Hodgson, G.L. et al., J.C.S. Perkin 1, 1973, 2113, (合成法, 絶対構造)

Kamikubo, T. et al., Chem. Lett., 1995, 95, (合成法)

Saito, M. et al., Tet. Lett., 1995, 36, 9003, (合成法)

§ β-Santala-3(15),10-dien-12-ol; (2S,4R,7R,10Z)-form

[化学名・別名] β-Santalol

[CAS No.] 77-42-9

[化合物分類] テルペノイド (β-Santalane sesquiterpenoid)

[一般的性質] Terpenoid numbering shown. Inversion of C-10 config. changes numbering C-12 vs C-13

[構造式]

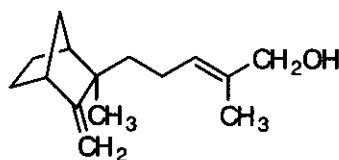
[基原] ビャクダンオイル (*Santalum album*)

[用途] 香水成分

[性状] オイル

[沸点] Bp<sub>17</sub> 177-178 °C

[比旋光度]: [α]<sub>D<sub>25</sub></sub><sup>56</sup> -87.1



-----文献-----

Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (aldehyde)

Baumann, M. et al., Annalen, 1979, 743, (合成法)

Christenson, P.A. et al., Phytochemistry, 1981, 20, 1139, (trans-β-Santalol)

Brunke, E.-J. et al., Annalen, 1982, 1105, (絶対構造)

Monti, H. et al., Tet. Lett., 1982, 23, 5539, (合成法)

Solas, D. et al., J.O.C., 1983, 48, 1988, (合成法, 成書)

Buchbauer, G. et al., Annalen, 1990, 119, (β-Santallic acid)

Krotz, A. et al., Tetrahedron: Asymmetry, 1990, 1, 537, (合成法)

Krotz, A. et al., Annalen, 1994, 601, (合成法)

α, T. et al., Phytochemistry, 1996, 41, 829, (β-Santaldiol)

§ β-Santala-3(15),10-dien-12-ol; (2S,4R,7R,10Z)-form, 12-Carboxylic acid

[化学名・別名] β-Santala-3(15),10-dien-12-oic acid. β-Santallic acid

[CAS No.] 73590-17-7

[化合物分類] テルペノイド (β-Santalane sesquiterpenoid)

[構造式]

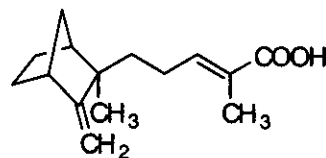
[分子式] C<sub>15</sub>H<sub>22</sub>O<sub>2</sub>

[分子量] 234.338

[正確な分子量] 234.16198

[基原] *Santalum album* のオイル

[性状] オイル



-----文献-----

Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (aldehyde)

Baumann, M. et al., Annalen, 1979, 743, (合成法)

Christenson, P.A. et al., Phytochemistry, 1981, 20, 1139, (trans-β-Santalol)

Brunke, E.-J. et al., Annalen, 1982, 1105, (絶対構造)

Monti, H. et al., Tet. Lett., 1982, 23, 5539, (合成法)

Solas, D. et al., J.O.C., 1983, 48, 1988, (合成法, 成書)

Buchbauer, G. et al., Annalen, 1990, 119, (β-Santallic acid)

Krotz, A. et al., Tetrahedron: Asymmetry, 1990, 1, 537, (合成法)

Krotz, A. et al., Annalen, 1994, 601, (合成法)

α, T. et al., Phytochemistry, 1996, 41, 829, (β-Santaldiol)

§ β-Santala-3(15),10-dien-12-ol; (2S,4R,7R,10E)-form

[化学名・別名]  $\beta$ -Santala-3(15), 10-dien-13-ol. *trans*- $\beta$ -Santalol

[CAS No.] 37172-32-0

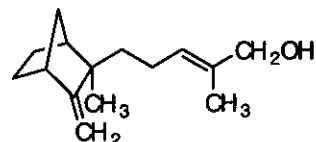
[化合物分類] テルペノイド ( $\beta$ -Santalane sesquiterpenoid)

[構造式]

[基原] *Santalum album*

[性状] オイル

[比旋光度]:  $[\alpha]_D^{21} -113.7$  (c, 0.3 in CHCl<sub>3</sub>) (synthetic)



-----文献-----

Demole, E. et al., *Helv. Chim. Acta*, 1976, 59, 737, (aldehyde)

Baumann, M. et al., *Annalen*, 1979, 743, (合成法)

Christenson, P.A. et al., *Phytochemistry*, 1981, 20, 1139, (*trans*- $\beta$ -Santalol)

Brunke, E.-J. et al., *Annalen*, 1982, 1105, (絶対構造)

Monti, H. et al., *Tet. Lett.*, 1982, 23, 5539, (合成法)

Solas, D. et al., *J.O.C.*, 1983, 48, 1988, (合成法, 成書)

Buchbauer, G. et al., *Annalen*, 1990, 119, ( $\beta$ -Santallic acid)

Krotz, A. et al., *Tetrahedron: Asymmetry*, 1990, 1, 537, (合成法)

Krotz, A. et al., *Annalen*, 1994, 601, (合成法)

$\alpha$ , T. et al., *Phytochemistry*, 1996, 41, 829, ( $\beta$ -Santaldiol)

### § $\beta$ -Santala-3(15),10-dien-12-ol; (2*S*,4*R*,7*R*,10*E*)-form, Aldehyde

[化学名・別名]  $\beta$ -Santal-3(15),10-dien-13-al.  $\beta$ -Santalal

[CAS No.] 59331-82-7

[化合物分類] テルペノイド ( $\beta$ -Santalane sesquiterpenoid)

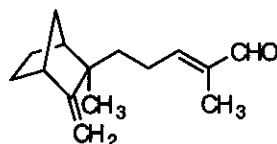
[構造式]

[分子式] C<sub>15</sub>H<sub>22</sub>O

[分子量] 218.338

[正確な分子量] 218.167065

[基原] 次の植物から分離:*Santalum album* のオイル



-----文献-----

Demole, E. et al., *Helv. Chim. Acta*, 1976, 59, 737, (aldehyde)

Baumann, M. et al., *Annalen*, 1979, 743, (合成法)

Christenson, P.A. et al., *Phytochemistry*, 1981, 20, 1139, (*trans*- $\beta$ -Santalol)

Brunke, E.-J. et al., *Annalen*, 1982, 1105, (絶対構造)

Monti, H. et al., *Tet. Lett.*, 1982, 23, 5539, (合成法)

Solas, D. et al., *J.O.C.*, 1983, 48, 1988, (合成法, 成書)

Buchbauer, G. et al., *Annalen*, 1990, 119, ( $\beta$ -Santallic acid)

Krotz, A. et al., *Tetrahedron: Asymmetry*, 1990, 1, 537, (合成法)

Krotz, A. et al., *Annalen*, 1994, 601, (合成法)

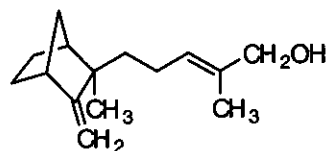
$\alpha$ , T. et al., *Phytochemistry*, 1996, 41, 829, ( $\beta$ -Santaldiol)

### § $\beta$ -Santala-3(15),10-dien-12-ol; (2*S*,4*R*,7*S*,10*Z*)-form

[化合物分類] テルペノイド ( $\beta$ -Santalane sesquiterpenoid)

[構造式]

[基原] *Santalum album*



-----文献-----

Demole, E. et al., *Helv. Chim. Acta*, 1976, 59, 737, (aldehyde)

Baumann, M. et al., *Annalen*, 1979, 743, (合成法)

Christenson, P.A. et al., *Phytochemistry*, 1981, 20, 1139, (*trans*- $\beta$ -Santalol)

Brunke, E.-J. et al., *Annalen*, 1982, 1105, (絶対構造)

Monti, H. et al., *Tet. Lett.*, 1982, 23, 5539, (合成法)

Solas, D. et al., *J.O.C.*, 1983, 48, 1988, (合成法, 成書)

Buchbauer, G. et al., *Annalen*, 1990, 119, ( $\beta$ -Santallic acid)

Krotz, A. et al., *Tetrahedron: Asymmetry*, 1990, 1, 537, (合成法)

Krotz, A. et al., *Annalen*, 1994, 601, (合成法)

$\alpha$ , T. et al., *Phytochemistry*, 1996, 41, 829, ( $\beta$ -Santaldiol)



§  $\beta$ -Santala-3(15),10-dien-12-ol; (2R,4S,7R,10Z)-form

[化学名・別名] *epi*- $\beta$ -Santalol

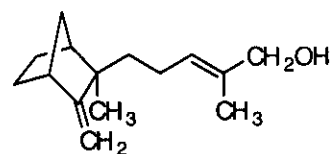
[CAS No.] 42495-69-2

[化合物分類] テルペノイド ( $\beta$ -Santalane sesquiterpenoid)

[構造式]

[基原] *Santalum album*

[性状] オイル



-----文献-----

Christenson, P.A. et al., *Phytochemistry*, 1981, 20, 1139, (trans- $\beta$ -Santalol)

Brunke, E.-J. et al., *Annalen*, 1982, 1105, (絶対構造)

Monti, H. et al., *Tet. Lett.*, 1982, 23, 5539, (合成法)

Solas, D. et al., *J.O.C.*, 1983, 48, 1988, (合成法, 成書)

Krotz, A. et al., *Tetrahedron: Asymmetry*, 1990, 1, 537, (合成法)

Krotz, A. et al., *Annalen*, 1994, 601, (合成法)

$\alpha$ , T. et al., *Phytochemistry*, 1996, 41, 829, ( $\beta$ -Santaldiol)

§  $\alpha$ -Santal-10-en-12-ol; (7R,10E)-form, Aldehyde

[化学名・別名]  $\alpha$ -Santal-10-en-12-al.  $\alpha$ -Santalal

[CAS No.] 59331-83-8

[化合物分類] テルペノイド ( $\alpha$ -Santalane sesquiterpenoid)

[構造式]

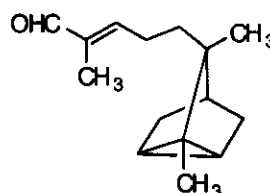
[分子式]  $C_{15}H_{22}O$

[分子量] 218.338

[正確な分子量] 218.167065

[基原] *Santalum album*

[性状] オイル



-----文献-----

Lewis, R.G. et al., *Tet. Lett.*, 1967, 401, (合成法)

Bohlmann, F. et al., *Tet. Lett.*, 1968, 1533, (分離, 合成法)

Corey, E.J. et al., *J.A.C.S.*, 1970, 92, 6314, (合成法)

Julia, M. et al., *Bull. Soc. Chim. Fr.*, 1973, 3065, (合成法)

Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1974, 12, 991, (レビュー, 毒性)

Sato, K. et al., *Bull. Chem. Soc. Jpn.*, 1976, 49, 3351, (合成法)

Demole, E. et al., *Helv. Chim. Acta*, 1976, 59, 737, (分離, aldehyde)

Bohlmann, F. et al., *Phytochemistry*, 1979, 18, 1997, (acid)

Nikiforov, A. et al., *Annalen*, 1990, 119, (分離, acid)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, OHG000

§ Santalone

[化学名・別名] 10,11,12,13-Tetranor- $\alpha$ -santalan-8-one

[CAS No.] 59300-51-5

[化合物分類] テルペノイド ( $\alpha$ -Santalane sesquiterpenoid)

[構造式]

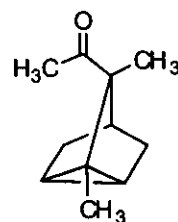
[分子式]  $C_{11}H_{16}O$

[分子量] 164.247

[正確な分子量] 164.120115

[基原] *Santalum album* のオイル

[性状] オイル



-----文献-----

Demole, E. et al., *Helv. Chim. Acta*, 1976, 59, 737

§ Teresantalol

[化学名・別名] 2,3-Dimethyltricyclo[2.2.1.0<sup>2,6</sup>]heptane-3-methanol (CAS 名)

[CAS No.] 29550-55-8

[化合物分類] テルペノイド (Tricyclic monoterpeneoid)

[構造式]

[分子式]  $C_{10}H_{16}O$

[分子量] 152.236

[正確な分子量] 152.120115

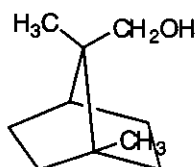
[基原] インドのビャクダンオイル (*Santalum album*)

[性状] 結晶 (petrol/ $C_6H_6$ )

[融点] Mp 115 °C

[沸点] Bp<sub>9</sub> 95-98 °C

[比旋光度]:  $[\alpha]_D +12.1$  (EtOH)



-----文献-----

Guha, P.C. et al., J. Indian Chem. Soc., 1944, 59, 271, (分離)

Nambara, T. et al., J. Chromatogr., 1974, 100, 180, (用途)

Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (分離)

Monti, S.A. et al., J.O.C., 1978, 43, 2282, (合成法)

### § Teresantalol; 8-Aldehyde

[化学名・別名] Teresantalal

[CAS No.] 59300-39-9

[化合物分類] テルペノイド (Tricyclic monoterpeneoid)

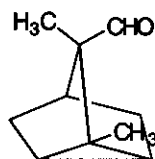
[構造式]

[分子式]  $C_{10}H_{14}O$

[分子量] 150.22

[正確な分子量] 150.104465

[基原] *Santalum album* のオイル



-----文献-----

Guha, P.C. et al., J. Indian Chem. Soc., 1944, 59, 271, (分離)

Nambara, T. et al., J. Chromatogr., 1974, 100, 180, (用途)

Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (分離)

Monti, S.A. et al., J.O.C., 1978, 43, 2282, (合成法)

### § Teresantalol; 8-Carboxylic acid

[化学名・別名]  $\alpha$ -Teresantalic acid

[CAS No.] 562-66-3

[化合物分類] テルペノイド (Tricyclic monoterpeneoid)

[構造式]

[分子式]  $C_{10}H_{14}O_2$

[分子量] 166.219

[正確な分子量] 166.09938

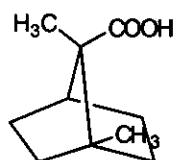
[基原] 次の植物から分離: *Santalum album*

[性状] 結晶 (EtOH)

[融点] Mp 158 °C

[沸点] Bp<sub>20</sub> 157-158 °C

[比旋光度]:  $[\alpha]_D^{20} -76.6$  ( $C_6H_6$ )



-----文献-----

Guha, P.C. et al., J. Indian Chem. Soc., 1944, 59, 271, (分離)

Nambara, T. et al., J. Chromatogr., 1974, 100, 180, (用途)

Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (分離)

Monti, S.A. et al., J.O.C., 1978, 43, 2282, (合成法)

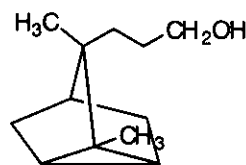
### § Tricycloekasantalol

[化学名・別名] 2,3-Dimethyltricyclo[2.2.1.0<sup>2,6</sup>]heptane-3-propanol (CAS 名)

[CAS No.] 16933-12-3

[化合物分類] テルペノイド ( $\alpha$ -Santalane sesquiterpenoid)

[構造式]  
 [分子式]  $C_{12}H_{20}O$   
 [分子量] 180.289  
 [正確な分子量] 180.151415  
 [基原] 次の植物から分離: oil of sandalwood (*Santalum album*)

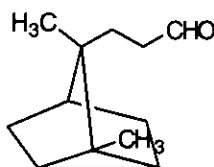


----- 文献 -----

Lewis, R.G. et al., Tet. Lett., 1967, 401, (合成法, IR, NMR)  
 Kretschmar, H.C. et al., Tet. Lett., 1970, 37, (分離)  
 Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (分離)

### § Tricycloekasantalol; Aldehyde

[化学名・別名] Tricycloekasantal  
 [CAS No.] 16933-18-9  
 [化合物分類] テルペノイド ( $\alpha$ -Santalane sesquiterpenoid)  
 [構造式]  
 [分子式]  $C_{12}H_{18}O$   
 [分子量] 178.274  
 [正確な分子量] 178.135765  
 [基原] *Santalum album* のオイル  
 [性状] オイル



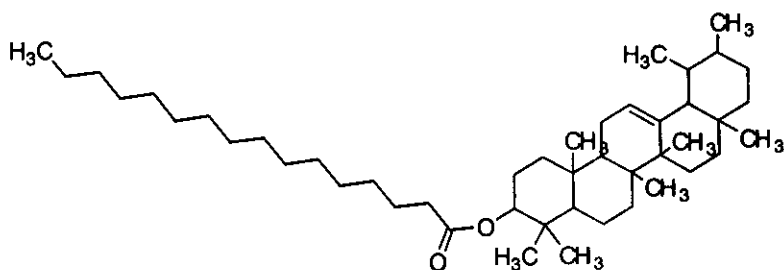
----- 文献 -----

Lewis, R.G. et al., Tet. Lett., 1967, 401, (合成法, IR, NMR)  
 Kretschmar, H.C. et al., Tet. Lett., 1970, 37, (分離)  
 Demole, E. et al., Helv. Chim. Acta, 1976, 59, 737, (分離)

### § 12-Ursen-3-ol; 3 $\beta$ -form, Hexadecanoyl

[化学名・別名]  $\alpha$ -Amyrin palmitate  
 [CAS No.] 22255-10-3  
 [化合物分類] テルペノイド (Ursane triterpenoid)  
 [構造式]

[分子式]  $C_{46}H_{80}O_2$   
 [分子量] 665.137  
 [正確な分子量] 664.61583  
 [基原] 次の植物から分離: *Viburnum* spp., *Santalum album*, *Sambucus* spp., その他  
 [用途] Trypsin and chymotrypsin inhibitor  
 [性状] プリズム結晶もしくは針状結晶 (EtOH/EtO)  
 [融点] Mp 73-74 °C  
 [比旋光度]:  $[\alpha]_D^{25} +52.5$  (c, 1.0 in  $C_6H_6$ )



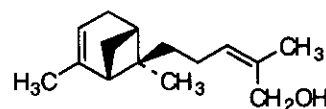
----- 文献 -----

Inoue, T. et al., Chem. Pharm. Bull., 1969, 17, 124, (palmitate)  
 Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn.,

### § § ビャクダン科オーストラリアンサンダルウッド (*Santalum spicatum* de Candolle) の材。

#### § $\alpha$ -Bergamotenol

[CAS No.] 88034-74-6  
 [関連 CAS No.] 65336-63-2, 176777-61-0  
 [化合物分類] テルペノイド (Miscellaneous bicyclic sesquiterpenoid)  
 [構造式]  
 [分子式]  $C_{15}H_{24}O$   
 [分子量] 220.354  
 [正確な分子量] 220.182715



[基原] *Hyptis suaveolens*, *Santalum album*, *Santalum spicatum*. 次を示す物質の成分: Guo Chan Tan Xiang Mu

[性状] オイル

[比旋光度]:  $[\alpha]_D -55.6$  (c, 0.39 in  $\text{CHCl}_3$ )

-----文献-----

Brunke, E.J. et al., *Dev. Food Sci.*, 1988, 18, 819-831, (レビュー)

Pant, A.K. et al., *J. Essent. Oil Res.*, 1992, 4, 9-13, (分離)

Yu, J.G. et al., *Yaoxue Xuebao*, 1993, 28, 840-844, (分離)

§ 2,6,10-Farnesatriene; (2E,6E)-form

[CAS No.] 7681-88-1

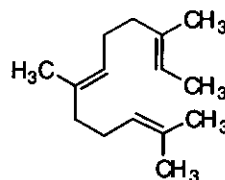
[化合物分類] テルペノイド (Simple farnesane sesquiterpenoid)

[構造式]

[基原] *Santalum spicatum* のオイル

[用途] Aphid alarm pheromone

[性状] オイル



-----文献-----

Birch, A.J. et al., *Aust. J. Chem.*, 1970, 23, 2337, (分離, 構造決定)

Nishino, C. et al., *Tetrahedron*, 1976, 32, 2875, (合成法)

§  $\beta$ -Santala-3(15),10-diene; (1R,2R)-form

[化学名・別名] Epi- $\beta$ -santalene

[CAS No.] 25532-78-9

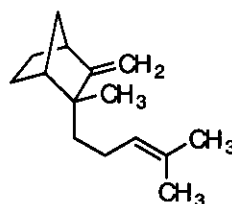
[化合物分類] テルペノイド ( $\beta$ -Santalane sesquiterpenoid)

[構造式]

[基原] *Santalum album*, *Santalum spicatum*, その他の植物. 次を示す物質の成分: Tan Xiang

[沸点]  $B_p$  105-107 °C

[比旋光度]:  $[\alpha]_D^{20} -26.6$  (c, 1 in  $\text{CHCl}_3$ )



-----文献-----

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

Hodgson, G.L. et al., *J.C.S. Perkin 1*, 1973, 2113, (合成法, 絶対構造)

Krotz, A. et al., *Annalen*, 1994, 601, (合成法)

Kamikubo, T. et al., *Chem. Lett.*, 1995, 95, (合成法)

Saito, M. et al., *Tet. Lett.*, 1995, 36, 9003, (合成法)

\*\*\*\*\*サンダルレッド (Red Sandalwood) \*\*\*\*\*

§ § ピアクダン科シタン (*Pterocarpus santalinus* L.) の材。

§ 2,4-Dihydroxybenzoic acid (CAS 名)

[化学名・別名]  $\beta$ -Resorcylic acid (旧 CAS 名). Resorcinol-4-carboxylic acid

[CAS No.] 89-86-1

[化合物分類] 単環芳香族 (Simple benzoic acids and ester)

[構造式]

[分子式]  $\text{C}_7\text{H}_6\text{O}_4$

[分子量] 154.122

[正確な分子量] 154.02661

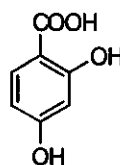
[基原] *Pterocarpus santalinus*, *Adenanthera pavonina*

[用途] Gives colour reaction with Fe; fluorescence reaction with B. Monomer for phenolic resins used as ion exchangers

[性状] 塊 ( $\text{CHCl}_3$ )

[融点]  $M_p$  152 °C で昇華,  $M_p$  175 °C.  $M_p$  218-219 °C (213 °C rapid heat)

[PKa 値]  $pK_{a1}$  3.11;  $pK_{a2}$  8.55;  $pK_{a3}$  14 (25 °C)



[傷害・毒性] 催奇形成作用  
[化学物質毒性データ総覧(RTECS)登録番号] VH3708050

-----文献-----

C.Djerassi et al., Dictionary of Natural Products, Chapman, Hall, 2002  
Coward, R.F. et al., J. Chromatogr., 1969, 45, 311, (ガスクロマト)  
Scriven, F.M. et al., J. Liq. Chromatogr., 1979, 2, 125, (HPLC)  
Venkataramaiah, V. et al., Indian J. Exp. Biol., 1980, 18, 887; CA, 93, 164513r, (生育)  
Achenbach, H. et al., Phytochemistry, 1988, 27, 1835, (分離, 誘導体)  
\*\*\*RTECS (化学物質毒性データ)\*\*\*

生体影響物質 : 生殖影響物質

\*\*\*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 : >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.

参考文献

JPETAB Journal of Pharmacology and Experimental Therapeutics. (Williams & Wilkins Co., 428 E. Preston St., Baltimore, MD 21202) V.1- 1909/10- [Vol.,頁,年(19-)] 196,478,1976

\*\*\*生殖に関するデータ\*\*\*

<<試験方法>> 最小毒性量(TDL<sub>0</sub>)試験.

曝露経路 : 皮下投与.

被験動物 : げっ歯類-ラット.

投与 : 642 mg/kg

雌雄投与期間 : 雌 11 日間(交配後)

毒性影響 : [生殖] [特定の发育異常] 筋肉骨格系.

参考文献

RCOCB8 Research Communications in Chemical Pathology and Pharmacology. (PJD Pub. Ltd., P.O. Box 966, Westbury, NY 11590) V.1- 1970- [Vol.,頁,年(19-)] 38,209,1982

\*\*\*米国に於ける状況\*\*\*

EPA TSCA Section 8(b) CHEMICAL INVENTORY

### § 6,7-Dihydroxy-3-(2,3,4-trihydroxyphenyl)-2H-1-benzopyran-2-one; 2',4'-Di-Me ether

[化学名・別名] 6,7-Dihydroxy-3-(3-hydroxy-2,4-dimethoxyphenyl) coumarin. Santalin AC

[CAS No.] 167425-76-5

[化合物分類] ベンゾピラノイド(6,7-Dioxygenated coumarin), フラボノイド(3-Arylcoumarin flavonoid)

[構造式]

[分子式] C<sub>17</sub>H<sub>14</sub>O<sub>7</sub>

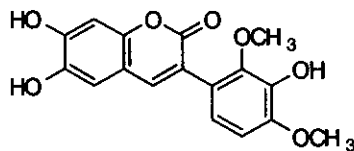
[分子量] 330.293

[正確な分子量] 330.073955

[基原] *Pterocarpus santalinus*

[性状] 淡黄色の針状結晶

[融点] Mp 292-295 °C



-----文献-----

Kinjo, J. et al., Tet. Lett., 1995, 36, 5599, (分離, H-NMR, C13-NMR)

### § 2,4,11-Eudesmanetriol; (2 α,4 α)-form

[化学名・別名] Pterocarptriol

[CAS No.] 52801-07-7

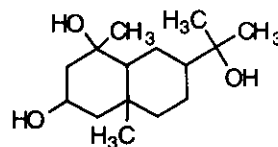
[化合物分類] テルペノイド(Simple eudesmane sesquiterpenoid)

[構造式]

[基原] *Pterocarpus santalinus* の心材

[性状] 結晶(CHCl<sub>3</sub>/MeOH)

[融点] Mp 168 °C



[比旋光度]:  $[\alpha]_D^{25} -38$  (c, 1 in MeOH)

-----文献-----

Kumar, N. et al., *Phytochemistry*, 1974, 13, 633

Li, S. et al., *Phytochemistry*, 1998, 49, 2035, (Pterodontoside A)

§ 2,4,11-Eudesmanetriol; (2  $\alpha$ ,4  $\alpha$ )-form, 2-Ketone

[化学名・別名] 4  $\alpha$ ,11-Dihydroxy-2-eudesmanone. Pterocarpdiolone

[CAS No.] 52801-08-8

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

[構造式]

[分子式]  $C_{15}H_{26}O_3$

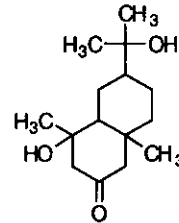
[分子量] 254.369

[正確な分子量] 254.188195

[基原] *Pterocarpus santalinus*

[性状] 粘調性液体

[比旋光度]:  $[\alpha]_D^{25} +11$  (c, 0.8 in  $CHCl_3$ )



-----文献-----

Kumar, N. et al., *Phytochemistry*, 1974, 13, 633

Li, S. et al., *Phytochemistry*, 1998, 49, 2035, (Pterodontoside A)

§ 11-Hydroxy-3-eudesmen-2-one

[化学名・別名] Isopterocarpolone

[CAS No.] 52801-06-6

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

[構造式]

[分子式]  $C_{15}H_{24}O_2$

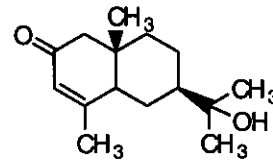
[分子量] 236.353

[正確な分子量] 236.17763

[基原] *Pterocarpus santalinus* の心材

[性状] 粘調性液体

[比旋光度]:  $[\alpha]_D^{22} +47$  (c, 0.9 in  $CHCl_3$ )



-----文献-----

Kumar, N. et al., *Phytochemistry*, 1974, 13, 633

§ 7-Hydroxy-6-methoxy-2H-1-benzopyran-2-one; O-[ $\alpha$ -L-Arabinopyranosyl-(1  $\rightarrow$  3)- $\beta$

-D-galactopyranosyl-(1  $\rightarrow$  6)- $\beta$ -D-glucopyranoside]

[CAS No.] 149597-09-1

[化合物分類] ベンゾピラノイド (6,7-Dioxygenated coumarin)

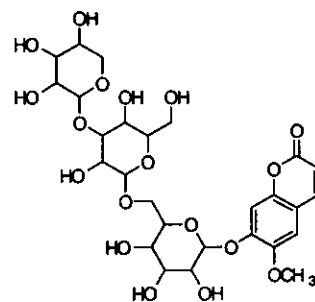
[構造式]

[分子式]  $C_{27}H_{36}O_{18}$

[分子量] 648.571

[正確な分子量] 648.19017

[基原] *Pterocarpus santalinus*



-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhaumluser Verlag, Basel, 1972, nos. 1328; 1329, (生育)

Tanaka, S. et al., *Arzneim.-Forsch.*, 1977, 27, 2039, (分離)

Herath, W.H.M. et al., *Phytochemistry*, 1978, 17, 1007, (分離)

Murray, R.D.H. et al., *The Natural Coumarins*, J. Wiley, 1982, (生育, レビュー)

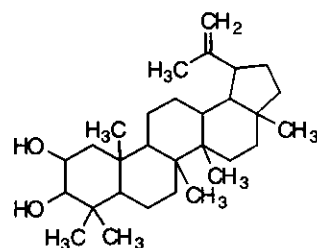
Wollenweber, E. et al., *Fitoterapia*, 1989, 60, 460, (分離, 誘導体)

Mizuno, M. et al., *Phytochemistry*, 1992, 31, 717, (誘導体)

§ 20(29)-Lupene-2,3-diol; (2  $\alpha$ ,3  $\alpha$ )-form

[CAS No.] 55476-83-0  
[化合物分類] テルペノイド (Lupane triterpenoid)

[構造式]  
[基原] *Pterocarpus santalinus*, *Euonymus revolutus*  
[性状] 結晶 (CHCl<sub>3</sub>/hexane)  
[融点] Mp 225-226 °C  
[比旋光度]: [α]<sub>D</sub> +25.4 (c, 0.2 in CHCl<sub>3</sub>)



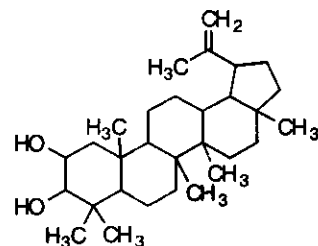
-----文献-----

Kumar, N. et al., *Phytochemistry*, 1975, 14, 521; 1976, 15, 1417, (分離)  
Ageta, H. et al., *Chem. Pharm. Bull.*, 1984, 32, 369, (分離, H-NMR)  
Hisham, A. et al., *Phytochemistry*, 1996, 42, 789, (分離, H-NMR, C13-NMR)

### § 20(29)-Lupene-2,3-diol; (2 α,3 β)-form

[CAS No.] 61448-03-1  
[化合物分類] テルペノイド (Lupane triterpenoid)  
[構造式]

[基原] *Pterocarpus santalinus*, *Salvia* spp., *Rhododendron macrocephalum*  
[性状] 結晶  
[融点] Mp 233-234 °C  
[比旋光度]: [α]<sub>D</sub> +12.5 (c, 0.2 in CHCl<sub>3</sub>)

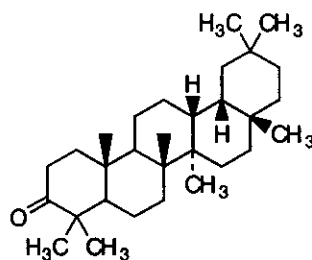


-----文献-----

Kumar, N. et al., *Phytochemistry*, 1975, 14, 521; 1976, 15, 1417, (分離)  
Ageta, H. et al., *Chem. Pharm. Bull.*, 1984, 32, 369, (分離, H-NMR)  
Hisham, A. et al., *Phytochemistry*, 1996, 42, 789, (分離, H-NMR, C13-NMR)  
Hussein, A.A. et al., *Phytochemistry*, 1997, 45, 1663, (2-Me ether)

### § 3-Oleananone

[CAS No.] 114717-93-0  
[化合物分類] テルペノイド (Oleanane triterpenoid)  
[構造式]  
[分子式] C<sub>30</sub>H<sub>50</sub>O  
[分子量] 426.724  
[正確な分子量] 426.386165  
[基原] *Pterocarpus santalinus*  
[性状] 結晶 (MeOH)  
[融点] Mp 233-235 °C  
[比旋光度]: [α]<sub>D</sub> +12.8 (c, 2.5 in CHCl<sub>3</sub>)

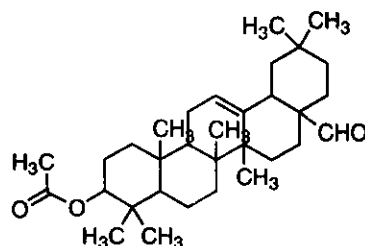


-----文献-----

Krishnaveni, K.S. et al., *Fitoterapia*, 2000, 71, 10-13, (分離, H-NMR, C13-NMR)

### § 12-Oleanene-3,28-diol; 3 β -form, 28-Aldehyde, 3-Ac

[化学名・別名] Acetyl oleanolic aldehyde  
[CAS No.] 1857-04-1  
[化合物分類] テルペノイド (Oleanane triterpenoid)  
[構造式]  
[分子式] C<sub>32</sub>H<sub>50</sub>O<sub>3</sub>  
[分子量] 482.745  
[正確な分子量] 482.375995  
[基原] *Madhuca incorruptible*, *Madhuca scleroxylon*, *Pterocarpus santalinus* の心材と辺材  
[性状] 結晶 (MeOH)  
[融点] Mp 225-228 °C  
[比旋光度]: [α]<sub>D</sub><sup>28</sup> -68 (c, 0.6 in CHCl<sub>3</sub>)



[溶解性]ヘキサンに難溶

-----文献-----

- Shamma, M. et al., J.O.C., 1959, 24, 726; 1962, 27, 4512, (分離, H-NMR)  
Kasprzyk, Z. et al., Phytochemistry, 1969, 8, 1921, (生合成)  
Yosioka, I. et al., Chem. Pharm. Bull., 1971, 19, 1186, (誘導体)  
Kamiya, K. et al., Phytochemistry, 1997, 44, 141, (Oleanolic aldehyde, H-NMR, C13-NMR)  
Takahashi, H. et al., Phytochemistry, 1999, 51, 543, (Coumaroylerythrodiol)

§ 2',4',5',6,7-Pentahydroxyisoflavone; 2',4',5',7-Tetra-Me ether

[化学名・別名]6-Hydroxy-2',4',5',7-tetramethoxyisoflavone

[化合物分類]フラボノイド (Isoflavones; 5 × O-置換基)

[構造式]

[分子式] C<sub>19</sub>H<sub>18</sub>O<sub>7</sub>

[分子量] 358.347

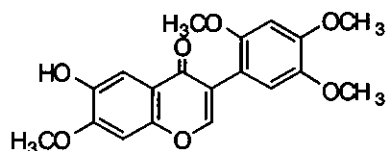
[正確な分子量] 358.105255

[基原] *Pterocarpus santalinus*

[性状] 無定型の粉末 (CHCl<sub>3</sub>/MeOH)

[融点] Mp 173-175 °C

[UV]: [neutral] λ<sub>max</sub> 263 (log ε 4.44); 324 (log ε 3.78) (MeOH)



-----文献-----

- Campbell, R.V.M. et al., J.C.S. (C), 1969, 1787, (分離)  
Campbell, R.V.M. et al., J.C.S. Perkin 1, 1973, 2222,  
Galina, E. et al., Phytochemistry, 1974, 13, 2593, (分離)  
Ingham, J.L., Prog. Chem. Org. Nat. Prod., 1983, 43, 1, (レビュー, 生育)  
Krishnaveni, K.S. et al., Phytochemistry, 2000, 53, 605, (6-Hydroxy-2',4',5',7-tetramethoxyisoflavone)

§ Santalin A

[化学名・別名]6-[(3,4-Dihydroxyphenyl) methyl]-2,10-dihydroxy-5-(4-hydroxy-2-methoxyphenyl)-1,3-dimethoxy-9H-benzo[a]xanthen-9-one (CAS 名)

[CAS No.] 38185-48-7

[化合物分類]フラボノイド (Biflavonoids and polyflavonoid) フラボノイド (3-Arylcoumarin flavonoid)

[構造式]

[分子式] C<sub>33</sub>H<sub>26</sub>O<sub>10</sub>

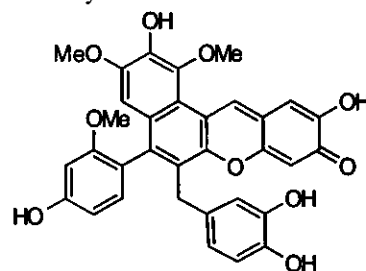
[分子量] 582.562

[正確な分子量] 582.1526

[基原] *Pterocarpus santalinus* の色素. また, カムウッドとコウキ(紅木)にも存在する

[性状] 赤色の針状結晶 (MeOH 溶液)

[融点] Mp 302-303 °C



-----文献-----

- Robertson, A. et al., J.C.S., 1954, 2794  
Mathieson, D.W. et al., J.C.S. Perkin 1, 1973, 184, (構造決定, NMR)  
Ravindranath, B. et al., Phytochemistry, 1973, 12, 2781, (UV, IR)  
Gurudutt, K.N. et al., Phytochemistry, 1974, 13, 2845, (構造決定)  
Arnone, A. et al., J.C.S. Perkin 1, 1975, 186, (構造決定, NMR)  
Arnone, A. et al., J.C.S. Perkin 1, 1977, 2118, (C13-NMR, 構造決定)  
Kinjo, J. et al., Tet. Lett., 1995, 36, 5599, (分離, H-NMR, C13-NMR)

§ Santalin A; 3''-Me ether

[化学名・別名] Santalin B

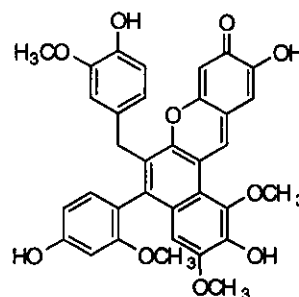
[CAS No.] 51033-46-6

[化合物分類]フラボノイド (Biflavonoids and polyflavonoid)

[構造式]

[分子式] C<sub>34</sub>H<sub>28</sub>O<sub>10</sub>

[分子量] 596.589





[正確な分子量] 596.16825

[基原] *Pterocarpus santalinus* の辺材の色素

[性状] 赤色の針状結晶 (MeOH 溶液)

[融点] Mp 292-294 °C

-----文献-----

Robertson, A. et al., J.C.S., 1954, 2794

Mathieson, D.W. et al., J.C.S. Perkin 1, 1973, 184, (構造決定, NMR)

Ravindranath, B. et al., Phytochemistry, 1973, 12, 2781, (UV, IR)

Gurudutt, K.N. et al., Phytochemistry, 1974, 13, 2845, (構造決定)

Arnone, A. et al., J.C.S. Perkin 1, 1975, 186, (構造決定, NMR)

Arnone, A. et al., J.C.S. Perkin 1, 1977, 2118, (C13-NMR, 構造決定)

Kinjo, J. et al., Tet. Lett., 1995, 36, 5599, (分離, H-NMR, C13-NMR)

### § Santalin A; Me ether (?)

[化学名・別名] Santalin C

[化合物分類] フラボノイド (Biflavonoids and polyflavonoid)

[構造式] 有効な構造式はない

[分子式] C<sub>34</sub>H<sub>28</sub>O<sub>10</sub>

[分子量] 596.589

[正確な分子量] 596.16825

[基原] 次の植物から分離: *Pterocarpus santalinus*

[性状] 橙色の針状結晶 (CHCl<sub>3</sub>/MeOH)

[融点] Mp 300 °C で分解

-----文献-----

Robertson, A. et al., J.C.S., 1954, 2794

Mathieson, D.W. et al., J.C.S. Perkin 1, 1973, 184, (構造決定, NMR)

Ravindranath, B. et al., Phytochemistry, 1973, 12, 2781, (UV, IR)

Gurudutt, K.N. et al., Phytochemistry, 1974, 13, 2845, (構造決定)

Arnone, A. et al., J.C.S. Perkin 1, 1975, 186, (構造決定, NMR)

Arnone, A. et al., J.C.S. Perkin 1, 1977, 2118, (C13-NMR, 構造決定)

Kinjo, J. et al., Tet. Lett., 1995, 36, 5599, (分離, H-NMR, C13-NMR)

### § Santalin Y

[CAS No.] 167425-77-6

[化合物分類] フラボノイド (3-Arylcoumarin flavonoid)

[構造式]

[分子式] C<sub>33</sub>H<sub>30</sub>O<sub>10</sub>

[分子量] 586.594

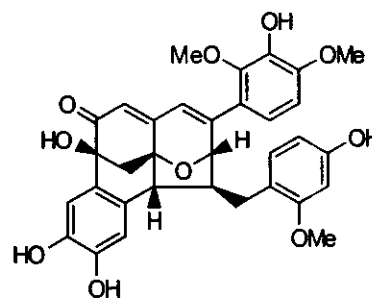
[正確な分子量] 586.1839

[基原] *Pterocarpus santalinus*

[性状] 黄色の針状結晶

[融点] Mp 244-248 °C

[その他のデータ] ラセミ体



-----文献-----

Kinjo, J. et al., Tet. Lett., 1995, 36, 5599, (分離, UV, IR, H-NMR, C13-NMR)

### § 3',4',5,7-Tetrahydroxyisoflavone; 7-Me ether, 3'-O-[3-O-E-cinnamoyl-β-D-glucopyranoside]

[化合物分類] フラボノイド (Isoflavones; 4 × O-置換基)

[構造式]

[分子式] C<sub>31</sub>H<sub>28</sub>O<sub>12</sub>

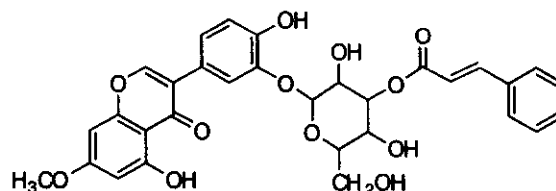
[分子量] 592.555

[正確な分子量] 592.15808

[基原] *Pterocarpus santalinus*

[性状] 無定形の黄色粉末 (MeOH)

[UV]: [neutral] λ<sub>max</sub> 265 (log ε 4.43); 322 (log ε 3.73) (MeOH)



-----文献-----

- Akisanya, A. et al., J.C.S., 1959, 2679, (分離)  
Wong, E. et al., J.O.C., 1963, 28, 2336, (分離, 構造決定, 合成法)  
Markham, K.R. et al., Phytochemistry, 1968, 7, 791, (分離)  
Dement, A.W. et al., Phytochemistry, 1972, 11, 1089, (分離)  
Ingham, J.L., Prog. Chem. Org. Nat. Prod., 1983, 43, 1, (レビュー, 生育)  
Krishnaveni, K.S. et al., Chem. Pharm. Bull., 2000, 48, 1373, (7-Me 3'-3-cinnamoylglucoside)

\*\*\*\*\*シイタケ (Shiitake) \*\*\*\*\*

§ § キシメジ科シイタケ (*Lentinus edodes* (Berk.) Sing.) の子実体。

§ 6-Amino-9H-purine-9-propanoic acid (CAS 名)

[化学名・別名] 3-(9-Adeniny) propionic acid

[CAS No.] 4244-47-7

[化合物分類] アルカロイド化合物 (Purine)

[構造式]

[分子式] C<sub>8</sub>H<sub>7</sub>N<sub>5</sub>O<sub>2</sub>

[分子量] 207.191

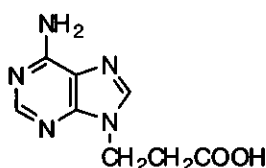
[正確な分子量] 207.075625

[基原] 次の植物から分離: *Lentinus edodes*

[用途] Exhibits anticholesteremic activity

[融点] Mp 277-278 °C で分解

[その他のデータ] λ<sub>max</sub> 259 (ε 13 800) (0.1N HCl), 262 nm (14 400) (0.1N NaOH)



-----文献-----

- Lira, E.P. et al., J.O.C., 1966, 31, 2188  
Chakraborti, S.K., Indian J. Chem., 1969, 7, 426, (合成法)  
Saito, Y. et al., Tet. Lett., 1970, 4863, (分離, 構造決定, 合成法)  
Japan. Pat., 1972, 33 196; CA, 78, 84435s  
Okumura, K. et al., J. Med. Chem., 1974, 17, 846

§ Bis[(methylthio)methyl] disulfide; 2,2,7,7-Tetraoxide

[化学名・別名] Bis(methylsulfonylmethyl) disulfide

[CAS No.] 74963-70-5

[化合物分類] 脂肪族化合物 (Disulfides, trisulfide)

[構造式]

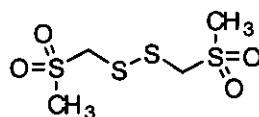
[分子式] C<sub>4</sub>H<sub>10</sub>O<sub>4</sub>S<sub>4</sub>

[分子量] 250.385

[正確な分子量] 249.94619

[基原] 次の植物から分離: マッシュルーム *Lentinus edodes*

[用途] 抗カビ剤



-----文献-----

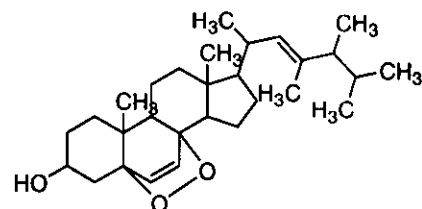
- Altamura, M.R. et al., J.O.C., 1963, 28, 2438, (合成法)  
Hase, T.A. et al., Synth. Commun., 1982, 12, 947, (合成法)  
Takazawa, H. et al., Yakugaku Zasshi, 1982, 102, 489, (tetraoxide)  
Weissflog, E., Phosphorus Sulfur Relat. Elem., 1983, 15, 27, (合成法)  
Boehme, H. et al., Sulfur Lett., 1984, 2, 151, (合成法)  
Burton, S.G. et al., Planta Med., 1992, 58, 295, (分離, IR, H-NMR)  
Kubota, K. et al., Biosci., Biotechnol., Biochem., 1994, 58, 430; 644, (分離, 合成法)  
Block, E. et al., J.O.C., 1994, 59, 2273, (合成法)  
Lim, H. et al., Phytochemistry, 1998, 48, 787, (4,4-dioxide)

§ 5,8-Epidioxy-23-methylergosta-6,22-dien-3-ol; (3 β, 22E, 24R)-form

[CAS No.] 211486-11-2

[化合物分類]ステロイド (Ergostane steroids;excluding withanolides and brassinolide) . (C28)

[構造式]



[基原] *Lentinus edodes*

[性状] 無定型の粉末

[比旋光度]:  $[\alpha]_D^{25} -37$  (c, 0.05 in CHCl<sub>3</sub>)

-----文献-----

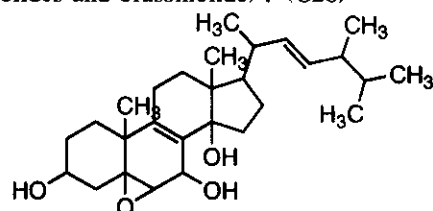
Yaoita, Y. et al., Chem. Pharm. Bull., 1998, 46, 944, (分離, H-NMR, C13-NMR)

§ 5,6-Epoxyergosta-8,22-diene-3,7,14-triol; (3 β,5 α,6 α,7 β,14 α,22E,24R)-form

[CAS No.] 211486-18-9

[化合物分類]ステロイド (Ergostane steroids;excluding withanolides and brassinolide) . (C28)

[構造式]



[基原] *Lentinus edodes*

[性状] 無定型の粉末

[比旋光度]:  $[\alpha]_D^{25} -19.6$  (c, 0.05 in CHCl<sub>3</sub>)

-----文献-----

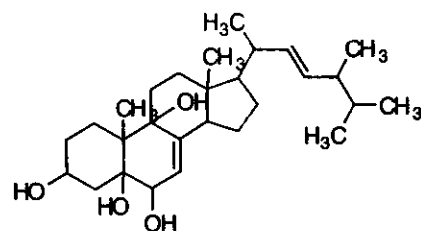
Yaoita, Y. et al., Chem. Pharm. Bull., 1998, 46, 944, (分離, H-NMR, C13-NMR)

§ Ergosta-7,22-diene-3,5,6,9-tetrol; (3 β,5 α,6 α,9 α,22E,24R)-form

[CAS No.] 211486-15-6

[化合物分類]ステロイド (Ergostane steroids;excluding withanolides and brassinolide) . (C28)

[構造式]



[基原] *Lentinus edodes* を含む食用マッシュルーム, *Flammulina velutipes*, *Hypsizigus marmoreus*, *Pleurotus ostreatus*, *Pholiota nameko*

[性状] 無定型の粉末

[比旋光度]:  $[\alpha]_D^{25} -28.8$  (c, 0.1 in CHCl<sub>3</sub>)

-----文献-----

Valisolalao, J. et al., Tetrahedron, 1983, 39, 2779, (Polyporus versicolor metab)

Migliuolo, A. et al., J. Nat. Prod., 1990, 53, 1414, (Spongia officinalis metab, 分離, H-NMR, C13-NMR)

Aiello, A. et al., Steroids, 1995, 60, 666, (6-sulfates, 分離, H-NMR, C13-NMR)

Yaoita, Y. et al., Chem. Pharm. Bull., 1998, 46, 944; 1999, 47, 847, (mushroom constit)

§ Ergosta-7,22-diene-3,5,6,9-tetrol; (3 β,5 α,6 α,9 α,22E,24R)-form, 22,23-Dihydro, 6-ketone

[化学名・別名] 3,5,9-Trihydroxyergost-7-en-6-one, 3,5,9-Trihydroxy-24-methylcholest-7-en-6-one

[CAS No.] 211486-13-4

[化合物分類]ステロイド (Ergostane steroids;excluding withanolides and brassinolide) . (C28)

[構造式]

[分子式] C<sub>28</sub>H<sub>46</sub>O<sub>4</sub>

[分子量] 446.669

[正確な分子量] 446.33961

[基原] 次の植物から分離: カビ類; *Lentinus edodes*, *Hypsizigus marmoreus*, *Pleurotus ostreatus*, *Pholiota nameko*

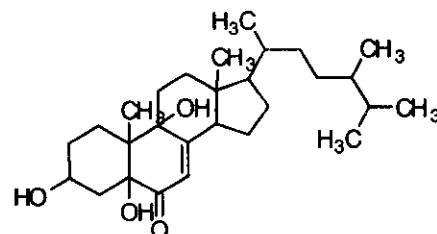
[性状] 無定型の粉末

[比旋光度]:  $[\alpha]_D^{25} -21.5$  (c, 0.09 in CHCl<sub>3</sub>)

[UV]: [neutral] λ<sub>max</sub> 236 (log ε 3.8) (MeOH)

-----文献-----

Valisolalao, J. et al., Tetrahedron, 1983, 39, 2779, (Polyporus versicolor metab)



Migliuolo, A. et al., J. Nat. Prod., 1990, 53, 1414, (Spongia officinalis metab, 分離, H-NMR, C13-NMR)  
Aiello, A. et al., Steroids, 1995, 60, 666, (6-sulfates, 分離, H-NMR, C13-NMR)  
Yaoita, Y. et al., Chem. Pharm. Bull., 1998, 46, 944; 1999, 47, 847, (mushroom constit)

### § Eritadenine; (2R,3R)-form

[化学名・別名] D-erythro-form

[CAS No.] 23918-98-1

[化合物分類] 炭水化物 (Aldonic acid) 炭水化物 (Nucleoside)

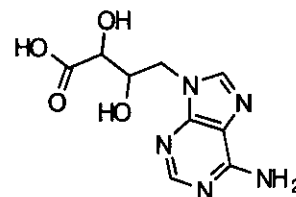
[構造式]

[基原] 次の植物から分離: 食用シイタケキノコ *Lentinus edodes*

[融点] Mp 261-263 °C で分解 (279 °C 分解)

[比旋光度]:  $[\alpha]_D +50$  (0.1M NaOH).  $[\alpha]_D +16$  (1M HCl)

[UV]: [acid]  $\lambda_{max}$  259 ( $\epsilon$  14129) (HCl) [neutral]  $\lambda_{max}$  261 ( $\epsilon$  14508) (H<sub>2</sub>O) [base]  $\lambda_{max}$  262 ( $\epsilon$  14300) (NaOH)



#### -----文献-----

Chibata, I. et al., *Experientia*, 1969, 25, 1237, (分離)  
Rokujo, T. et al., *Life Sci.*, 1970, 9, 379, (薬理)  
Kamiya, T. et al., *Tetrahedron*, 1972, 28, 899, (合成法, 絶対構造)  
Kawazu, M. et al., *J.O.C.*, 1973, 38, 2887, (合成法, H-NMR)  
Okumura, K. et al., *J. Med. Chem.*, 1974, 17, 846  
Holy, A. et al., *Coll. Czech. Chem. Comm.*, 1982, 47, 1392, (合成法, 薬理)

### § Eritadenine; (2R,3R)-form, 3-Deoxy

[化学名・別名] Deoxyeritadenine

[CAS No.] 31701-90-3

[化合物分類] 炭水化物 (Nucleoside)

[構造式]

[分子式] C<sub>9</sub>H<sub>11</sub>N<sub>5</sub>O<sub>3</sub>

[分子量] 237.218

[正確な分子量] 237.08619

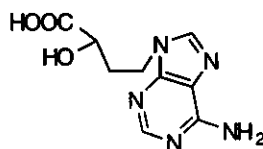
[基原] 食用シイタケキノコ *Lentinus edodes*

[用途] 弱いコレステロール低下活性を示す

[融点] Mp 270-271 °C で分解

[比旋光度]:  $[\alpha]_D +18.4$  (c, 1.0 in 0.1N NaOH)

[UV]: [base]  $\lambda_{max}$  262 ( $\epsilon$  14300) (0.1 M NaOH) [acid]  $\lambda_{max}$  262 ( $\epsilon$  13900) (0.1 M HCl)



#### -----文献-----

Chibata, I. et al., *Experientia*, 1969, 25, 1237, (分離)  
Rokujo, T. et al., *Life Sci.*, 1970, 9, 379, (薬理)  
Kamiya, T. et al., *Tetrahedron*, 1972, 28, 899, (合成法, 絶対構造)  
Kawazu, M. et al., *J.O.C.*, 1973, 38, 2887, (合成法, H-NMR)  
Okumura, K. et al., *J. Med. Chem.*, 1974, 17, 846  
Holy, A. et al., *Coll. Czech. Chem. Comm.*, 1982, 47, 1392, (合成法, 薬理)

### § Hexathiepane (CAS 名)

[化学名・別名] 1,2,3,4,5,6-Hexathiacycloheptane

[CAS No.] 17233-71-5

[化合物分類] 脂肪族化合物 (Simple heteroalicyclics (miscellaneous heteroatom))

[構造式]

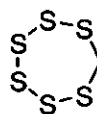
[分子式] CH<sub>2</sub>S<sub>6</sub>

[分子量] 206.423

[正確な分子量] 205.84807

[基原] *Lentinus edodes* の微量成分

[融点] Mp 90 °C



#### -----文献-----

Katsura, M. et al., *Chem. Pharm. Bull.*, 1967, 15, 988, (分離, 合成法)