

Wu, S.H., J. Chromatogr., 1982, 245, 268, (分離, hplc)

§ **Glycinoeclepin B**

[CAS No.] 103847-17-2

[化合物分類]テルペノイド (Cycloartane triterpenoids)

[構造式]

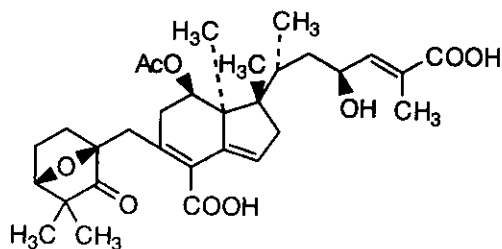
[分子式]  $C_{31}H_{42}O_6$

[分子量] 558.667

[正確な分子量] 558.282885

[天然基原] *Phaseolus vulgaris* の根

UV: [neutral]  $\lambda_{max}$  252 ( $\epsilon$  9500) (MeOH) (Derep)



-----文献-----

Fukuzawa, A. et al., Tet. Lett., 1985, 26, 5539

Corey, E.J. et al., J.A.C.S., 1990, 112, 8997, (合成法)

§ **Glycinoeclepin C**

[化合物分類]テルペノイド (Cycloartane triterpenoids)

[構造式]

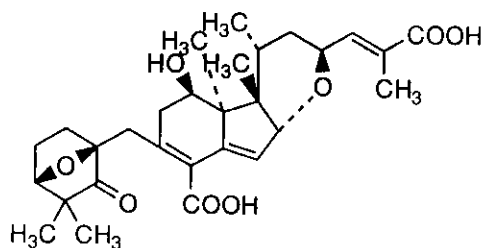
[分子式]  $C_{29}H_{38}O_8$

[分子量] 514.614

[正確な分子量] 514.25667

[天然基原] *Phaseolus vulgaris* の根

UV: [neutral]  $\lambda_{max}$  252 ( $\epsilon$  9500) (MeOH) (Derep)



-----文献-----

Fukuzawa, A. et al., Tet. Lett., 1985, 26, 5539

§ **3-Hydroxy-5,7-megastigmadien-9-one; (3R,7E)-form**

[化学名・別名] 3-Hydroxy- $\beta$ -ionone

[化合物分類]テルペノイド (Megastigmene nortriterpenoids)

[構造式]

[分子式]  $C_{13}H_{20}O_2$

[分子量] 208.3

[正確な分子量] 208.14633

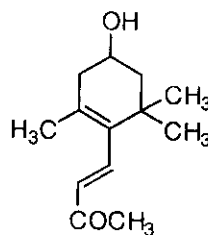
[天然基原] 次の植物から分離: *Phaseolus vulgaris*

[用途] 成長阻害因子

[性状] オイル

[比旋光度]:  $[\alpha]_D^{22}$  -140.5 (c, 0.1 in  $CHCl_3$ )

[その他のデータ]  $\lambda_{max}$  221, 290 nm (EtOH)



-----文献-----

Leppik, R.A. et al., Phytochemistry, 1972, 11, 2055, (分離)

Mori, K. et al., Agric. Biol. Chem., 1973, 37, 2899, (合成法)

Miyase, T. et al., Chem. Pharm. Bull., 1987, 35, 1109, (Icariside B<sub>2</sub>)

Kato-Noguchi, H. et al., Phytochemistry, 1993, 33, 553, (分離, H-NMR, C13-NMR)

Suchy, V. et al., Coll. Czech. Chem. Comm., 1995, 60, 1380, (Icariside B<sub>2</sub>, H-NMR, C13-NMR)

§ **2-C-(Hydroxymethyl)ribonic acid; D-form, 5-O-Phosphate**

[CAS No.] 112160-91-5

[化合物分類]炭水化物 (Aldonic acids), 炭水化物 (Sugar phosphates)

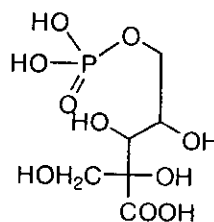
[構造式]

[分子式]  $C_6H_{13}O_{10}P$

[分子量] 276.136

[正確な分子量] 276.024637

[天然基原] 次の植物から分離: *Phaseolus vulgaris* の葉



[用途] Inhibitor of ribulose 1,5-bisphosphate carboxylase

文献

Beck, E. et al., *Plant Physiol.*, 1989, 90, 13, (H-NMR, C13-NMR)

Moore, B.D. et al., *Phytochemistry*, 1993, 34, 703, (生育)

§ 3-Hydroxystigmasta-5,22-dien-7-one; (3  $\beta$ , 22E)-form

[化学名・別名] 7-Oxostigmasterol

[CAS No.] 36449-99-7

[化合物分類] ステロイド (Stigmastane steroids). (C29).

[構造式]

[分子式]  $C_{29}H_{48}O_2$

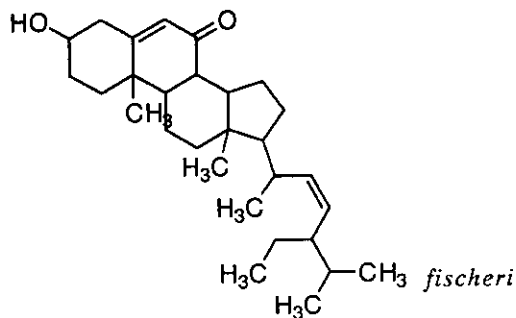
[分子量] 426.881

[正確な分子量] 426.34978

[天然基原] 次の植物から分離: *Cannabis sativa*, *Euphorbia ana*, *Iris missouriensis*, *Phaseolus vulgaris*

[性状] 針状結晶 (MeOH/petrol)

[融点] Mp 162 °C



文献

Schroeder, G. et al., *Phytochemistry*, 1980, 19, 2213, (分離)

Wong, S.M. et al., *J. Nat. Prod.*, 1986, 49, 330, (分離)

Kovganko, N.V. et al., *Khim. Prir. Soedin.*, 1996, 32, 206-211; *Chem. Nat. Compd. (Engl. Transl.)*, 1996, 32, 183-186, (合成法)

§ 6-Hydroxystigmasta-4,22-dien-3-one; (6  $\beta$ , 22E)-form

[CAS No.] 36450-01-8

[化合物分類] ステロイド (Stigmastane steroids). (C29).

[構造式]

[分子式]  $C_{29}H_{48}O_2$

[分子量] 426.881

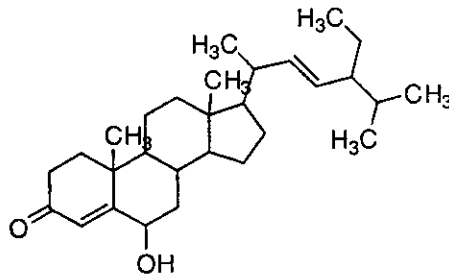
[正確な分子量] 426.34978

[天然基原] *Phaseolus vulgaris* の根, *Phoenix dactylifera* の茎

[性状] 結晶 (EtOH)

[融点] Mp 210-212 °C

[比旋光度]:  $[\alpha]_D^{25} +8$  (CHCl<sub>3</sub>)



文献

Katsui, N. et al., *Bull. Chem. Soc. Jpn.*, 1972, 45, 223, (分離)

Fernandez, M.I. et al., *Phytochemistry*, 1983, 22, 2087, (分離)

Galagovsky, L.R. et al., *J. Chem. Res., Synop.*, 1990, 366, (合成法, MR)

§ 6-Hydroxystigmast-4-en-3-one; (6  $\beta$ , 24R)-form

[CAS No.] 36450-02-9

[化合物分類] ステロイド (Stigmastane steroids). (C29).

[構造式]

[分子式]  $C_{29}H_{48}O_2$

[分子量] 428.697

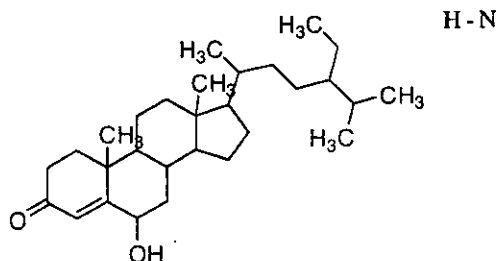
[正確な分子量] 428.36543

[天然基原] 次の植物を含む色々な植物属から分離: *Phaseolus vulgaris*, *Quercus* spp., *Sambucus* sp.

[性状] 針状結晶 (petrol)

[融点] Mp 213-215 °C

[比旋光度]:  $[\alpha]_D^{25} +29$  (CHCl<sub>3</sub>)



文献

Katsui, N. et al., *Bull. Chem. Soc. Jpn.*, 1972, 45, 223, (分離)

Tunmann, P. et al., *Arch. Pharm. (Weinheim, Ger.)*, 1974, 307, 966, (分離)

Hui, W.-H. et al., *J.C.S. Perkin 1*, 1977, 897, (分離)

Khan, A.Q. et al., *Phytochemistry*, 1989, 28, 2859, (分離, H-NMR, C13-NMR)

Della Greca, M. et al., *J. Nat. Prod.*, 1990, 53, 1430, (分離, H-NMR, C13-NMR)

Arai, Y. et al., *Phytochemistry*, 1998, 48, 471-474, (分離, H-NMR, C13-NMR)

§ **Malic acid; (S)-form, O-(3,4-Dihydroxycinnamoyl)**

[化学名・別名] Phaselic acid, Caffeylmalic acid

[CAS No.] 53755-04-7

[化合物分類] 炭水化物 (Aldaric acids)

[構造式]

[分子式]  $C_{13}H_{12}O_8$

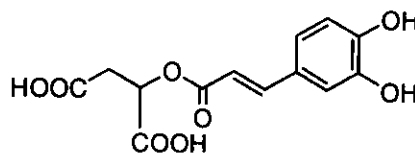
[分子量] 296.233

[正確な分子量] 296.05322

[天然基原] 次の植物から分離: サヤインゲン (*Phaseolus vulgaris*) の葉, *Trifolium pratense*

[性状] 黄色がかった吸湿性のガラス状結晶

[比旋光度]:  $[\alpha]_D^{20} +31.5$  (c, 1.36 in H<sub>2</sub>O),  $[\alpha]_D^{25} +28.3$  (H<sub>2</sub>O)



----- 文献 -----

Scarpati, M.L. et al., *Gazz. Chim. Ital.*, 1960, 90, 212, (Phaselic acid)

Hahn, R. et al., *Planta Med.*, 1993, 59, 71; 189, (Phaselic acid)

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

[化学名・別名] 24-α-Methylphenol

[CAS No.] 33903-17-2

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

[構造式]

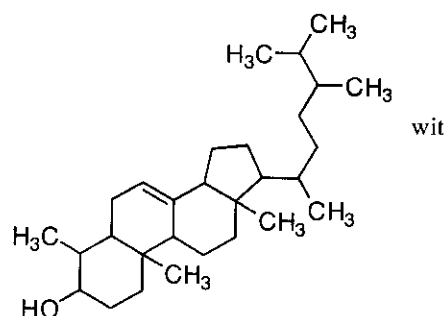
[分子式]  $C_{29}H_{50}O$

[分子量] 414.713

[正確な分子量] 414.386165

[天然基原] 次の植物から分離: アメリカトガサワラの辺材, *Phaseolus vulgaris* の種子, その他の植物

[融点] Mp 140-141 °C (as acetate)



----- 文献 -----

Conner, A.H. et al., *Phytochemistry*, 1981, 20, 2543, (分離, H-NMR)

Akihisa, T. et al., *Phytochemistry*, 1989, 28, 1219, (分離, H-NMR, Mass)

§ **2-C-Methyl-1,4-erythrone; D-form**

[CAS No.] 18465-71-9

[化合物分類] AF8400, 炭水化物 (Other sugar acids), 炭水化物 (Branched chain sugars)

[構造式]

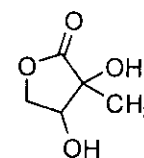
[分子式]  $C_5H_8O_4$

[分子量] 132.116

[正確な分子量] 132.04226

[天然基原] *Astragalus lusitanicus*, *Oriza japonica*, *Trifolium incarnatum*, *Phaseolus vulgaris*

[比旋光度]:  $[\alpha]_D -58.6$  (CHCl<sub>3</sub>)



----- 文献 -----

Ishizu, A. et al., *Acta Chem. Scand.*, 1967, 21, 424, (isopropylidene)

De Pascual Teresa, J. et al., *Tet. Lett.*, 1980, 1359, (分離, di-Ac, isopropylidene)

Ono, H. et al., *Biosci., Biotechnol., Biochem.*, 2000, 64, 1970-1973, (分離, H-NMR, C13-NMR)

§ **25-Methyl-24-methylenecholest-5-en-3-ol; 3β-form**

[化学名・別名] 25-Methyl-24-methylenecholesterol

[CAS No.] 89702-24-9

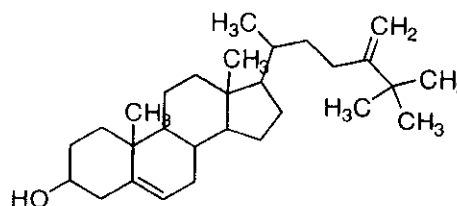
[化合物分類] ステロイド (Ergostane steroids; excluding withanolides and brassinolides). (C28).

[構造式]

[分子式]  $C_{29}H_{48}O$

[分子量] 412.698

[正確な分子量] 412.370515



[天然基原] *Brassica juncea*, *Helianthus annuus*, *Phaseolus vulgaris*, *Wrightia tinctoria*

[性状] 結晶 (EtOH)

[融点] Mp 158.5-160 °C

-----文献-----

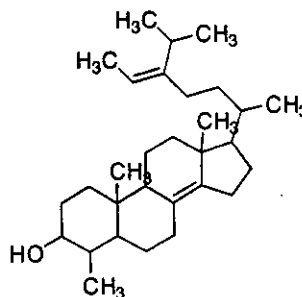
Matsumoto, T. et al., *Phytochemistry*, 1983, 22, 2619; 1984, 23, 921; 1988, 27, 629; 3231, (分離)

§ 4-Methylstigmasta-8(14),24(28)-dien-3-ol; (3 $\beta$ ,4 $\alpha$ ,5 $\alpha$ ,24Z)-form

[CAS No.] 78285-84-4

[化合物分類] ステロイド (Stigmastane steroids). (C29).

[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

[天然基原] *Glenodinium* sp., *Phaseolus vulgaris*

-----文献-----

Kokke, W.C.M.C. et al., *Phytochemistry*, 1981, 20, 127, (分離)

Bohlin, L. et al., *Phytochemistry*, 1981, 20, 2397, (誘導体)

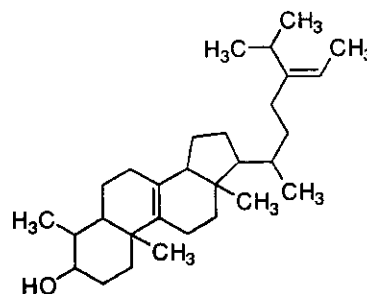
Akihisa, T. et al., *Phytochemistry*, 1989, 28, 1219, (分離)

§ 4-Methylstigmasta-8,24(28)-dien-3-ol; (3 $\beta$ ,4 $\alpha$ ,5 $\alpha$ ,24Z)-form

[CAS No.] 71418-13-8

[化合物分類] ステロイド (Stigmastane steroids). (C29).

[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

[天然基原] *Phaseolus vulgaris*, *Rubus fruticosus*

[融点] Mp 130-132 °C (as acetate)

-----文献-----

Schmitt, P. et al., *Phytochemistry*, 1987, 26, 2709, (分離)

Akihisa, T. et al., *Phytochemistry*, 1989, 28, 1219, (分離)

§ Octanedioic acid (CAS 名)

[化学名・別名] Suberic acid (旧 CAS 名). 1,6-Hexanedicarboxylic acid

[CAS No.] 505-48-6

[化合物分類] 脂肪族化合物 (Saturated unbranched carboxylic acids and lactones)

[構造式] HOOC(CH<sub>2</sub>)<sub>6</sub>COOH

[分子式] C<sub>8</sub>H<sub>14</sub>O<sub>4</sub>

[分子量] 174.196

[正確な分子量] 174.08921

[天然基原] 次の植物から分離: *Anthyllis sericea* の茎と葉, *Phaseolus vulgaris* の根. Manuf. by oxidative cleavage of cyclooctene

[用途] プラスチック産業に用いられる. ポリエステルとポリアミドの単量体

[性状] 結晶 (H<sub>2</sub>O or C<sub>6</sub>H<sub>6</sub>/EtOH)

[融点] Mp 144 °C

[沸点] Bp<sub>100</sub> 279 °C

[溶解性] 水に不溶; エーテル, ベンゼンに可溶

[PKa 値] pK<sub>a1</sub> 4.53; pK<sub>a2</sub> 5.52 (25 °C, 0.1 M KNO<sub>3</sub>)

[その他のデータ] Subl. >300 °C

[販売元] Aldrich:S520-0; Fluka:60930; Sigma:S7126

-----文献-----

Takasugi, M. et al., *Chem. Lett.*, 1973, 445, (分離)

Marco, J.A. et al., *Phytochemistry*, 1978, 17, 1438, (分離)

§ 12,15-Oleanadiene-3,23-diol; 3  $\beta$ -form, 3-O-[ $\alpha$ -L-Rhamnopyranosyl-(1  $\rightarrow$  6) [ $\alpha$ -D-galactopyranosyl-(1  $\rightarrow$  2)]- $\beta$ -D-glucopyranosyl-(1  $\rightarrow$  4)- $\alpha$ -D-galactopyranosyl-(1  $\rightarrow$  2)- $\alpha$ -L-arabinopyranosyl-(1  $\rightarrow$  3)]- $\beta$ -D-glucuronide]

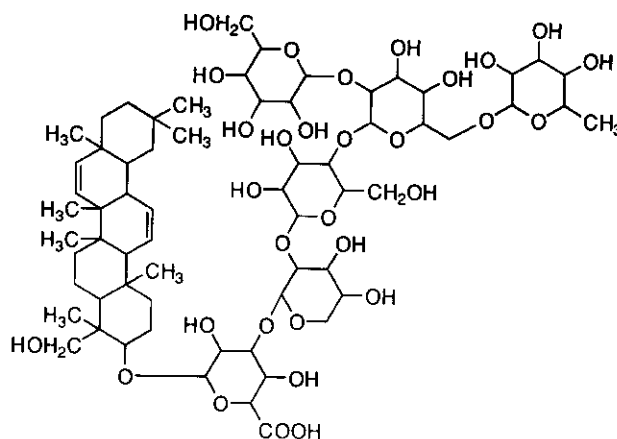
[化学名・別名]Phaseolside D

[CAS No.]30937-16-7

[化合物分類]テルペノイド

(Oleanane triterpenoids)

[構造式]



[分子式]  $C_{65}H_{104}O_{51}$

[分子量] 1381.518

[正確な分子量] 1380.656165

[天然基原] 次の植物から分離: *Phaseolus*

*ulgaris*

-----文献-----

Chirva, V.Y. et al., *Khim. Prir. Soedin.*, 1970, 6, 377; 559; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, 6, 386; 575, (分離, 構造決定)

Lazur'evskii, G.V. et al., *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1971, 199, 226; *CA*, 75, 115903, (構造決定)

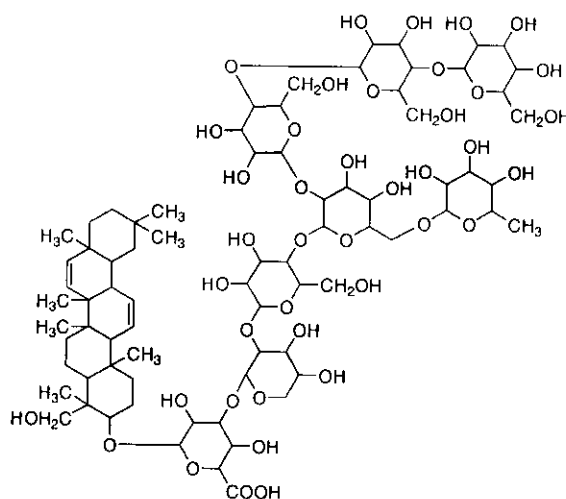
§ 12,15-Oleanadiene-3,23-diol; 3  $\beta$ -form, 3-O-[ $\beta$ -D-Glucopyranosyl-(1  $\rightarrow$  4)- $\beta$ -D-glucopyranosyl-(1  $\rightarrow$  4)- $\alpha$ -D-galactopyranosyl-(1  $\rightarrow$  2) [ $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  6)]- $\beta$ -D-glucopyranosyl-(1  $\rightarrow$  4)- $\alpha$ -D-galactopyranosyl-(1  $\rightarrow$  2)- $\alpha$ -L-arabinopyranosyl-(1  $\rightarrow$  3)]- $\beta$ -D-glucuronide]

[化学名・別名]Phaseolside E

[CAS No.]30915-09-4

[化合物分類]テルペノイド(Oleanane triterpenoids)

[構造式]



[分子式]  $C_{77}H_{124}O_{41}$

[分子量] 1705.802

[正確な分子量] 1704.761815

[天然基原] 次の植物から分離: *Phaseolus vulgaris*

-----文献-----

Chirva, V.Y. et al., *Khim. Prir. Soedin.*, 1970, 6, 377; 559; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, 6, 386; 575, (分離, 構造決定)

Lazur'evskii, G.V. et al., *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1971, 199, 226; *CA*, 75, 115903, (構造決定)

§ 12-Oleanene-3,22,24-triol; (3  $\beta$ , 22  $\beta$ )-form, 24-O- $\beta$ -D-Glucopyranoside

[CAS No.]115334-08-2

[化合物分類]テルペノイド(Oleanane triterpenoids)

[構造式]

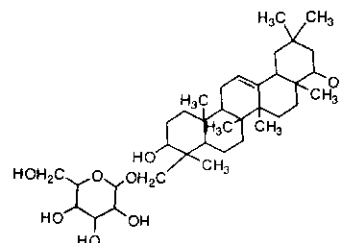
[分子式]  $C_{36}H_{60}O_8$

[分子量] 620.865

[正確な分子量] 620.42882

[天然基原] サヤインゲンの種子(*Phaseolus vulgaris*)

[性状] 結晶 (MeOH)



[比旋光度]:  $[\alpha]_D^{25} +57$  (CHCl<sub>3</sub>)

-----文献-----

Willner, D. et al., J.C.S., 1964, 5885, (分離)

Kaneda, M. et al., Chem. Pharm. Bull., 1984, 32, 1287, (分離)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1985, 33, 4267, (分離)

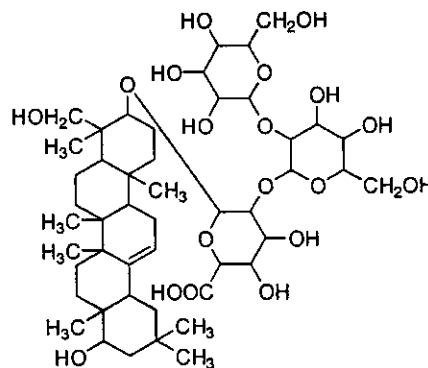
§ 12-Oleanene-3,22,24-triol; (3 $\beta$ ,22 $\beta$ )-form, 3-O-[ $\beta$ -D-Glucopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-galactopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-glucuronopyranoside]

[化学名・別名] Soyasaponin V

[CAS No.] 114590-20-4

[化合物分類] テルペノイド (Oleanane triterpenoids)

[構造式]



[分子式] C<sub>48</sub>H<sub>78</sub>O<sub>19</sub>

[分子量] 959.133

[正確な分子量] 958.513735

[天然基原] ダイズの種子 (*Glycine max*), サヤインゲン (*Phaseolus ris*)

*vulga*

-----文献-----

Curl, C.L. et al., J. Sci. Food Agric., 1988, 43, 101, (Soyasaponin V)

§ 12-Oleanene-3,22,24-triol; (3 $\beta$ ,22 $\beta$ )-form, 3-O-[ $\beta$ -D-Glucopyranosyl-(1 $\rightarrow$ 3)-[ $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 4)]- $\beta$ -D-glucopyranoside]

[化学名・別名] Phaseoluside A

[CAS No.] 137231-80-2

[化合物分類] テルペノイド (Oleanane triterpenoids)

[構造式]

[分子式] C<sub>48</sub>H<sub>80</sub>O<sub>18</sub>

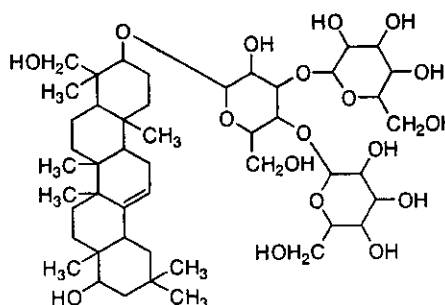
[分子量] 945.149

[正確な分子量] 944.53447

[天然基原] 次の植物から分離: サヤインゲンの種子油  
*Phaseolus vulgaris*)

[融点] Mp 245-248 °C (分解)

[比旋光度]:  $[\alpha]_D^{25} +25.1$  (c, 1 in Py)



-----文献-----

Jain, D.C. et al., Planta Med., 1991, 57, 94, (Phaseoluside A)

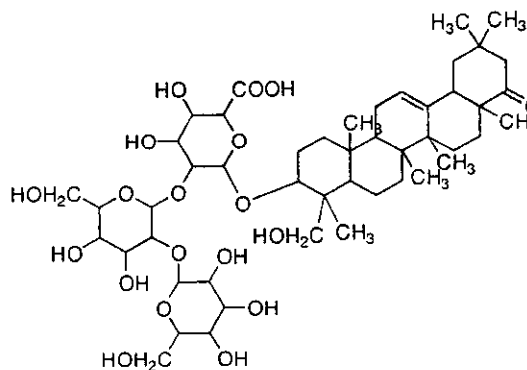
§ 12-Oleanene-3,22,24-triol; (3 $\beta$ ,22 $\beta$ )-form, 3-O-[ $\beta$ -D-Glucopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-galactopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-glucuronopyranoside]

[化学名・別名] Sandosaponin A

[CAS] No.] 135272-91-2

[化合物分類] テルペノイド  
(Oleanane triterpenoids)

[構造式]



[分子式] C<sub>48</sub>H<sub>76</sub>O<sub>19</sub>

[分子量] 957.117

[正確な分子量] 956.498085

[天然基原] サヤインゲン (*Phaseolus vulgaris*) の種子

[性状] 結晶 (MeOH 溶液)

[融点] Mp 200-201 °C

[比旋光度]:  $[\alpha]_D^{25} -5.8$  (c, 0.8 in MeOH)

-----文献-----

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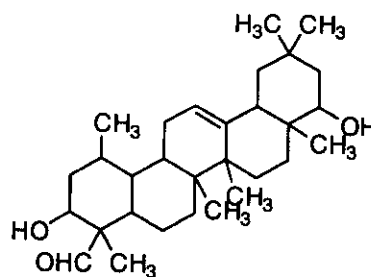
Yoshikawa, M. et al., Chem. Pharm. Bull., 1997, 45, 877-882, (Sandosapogenol, Sandosaponins)

§ 12-Oleanene-3,22,24-triol; (3 $\beta$ ,22 $\beta$ )-form, 24-Aldehyde

[化学名・別名] 3,22-Dihydroxy-12-oleanen-24-al. Sandosapogenol

[化合物分類] テルペノイド (Oleanane triterpenoids)

[構造式]



[分子式] C<sub>30</sub>H<sub>48</sub>O<sub>3</sub>

[分子量] 456.707

[正確な分子量] 456.360345

[天然基原] サヤインゲン (*Phaseolus vulgaris*) の種子から得られるサポゲニン

[性状] 粉末

[比旋光度]:  $[\alpha]_D^{24} +61.2$  (c, 1.38 in CHCl<sub>3</sub>)

-----文献-----

Yoshikawa, M. et al., Chem. Pharm. Bull., 1997, 45, 877-882, (Sandosapogenol, Sandosaponins)

§ 12-Oleanene-3,22,24-triol; (3 $\beta$ ,22 $\beta$ )-form, 24-Aldehyde, 3-O- $[\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-galactopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-glucuronopyranoside]

[化学名・別名] Sandosaponin B

[化合物分類] テルペノイド (Oleanane triterpenoids)

[構造式]

[分子式] C<sub>48</sub>H<sub>76</sub>O<sub>19</sub>

[分子量] 957.117

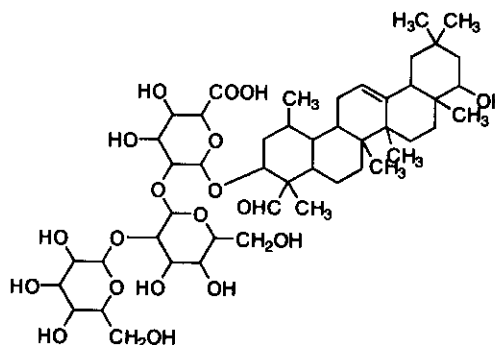
[正確な分子量] 956.498085

[天然基原] サヤインゲン (*Phaseolus vulgaris*) の種子

[性状] 結晶 (MeOH 溶液)

[融点] Mp 212-213 °C

[比旋光度]:  $[\alpha]_D^{28} +34.8$  (c, 0.3 in MeOH)



-----文献-----

Yoshikawa, M. et al., Chem. Pharm. Bull., 1997, 45, 877-882, (Sandosapogenol, Sandosaponins)

§ Orotidine

[化学名・別名] 1,2,3,6-Tetrahydro-2,6-dioxo-3- $\beta$ -D-ribofuranosyl-4-pyrimidinecarboxylic acid (CAS 名), 3- $\beta$ -D-Ribofuranosylorotic acid (旧 CAS 名), 6-Carboxyuridine (旧 CAS 名)

[CAS No.] 314-50-1

[化合物分類] 炭水化物 (Nucleosides)

[構造式]

[分子式] C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O<sub>8</sub>

[分子量] 288.213

[正確な分子量] 288.059368

[天然基原] 細菌によって生産される。また植物にも存在する。例えば、*Phaseolus vulgaris* と *Xanthium pensylvanicum* から分離される

[用途] ピリミジンヌクレオチド生合成の中間体

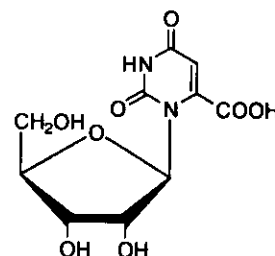
[融点] Mp 200 °C (turns brown near)

UV: [acid]  $\lambda_{max}$  267 (ε 9570) (0.1 N HCl) (Derep) [base]  $\lambda_{max}$  265 (ε 8960) (0.1 N NaOH) (Derep)

[neutral]  $\lambda_{max}$  268 (ε 8900) (MeOH) (Derep)

[その他のデータ]  $\lambda_{max}$  268 (ε 8900) (MeOH), 267 (9570) (0.1 M HCl), 265 nm (8960) (0.1 M NaOH)

[販売元] Sigma:O9505



-----文献-----

Hruska, F.E., J.A.C.S., 1971, 93, 1795, (conformn, H-NMR)

Hermann, E.C. et al., Anal. Biochem., 1973, 53, 478, (chromatog, phosphate)

Holy, A., Coll. Czech. Chem. Comm., 1975, 40, 738, (合成法)

§ Phaseolamin (CAS 名)

[CAS No.] 56996-83-9

[化合物分類] アミノ酸とペプチド (Other proteins)

[構造式] 不明

[一般的性質] Protein

[天然基原] 次の植物から分離: インゲン豆 *Phaseolus vulgaris*

[用途]  $\alpha$ -amylase 阻害因子

-----文献-----

Marshall, J.J. et al., J. Biol. Chem., 1975, 250, 8030, (分離)

### § Phaseollin

[化学名・別名] 6b,12b-Dihydro-3,3-dimethyl-3H,7H-furo[3,2-c:5,4-f]bis[1]benzopyran-10-ol (CAS 名). Phaseolin

[CAS No.] 13401-40-6

[化合物分類] フラボノイド (Simple pterocarpin flavonoids), フラボノイド (Cyclised C-isopentenylated flavonoids), 薬物: 抗菌性剤 (Antibacterial agents), 薬物: 抗カビ薬 (Antifungal agents)

[構造式]

[分子式]  $C_{29}H_{18}O_4$

[分子量] 322.36

[正確な分子量] 322.12051

[天然基原] 次の植物から分離: *Phaseolus vulgaris*. また

*a abyssinica*, *Vigna unguiculata*

[用途] 細菌, カビ, 酵母に対して活性を有する. ファイキシン

[融点] Mp 177-178 °C

[比旋光度]:  $[\alpha]_D -145$  (c, 0.17 in EtOH)

[溶解性] BERDY SOL: メタノール, エーテル, 塩基に可溶; 水に易溶

[PKa 値] pKa 9.13

[Log P 計算値] Log P 3.96 (未確認値) (計算値)

UV: [neutral]  $\lambda_{max}$  207 ( $\epsilon$  47900); 230 ( $\epsilon$  25100); 280 ( $\epsilon$  9330); 286 ( $\epsilon$  7940); 315 ( $\epsilon$  2190) (MeOH) (Derep) [neutral]  $\lambda_{max}$  279 ( $\epsilon$  9120); 286 ( $\epsilon$  7940); 315 ( $\epsilon$  2190) (EtOH) (Berdy) [base]  $\lambda_{max}$  281 ( $\epsilon$  11480); 292 ( $\epsilon$  10960); 377 ( $\epsilon$  2880) (EtOH-NaOH) (Berdy)

-----文献-----

Perrin, O.R., Tet. Lett., 1964, 438, (分離)

Cruickshank, I. et al., Phytopathol. Z., 1971, 70, 209, (分離)

DeMartinis, C. et al., Tetrahedron, 1978, 34, 1849, (結晶構造)

Kamat, V.S. et al., Heterocycles, 1981, 15, 1163, (分離)

Kitagawa, I. et al., Chem. Pharm. Bull., 1994, 42, 1056, (1-Methoxyphaseollin)

### § Phaseollinisoflavan

[化学名・別名] 3,4-Dihydro-2,2-dimethyl[3,6'-bi-2H-1-benzopyran]-5',7-diol (CAS 名)

[CAS No.] 40323-57-7

[化合物分類] フラボノイド (Isoflavans), フラボノイド (Cyclised C-isopentenylated flavonoids)

[構造式]

[分子式]  $C_{29}H_{20}O_4$

[分子量] 324.376

[正確な分子量] 324.13616

[一般的性質] Isoflavanoid numbering shown

[天然基原] 次の植物から得られるファイトアレキシン:

*us vulgaris*, その他の *Phaseolus* spp., *Glycyrrhiza glabra*

[用途] カビ成長抑制因子

[比旋光度]:  $[\alpha]_D -9$  (c, 0.1 in MeOH)

-----文献-----

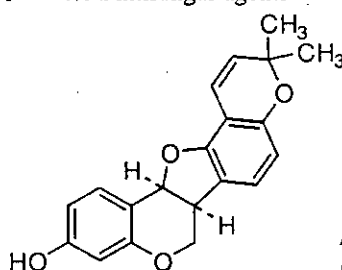
Burden, R.S. et al., Tet. Lett., 1972, 4175, (分離, 構造決定, UV, H-NMR)

v. Etten, H.D., Phytochemistry, 1973, 12, 1791, (誘導體)

Seifert, K. et al., Z. Naturforsch., C, 1993, 48, 550, (分離, H-NMR, C13-NMR)

Tanaka, H. et al., Phytochemistry, 1998, 47, 1397-1400, (分離, CD, H-NMR, C13-NMR)

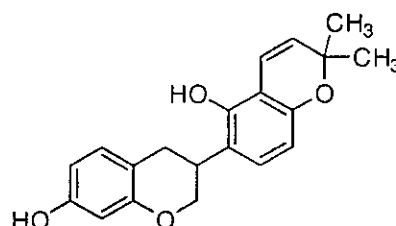
### § Phaseollinisoflavan; 2'-Me ether



Erythrin

トアレ

Absolute configuration



Phaseol



### § Phaseollinisoflavan; 2'-Me ether

[化学名・別名] 2'-O-Methylphaseollinisoflavan, 2'-Methoxyphaseollinisoflavan (incorr.)

[CAS No.] 49594-01-6

[化合物分類] フラボノイド (Isoflavans), フラボノイド (Cyclised C-isopentenylated flavonoids)

[構造式]

[分子式]  $C_{21}H_{22}O_4$

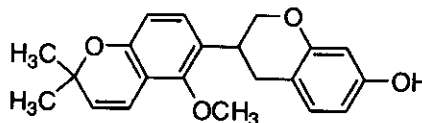
[分子量] 338.402

[正確な分子量] 338.15181

[天然基原] *Phaseolus vulgaris*

[比旋光度]:  $[\alpha]_D^{24} +19.5$  (EtOH)

UV: [neutral]  $\lambda_{max}$  228 ( $\epsilon$  39800); 271 ( $\epsilon$  9120); 280 ( $\epsilon$  9330); 313 ( $\epsilon$  2040) (EtOH) (Berdy)



-----文献-----

Burden, R.S. et al., Tet. Lett., 1972, 4175, (分離, 構造決定, UV, H-NMR)

v. Etten, H.D., Phytochemistry, 1973, 12, 1791, (誘導體)

Seifert, K. et al., Z. Naturforsch., C, 1993, 48, 550, (分離, H-NMR, C13-NMR)

Tanaka, H. et al., Phytochemistry, 1998, 47, 1397-1400, (分離, CD, H-NMR, C13-NMR)

### § Phaseoloside A

[化合物分類] テルペノイド (Terpenoids 構造は未知)

[一般的性質] Triterpene glycoside of unknown struct.

[天然基原] *Phaseolus vulgaris*

[その他のデータ] 物理化学的性質に関する事柄はない

-----文献-----

Chirva, V.Y. et al., Khim. Prir. Soedin., 1970, 6, 377; Chem. Nat. Compd. (Engl. Transl.), 386

### § Phaseoloside B

[化合物分類] テルペノイド (Terpenoids 構造は未知)

[一般的性質] Triterpene glycoside of unknown struct.

[天然基原] *Phaseolus vulgaris*

[その他のデータ] 物理化学的性質に関する事柄はない

-----文献-----

Chirva, V.Y. et al., Khim. Prir. Soedin., 1970, 6, 377; Chem. Nat. Compd. (Engl. Transl.), 386

### § Phaseoloside C

[化合物分類] テルペノイド (Terpenoids 構造は未知)

[一般的性質] Triterpene glycoside of unknown struct.

[天然基原] *Phaseolus vulgaris*

[その他のデータ] 物理化学的性質に関する事柄はない

-----文献-----

Chirva, V.Y. et al., Khim. Prir. Soedin., 1970, 6, 377; Chem. Nat. Compd. (Engl. Transl.), 386

### § Phaseothione

[化合物分類] テルペノイド (Terpenoids 構造は未知)

[一般的性質] Mercaptopeptide of unknown struct.

[天然基原] *Glycine max*, *Phaseolus limensis*, *Phaseolus vulgaris*, *Trifolium repens*

-----文献-----

Price, C.A., Nature (London), 1957, 180, 148, (分離)

### § Stigmasta-5,28-diene-3,24-diol; 3 $\beta$ -form, 3-O- $\beta$ -D-Glucopyranoside

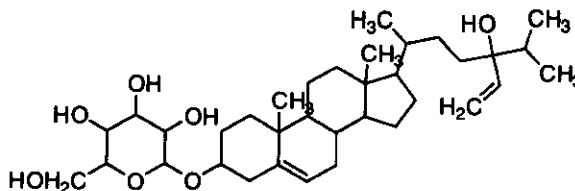
[化合物分類] ステロイド (Stigmastane steroids).

(C29).

[構造式]

[分子式]  $C_{35}H_{58}O_7$

[分子量] 590.839

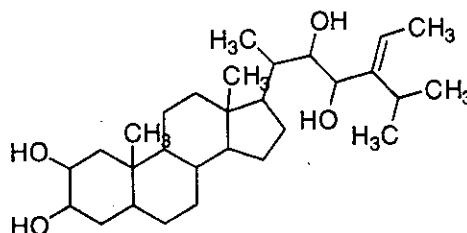


-----文献-----

Ikekawa, N. et al., Chem. Ind. (London), 1966, 1179  
 Kim, S.-K., J. Plant Biol., 1994, 37, 441; CA, 123, 79492b, (配糖体)

§ Stigmast-24 (28)-ene-2,3,22,23-tetrol; (2 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ ,22R,23R,24(28)E)-form

[化学名・別名] 6-Deoxohomodolichosterone  
 [CAS No.] 110345-06-7  
 [化合物分類] ステロイド (Stigmastane steroids). (C29)  
 [構造式]  
 [分子式] C<sub>29</sub>H<sub>50</sub>O<sub>4</sub>  
 [分子量] 462.712  
 [正確な分子量] 462.37091  
 [天然基原] *Phaseolus vulgaris* の種子  
 [性状] 結晶 (MeOH)  
 [融点] Mp 225-227 °C



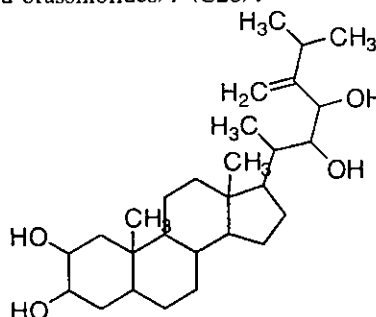
-----文献-----

Takatsuti, S. et al., J.C.S. Perkin 1, 1986, 2269  
 Yokota, T. et al., Agric. Biol. Chem., 1987, 51, 1625

§ 2,3,22,23-Tetrahydroxyergost-24 (28)-en-6-one; (2 $\alpha$ ,3 $\alpha$ ,5 $\alpha$ ,22R,23R)-form, 6-Deoxo

[化学名・別名] 5 $\alpha$ -Ergost-24 (28)-ene-2 $\alpha$ ,3 $\alpha$ ,22R,23R-tetrol (CAS 名). 6-Deoxodolichosterone  
 [CAS No.] 87833-55-4  
 [化合物分類] ステロイド (Ergostane steroids; excluding withanolides and brassinolides). (C28).  
 [構造式]

[分子式] C<sub>28</sub>H<sub>48</sub>O<sub>4</sub>  
 [分子量] 448.685  
 [正確な分子量] 448.35526  
 [天然基原] *Phaseolus vulgaris*, *Dolichos lablab*  
 [性状] 結晶 (EtOAc/MeOH)  
 [融点] Mp 219-220.5 °C  
 [比旋光度]:  $[\alpha]_D^{25} +33.2$  (c, 0.51 in MeOH)

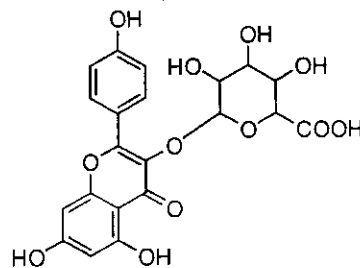


-----文献-----

Singh, H. et al., Indian J. Chem., Sect. B, 1986, 25, 989, (レビュー)  
 Adam, G. et al., Phytochemistry, 1986, 25, 1787, (レビュー)

§ 3,4',5,7-Tetrahydroxyflavone; 3-O- $\beta$ -D-Glucuronopyranoside

[化学名・別名] Kaempferol 3-glucuronoside  
 [CAS No.] 22688-78-4  
 [化合物分類] フラボノイド (Flavonols; 4 × O-置換基)  
 [構造式]  
 [分子式] C<sub>21</sub>H<sub>18</sub>O<sub>12</sub>  
 [分子量] 462.366  
 [正確な分子量] 462.07983  
 [天然基原] 次の植物から分離: *Euphorbia lathyris* の葉, *Euphorbia cyparissias*, *Anemone alpina*, *Phaseolus vulgaris*, その他多くの植物  
 [融点] Mp 189-190.5 °C



-----文献-----

Oesch, J. et al., J.C.S., 1914, 105, 2350, (分離)  
 Hasegawa, M., Acta Phytochim., 1940, 11, 299; CA, 35, 1403, (分離)  
 Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1497; 1498; 1504  
 Nakano, K. et al., Phytochemistry, 1983, 22, 1249, (分離)  
 The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

§ 2',4',5,7-Tetrahydroxyisoflavanone

§ 2',4',5,7-Tetrahydroxyisoflavanone

[化学名・別名] 2,3-Dihydro-5,7-dihydroxy-3-(2,4-dihydroxyphenyl)-4H-1-benzopyran-4-one (CAS 名).

Dalbergioidin

[CAS No.] 30368-42-4

[関連 CAS No.] 66152-08-7

[化合物分類] フラボノイド (Isoflavanones)

[構造式]

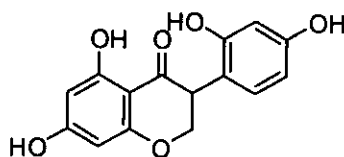
[分子式] C<sub>15</sub>H<sub>12</sub>O<sub>6</sub>

[分子量] 288.256

[正確な分子量] 288.06339

[天然基原] 次の植物から分離: *Dolichos biflorus*, *Lablab niger*, *Lespedeza cyrtobotrya*, *Macrotyloma axillare*, *Ougeinia dalbergioides*, *Phaseolus vulgaris*, *Stizolobium deeringianum* (すべてのマメ科, マメ亜科)

UV: [neutral] λ<sub>max</sub> 201 ; 289 ; 291 (ε 7000) (MeOH) (Berdy) [neutral] λ<sub>max</sub> 288 (ε 22000) (EtOH) (Berdy) [base] λ<sub>max</sub> 323 (MeOH-NAOH) (Berdy)



-----文献-----

Woodward, M.D., *Phytochemistry*, 1979, 18, 363, (分離)

Ingham, J.L., *Prog. Chem. Org. Nat. Prod.*, 1983, 43, 1, (レビュー, 生育)

§ 2',4',5,7-Tetrahydroxyisoflavone

[化学名・別名] 3-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one (CAS 名).

2'-Hydroxygenistein

[CAS No.] 1156-78-1

[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>15</sub>H<sub>10</sub>O<sub>6</sub>

[分子量] 286.24

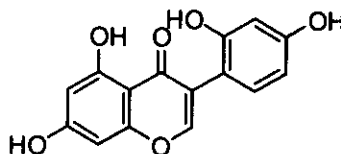
[正確な分子量] 286.04774

[天然基原] 次の植物から分離: *Apios tuberosa*, *Argyrocystis battandieri*, *Cajanus cajan*, *Crotalaria juncea*, *Dolichos biflorus*, *Hardenbergia violacea*, *Lablab niger*, *Laburnum anagyroides*, *Lupinus albus*, *Moghania macrophylla*, *Neonotonia wightii*, *Phaseolus vulgaris*, *Phaseolus coccineus*, *Spartium junceum*, *Stizolobium deeringianum* (すべてのマメ科, マメ亜科)

[性状] 結晶 (CHCl<sub>3</sub>/MeOH)

[融点] Mp 270-273 °C

UV: [neutral] λ<sub>max</sub> 209 ; 262 ; 288 (MeOH) (Berdy)



-----文献-----

Braz Filho, R. et al., *Phytochemistry*, 1976, 15, 1029, (分離, UV, IR, H-NMR, Mass, 誘導体)

Ingham, J.L., *Z. Naturforsch., C*, 1976, 31, 504; 1977, 32, 1018, (分離)

Prasad, J.S. et al., *Phytochemistry*, 1977, 16, 1120, (分離, UV, H-NMR, 構造決定)

Ingham, J.L., *Prog. Chem. Org. Nat. Prod.*, 1983, 43, 1, (レビュー, 生育)

Sanduja, R. et al., *J. Chem. Res., Synop.*, 1985, 56, (分離, 誘導体)

Adeesanya, S.A. et al., *Phytochemistry*, 1985, 24, 2699, (分離, 誘導体)

§ 2,3,22,23-Tetrahydroxy-25-methylergost-24(28)en-6-one; (2α,3α,5α,22R,23R)-form

[化学名・別名] 25-Methyldiolichosterone

[CAS No.] 111618-87-2

[化合物分類] ステロイド (Ergostane steroids; excluding withanolides and brassinolides). (C<sub>28</sub>).

[構造式]

[分子式] C<sub>29</sub>H<sub>48</sub>O<sub>5</sub>

[分子量] 476.695

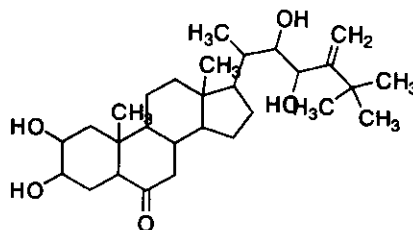
[正確な分子量] 476.350175

[天然基原] *Phaseolus vulgaris* の未熟な種子

[性状] 針状結晶 (MeOH)

[融点] Mp 254 °C (246-247 °C)

[比旋光度]: [α]<sub>D</sub><sup>22</sup> +4.3 (c, 0.13 in MeOH)



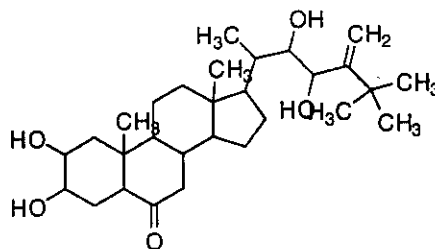
-----文献-----

§ 2,3,22,23-Tetrahydroxy-25-methylergost-24(28)en-6-one; (2 $\beta$ ,3 $\alpha$ ,5 $\alpha$ ,22R,23R)-form

[CAS No.] 121398-03-6

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

[構造式]



[分子式] C<sub>29</sub>H<sub>48</sub>O<sub>5</sub>

[分子量] 476.695

[正確な分子量] 476.350175

[天然基原] *Phaseolus vulgaris* の未熟な種子

-----文献-----

Kim, S.K. et al., Agric. Biol. Chem., 1987, 51, 2303, (分離)

Mori, K. et al., Annalen, 1988, 815, (合成法)

Japan. Pat., 1988, 88 255 297; CA, 111, 36804, (分離)

§ 2,3,22,23-Tetrahydroxy-25-methylergost-24(28)en-6-one; (2 $\beta$ ,3 $\beta$ ,5 $\alpha$ ,22R,23R)-form

[CAS No.] 114958-54-2

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

[構造式]

[分子式] C<sub>29</sub>H<sub>48</sub>O<sub>5</sub>

[分子量] 476.695

[正確な分子量] 476.350175

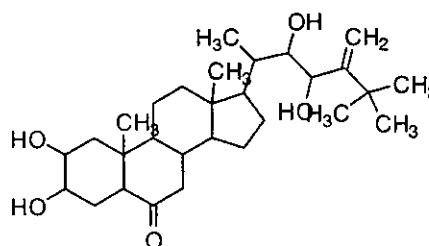
[天然基原] *Phaseolus vulgaris* の未熟な種子

[性状] プリズム結晶 (MeOH)

[融点] Mp 248 °C

[比旋光度]: [α]<sub>D</sub><sup>22</sup> +4.6 (c, 0.18 in CHCl<sub>3</sub>)

[その他のデータ] Sinters at 243 °C



-----文献-----

Kim, S.K. et al., Agric. Biol. Chem., 1987, 51, 2303, (分離)

Mori, K. et al., Annalen, 1988, 815, (合成法)

Japan. Pat., 1988, 88 255 297; CA, 111, 36804, (分離)

§ 2',4',5,7-Tetrahydroxy-8-prenylisoflavanone

[化学名・別名] 3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one (CAS名). Kievitone. Vignatin.

eolus substance II

[CAS No.] 40105-60-0

[化合物分類] フラボノイド (Isoflavanones)

[構造式]

[分子式] C<sub>20</sub>H<sub>20</sub>O<sub>6</sub>

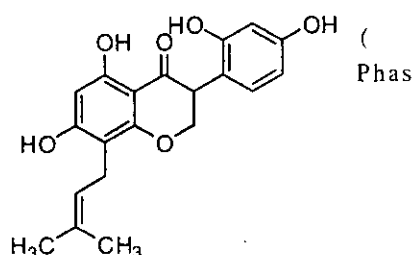
[分子量] 356.374

[正確な分子量] 356.12599

[天然基原] 次の植物から分離: *Dolichos biflorus*, *Lablab niger*, *Macroptilium atropurpureum*, *Macrotyloma axillare*, *Mucuna utilis*, *Phaseolus aureus*, *Phaseolus calcaratus*, *Phaseolus lunatus*, *Phaseolus vulgaris*, *Stizolobium deeringianum*, *Vigna unguiculata* (すべてのマメ科, マメ亜科)

[溶解性] BERDY SOL: メタノール, 塩基, エーテルに可溶; 水, ヘキサンに難溶

UV: [neutral] λ<sub>max</sub> 210; 293 (ε 16600); 330 (ε 3800); 340 (MeOH) (Berdy)



-----文献-----

Burden, R.S. et al., Tet. Lett., 1972, 4175, (分離)

Kuhn, P.J. et al., Phytochemistry, 1977, 16, 296, (Kievitone hydrate)

Ingham, J.L., Prog. Chem. Org. Nat. Prod., 1983, 43, 1, (レビュー, 生育)

O'Neill, M.J. et al., Phytochemistry, 1986, 25, 1315, (Kievitol, 5-Deoxykievitol)

§ 2',4',5,7-Tetrahydroxy-8-prenylisoflavanone; 5-Deoxy

[化学名・別名] 2',4',7-Trihydroxy-8-prenylisoflavanone. 5-Deoxykievitone

[CAS No.] 74161-24-3

[化合物分類] フラボノイド (Isoflavanones)

[構造式]

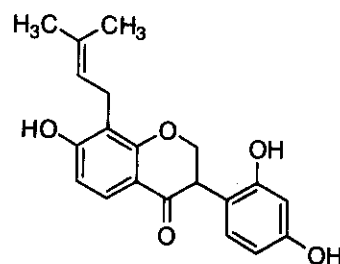
[分子式] C<sub>20</sub>H<sub>20</sub>O<sub>5</sub>

[分子量] 340.375

[正確な分子量] 340.131075

[天然基原] 次の植物のさやから分離: *Phaseolus vulgaris*, *Phaseolus mungo*

UV: [neutral] λ<sub>max</sub> 286 (MeOH) (Berdy) [base] λ<sub>max</sub> 340 (MeOH-NAOH) (Berdy)



-----文献-----

Burden, R.S. et al., Tet. Lett., 1972, 4175, (分離)

Granamanickam, S.S., Experientia, 1979, 35, 323, (分離)

Ingham, J.L., Prog. Chem. Org. Nat. Prod., 1983, 43, 1, (レビュー, 生育)

§ 2',4',5,7-Tetrahydroxy-3'-prenylisoflavone

[化学名・別名] [2,4-Dihydroxy-3-(3-methyl-2-butenyl) phenyl]-5,7-dihydroxy-4H-1-benzopyran-4-one (CAS名). 3'-Isopentenyl-2',4',5,7-tetrahydroxyisoflavone. Licoisoflavone A. Phaseoluteone

[CAS No.] 66056-19-7

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

[構造式]

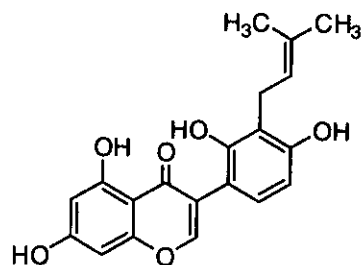
[分子式] C<sub>20</sub>H<sub>18</sub>O<sub>6</sub>

[分子量] 354.359

[正確な分子量] 354.11034

[天然基原] *Glycyrrhiza* spp.の根, また *Hardenbergia violacea*, *Phaseolus vulgaris*

[性状] 青白い黄色のプリズム結晶 (MeOH 溶液)



-----文献-----

Kinoshita, T. et al., Chem. Pharm. Bull., 1978, 26, 141, (分離, 構造決定)

Komatsu, M. et al., Chem. Pharm. Bull., 1978, 26, 3863, (Sophoraisoflavanone A)

Woodward, M.D., Phytochemistry, 1979, 18, 363, (分離, UV, H-NMR, IR)

Tsukayama, M. et al., Bull. Chem. Soc. Jpn., 1985, 58, 136, (合成法)

Shibuya, Y. et al., Z. Naturforsch., C, 1991, 46, 513, (配糖体)

§ 2',4',5,7-Tetrahydroxy-8-prenylisoflavone

[化学名・別名] 2,3-Dehydrokievitone

[CAS No.] 74161-25-4

[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>20</sub>H<sub>18</sub>O<sub>6</sub>

[分子量] 354.359

[正確な分子量] 354.11034

[天然基原] 次の植物から分離: *Lupinus luteus*, *Phaseolus lunatus*,

*Phaseolus aureus*, *Phaseolus vulgaris*

UV: [neutral] λ<sub>max</sub> 265 (MeOH) (Berdy) [base] λ<sub>max</sub> 281 (MeOH-NAOH) (Berdy)

[傷害・毒性] BERDY HAZD : 50 %致死量 (LD<sub>50</sub>) (マウス, 静脈内) 83 mg/kg, 50 %致死量 (LD<sub>50</sub>) (マウス, 腹膜内) 3.2 mg/kg

[化学物質毒性データ総覧 (RTECS) 登録番号] DJ2982700

-----文献-----

O'Neill, M.J. et al., Phytochemistry, 1986, 25, 1315, (2,3-Dehydrokievitone)

\*\*\*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).

被験動物 : げっ歯類-マウス.  
投与量・期間 : 830 ug/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

"CRC Handbook of Antibiotic Compounds," 12,351,1985

§ Thymidine (旧 CAS 名)

[化学名・別名] 1-(2-Deoxy-β-D-erythro-pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione (CAS 名). 1-(2-Deoxy-β-D-ribofuranosyl)-5-methyluracil. Thymine 2-desoxyribose. Thymosine. NSC 21548

[CAS No.] 50-89-5

[関連 CAS No.] 50-88-4

[化合物分類] 炭水化物 (Nucleosides)

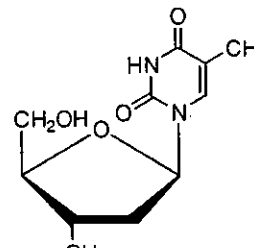
[構造式]

[分子式] C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O<sub>5</sub>

[分子量] 242.231

[正確な分子量] 242.090273

[天然基原] 植物基原から分離, 例えば, *Phaseolus vulgaris* の発芽種子. DNA の主成分



[融点] Mp 186-187 °C

[比旋光度]: [α]<sub>D</sub><sup>25</sup> +18.5 (H<sub>2</sub>O). [α]<sub>D</sub><sup>25</sup> +30.6 (c, 1.0 in H<sub>2</sub>O)

[PKa 値] pK<sub>a1</sub> 9.8; pK<sub>a2</sub> 12.9 (25 °C)

[その他のデータ] λ<sub>max</sub> 267 (ε 9 700) and 206.5 nm (9 800) (pH 7.2)

[傷害・毒性] 催奇形成作用に関する研究がある (多量投与時), ヒトにおいて有害作用 (多量投与時), 抗腫瘍性剤 (and in co-administration with methotrexate, see Methotrexate). 50 % 致死量 (LD<sub>50</sub>) (マウス, 腹膜内) 2512 mg/kg

[化学物質毒性データ総覧 (RTECS) 登録番号] XP2071000

[販売元] Aldrich:85500-6; Fluka:89270; Sigma:J5273

§ 2',4',7-Trihydroxyisoflavan

[化学名・別名] 4-(3,4-Dihydro-7-hydroxy-2H-1-benzopyran-4-yl)-1,3-benzenediol (CAS 名). 3,4-Dihydro-3-(2,4-dihydroxyphenyl)-7-hydroxy-2H-1-benzopyran. Demethylvestitol

[CAS No.] 65332-45-8

[関連 CAS No.] 64190-84-7, 75556-92-2

[化合物分類] フラボノイド (Isoflavans)

[構造式]

[分子式] C<sub>15</sub>H<sub>10</sub>O<sub>4</sub>

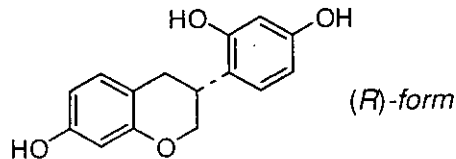
[分子量] 258.273

[正確な分子量] 258.08921

[一般的性質] Compds. in both enantiomeric series appear to occur naturally but in most cases the abs. config. was not detd.

[天然基原] 次の植物から分離: *Anthyllis vulneraria*, *Erythrina sandwicensis*, *Hosackia americana*, *Lablab niger*, *Lotus* spp., *Phaseolus vulgaris*, *Tetragonolobus* spp. as a phytoalexin

UV: [neutral] λ<sub>max</sub> 209; 283 (EtOH) (Berdy) [base] λ<sub>max</sub> 219; 297 (EtOH-NaOH) (Berdy)



(R)-form

-----文献-----

Braz Filho, R. et al., *Phytochemistry*, 1975, 14, 1454, (分離)

Ingham, J.L. et al., *Phytochemistry*, 1977, 16, 1279; 1979, 18, 1711, (分離, 構造決定)

Ingham, J.L. et al., *Prog. Chem. Org. Nat. Prod.*, 1983, 43, 1, (レビュー, 生育)

Herath, H.M.T.B. et al., *Phytochemistry*, 1998, 47, 117-119, (分離, H-NMR, C13-NMR)

§ 2',4',7-Trihydroxyisoflavanone; (±)-form

[化合物分類] フラボノイド (Isoflavanones)

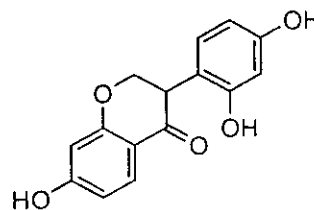
[構造式]

[分子式] C<sub>15</sub>H<sub>10</sub>O<sub>3</sub>

[分子量] 272.257

[正確な分子量] 272.068475

[天然基原] 次の植物から分離: *Phaseolus vulgaris* のさや, また *us coccineus* から得られる



*Phaseol*

*Phaseolus coccineus* から得られる

-----文献-----

Woodward, M.D., *Phytochemistry*, 1980, 19, 921, (分離, UV, H-NMR)

Ingham, J.L., *Planta Med.*, 1982, 45, 46, (分離)

Adesanya, S.A. et al., *Phytochemistry*, 1985, 24, 2699, (分離)

Jain, A.C. et al., *Indian J. Chem., Sect. B*, 1987, 26, 136, (合成法)

§ 2',4',7-Trihydroxyisoflavone

[化学名・別名] 3-(2,4-Dihydroxyphenyl)-7-hydroxy-4H-1-benzopyran-4-one (CAS 名). 2'-Hydroxydaidzein

[CAS No.] 7678-85-5

[化合物分類] フラボノイド (Isoflavones; 3 × O-置換基)

[構造式]

[分子式]  $C_{15}H_{10}O_5$

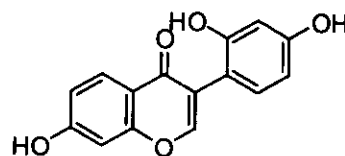
[分子量] 270.41

[正確な分子量] 270.052825

[天然基原] 次の植物から分離: pods of *Phaseolus vulgaris*, *Phaseolus lunatus*

[性状] 結晶 (MeOH)

[融点] Mp 275 °C で分解 (synthetic)



-----文献-----

O'Neill, M.J. et al., *Phytochemistry*, 1986, 25, 1315, (分離)

§ 9,10,13-Trihydroxyoctadecanoic acid

[化学名・別名] 9,10,13-Trihydroxystearic acid

[CAS No.] 50439-74-2

[化合物分類] 脂肪族化合物 (Saturated unbranched carboxylic acids and lactones)

[構造式]  $H_3C(CH_2)_4CH(OH)CH_2CH_2CH(OH)CH(OH)(CH_2)_7COOH$

[分子式]  $C_{18}H_{36}O_5$

[分子量] 332.479

[正確な分子量] 332.256275

[天然基原] *Phaseolus vulgaris* の根

[用途] Hatching stimulant of nematode eggs

[融点] Mp 135-137 °C

-----文献-----

Takasugi, M. et al., *Chem. Lett.*, 1973, 445, (分離, H-NMR, Mass)

§ § マメ科ソラマメ (*Vicia faba* L.) の果実, 種子または発芽種子 (モヤシ)。

§ Abscisic acid; (S)-form, 14-Hydroxy

[化学名・別名] Nigellinic acid

[CAS No.] 91897-25-5

[化合物分類] テルペノイド (Cyclofarnesane sesquiterpenoids)

[構造式]

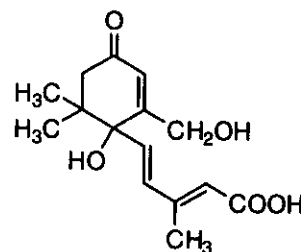
[分子式]  $C_{15}H_{20}O_5$

[分子量] 280.32

[正確な分子量] 280.131075

[天然基原] 次の植物から分離: *Xanthium strumarium*, *Nigella damascena*, *Vicia faba* の葉

[性状] ガム



-----文献-----

Boyer, G.L. et al., *Phytochemistry*, 1986, 25, 1103, (Nigellinic acid)

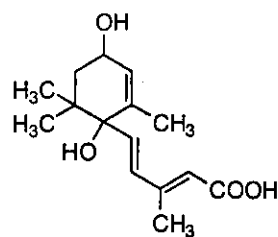
§ Abscisic acid; (S)-form, 3 α-Alcohol

[化学名・別名] 4'-Dihydroabscisic acid

[CAS No.] 84026-26-6

[化合物分類] テルペノイド (Cyclofarnesane sesquiterpenoids)

[構造式]



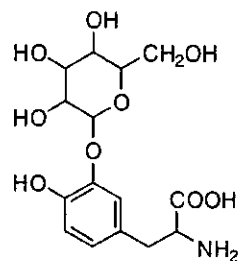
[分子式]  $C_{15}H_{22}O_4$   
 [分子量] 266.336  
 [正確な分子量] 266.15181  
 [天然基原] 次の植物から分離: ソラマメ (*Vicia faba*) の未熟な種子

-----文献-----

Dathe, W. et al., *Phytochemistry*, 1982, 21, 1798, (4'-Dihydroabscisic acid)

§ 2-Amino-3-(3,4-dihydroxyphenyl) propanoic acid; (S)-form, 3'-O-β-D-Glucopyranoside

[CAS No.] 2275-95-8  
 [化合物分類] アミノ酸とペプチド (Non-protein α-aminoacids)  
 [構造式]



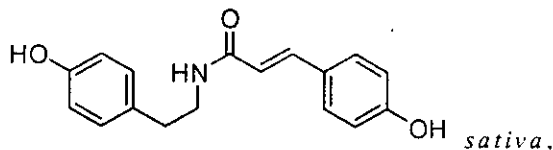
[分子式]  $C_{15}H_{21}NO_9$   
 [分子量] 359.332  
 [正確な分子量] 359.121634  
 [天然基原] 次の植物から分離: *Pisum sativum*, *Vicia faba*  
 [性状] 樹脂もしくはシロップ

-----文献-----

Fellman, J.H. et al., *Biochim. Biophys. Acta*, 1975, 381, 9, (分離, 誘導體)  
 Bartholini, G. et al., *Pharmacol. Ther.*, Part B, 1975, 1, 407, (レビュー, 薬理)  
 Gomez, R. et al., *Anal. Profiles Drug Subst.*, 1976, 5, 189, (レビュー)  
 Nutt, J.G. et al., *Clin. Neuropharmacol.*, 1984, 7, 35, (レビュー, 代謝)  
 Laycock, M.V. et al., *J. Nat. Prod.*, 1984, 47, 1033, (分離, sulfate)

§ 4-(2-Aminoethyl) phenol; N-(4-Hydroxy-E-cinnamoyl)

[化学名・別名] *N-p-trans-Coumaroyltyramine*. *N-(p-Hydroxyphenyl) ethyl p-hydroxycinnamide*. Papazaine  
 [CAS No.] 36417-86-4  
 [化合物分類] アルカロイド化合物 (Cinnamic acid amides), アルカロイド化合物 (Simple tyramine alkaloids)  
 [構造式]



[分子式]  $C_{17}H_{17}NO_3$   
 [分子量] 283.326  
 [正確な分子量] 283.120844  
 [天然基原] *Actinodaphne* spp., *Allium chinense*, *Cannabis*  
*Evodia belahe*, *Fumaria indica*, *Vicia faba*

[性状] 結晶 (MeOH)

[融点] Mp 260-261 °C

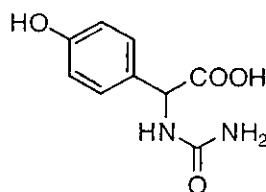
[傷害・毒性] 50 % 致死量 (LD<sub>50</sub>) (マウス, 腹膜内) 780 mg/kg

-----文献-----

Butenandt, A. et al., *Arch. Biochem. Biophys.*, 1959, 83, 76, (*N*-Acetyltyramine)  
 Rondest. J. et al., *Bull. Soc. Chim. Fr.*, 1968, 2411-2414, (*N*-4-hydroxycinnamoyl)

§ 2-Amino-2-(4-hydroxyphenyl) acetic acid; (±)-form, N-Carbamoyl

[CAS No.] 32507-69-0  
 [その他の CAS No.] 72500-37-9  
 [化合物分類] アミノ酸とペプチド (Non-protein α-aminoacids)  
 [構造式]



[分子式]  $C_9H_{10}N_2O_3$

[分子量] 210.189

[正確な分子量] 210.064058

[天然基原] 次の植物の葉から分離: *Vicia faba*

-----文献-----

Larsen, P.O. et al., *Biochim. Biophys. Acta*, 1975, 381, 397-408, (分離)  
 Smith, G.A. et al., *J.C.S. Perkin 1*, 1975, 2108-2115, (分離)



Blackburn, K.J. et al., Br. J. Pharmacol., 1979, 66, 443P-444P, (薬理)  
McGahren, W.J. et al., J.A.C.S., 1980, 102, 1671-1684, (分離)  
Yoshioka, R. et al., Bull. Chem. Soc. Jpn., 1987, 60, 649-652, (分割, 成書)

§ Arginine; (S)-form, N<sup>2</sup>-(3-Carboxy-2-hydroxypropanoyl)

[化学名・別名] N<sup>2</sup>-(2-Hydroxysuccinoyl) arginine. N<sup>2</sup>-(3-Carboxy-2-hydroxy-1-oxopropyl) arginine

[CAS No.] 87605-92-3

[化合物分類] アミノ酸とペプチド (Non-protein α-aminoacids)

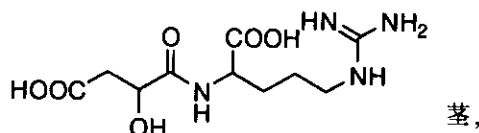
[構造式]

[分子式] C<sub>10</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>

[分子量] 290.275

[正確な分子量] 290.122636

[天然基原] the seeds of *Vicia faba* の種子, *Smilax china* の塊  
リンゴとセイヨウナシの木のシュート



-----文献-----

Greenstein, J.P. et al., Chemistry of the Amino Acids, Wiley, N.Y., 1961, 3, 1841, (レビュー)  
Weisburger, J.H. et al., Toxicol. Appl. Pharmacol., 1969, 14, 163-175, (arginine glutamate, 薬理)  
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2392, (生育)  
Kasai, T. et al., Phytochemistry, 1983, 22, 147-149; 1984, 23, 19-22, (N-succinoyl derivs)  
Zieve, L. et al., Metab. Brain Dis., 1986, 1, 25-35; 1989, 4, 113-120, (arginine glutamate, 薬理, 毒)  
Velianou, J.L. et al., Expert Opin. Invest. Drugs, 1999, 8, 1785-1793, (レビュー)

§ Brassinolide; 24-Epimer

[化学名・別名] 24-Epibrassinolide. Epibrassinolide R

[CAS No.] 78821-43-9

[化合物分類] ステロイド (Withanolide and brassinolide steroids). (C28).

[構造式]

[分子式] C<sub>28</sub>H<sub>48</sub>O<sub>6</sub>

[分子量] 480.684

[正確な分子量] 480.34509

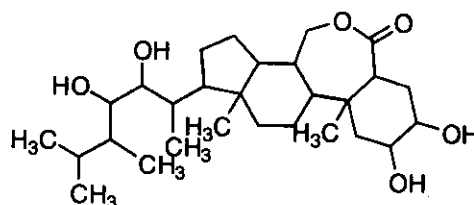
[天然基原] *Vicia faba* の花粉

[用途] 植物成長促進剤

[性状] 結晶

[融点] Mp 256-258 °C

[販売元] Sigma:E1641



-----文献-----

Ikekawa, N. et al., Chem. Pharm. Bull., 1988, 36, 405, (24-epi-Brassinolide)

§ 4-Chlorotryptophan; (S)-form

[化学名・別名] L-form

[CAS No.] 52448-14-3

[化合物分類] アミノ酸とペプチド (Non-protein α-aminoacids)

[構造式]

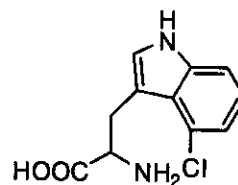
[分子式] C<sub>11</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>2</sub>

[分子量] 238.673

[正確な分子量] 238.050905

[天然基原] 次の植物から分離: *Achromobacter petrophilum* の細菌培養, エンドウ豆 *Pisum sativum* の種子  
タンパク. また *Vicia faba* の種子からも得られる

[比旋光度]: [α]<sub>D</sub><sup>25</sup> -45 (c, 0.13 in AcOH 溶液)



-----文献-----

Marumo, S. et al., Planta, 1970, 90, 208, (分離)  
Japan. Pat., 1973, 73 98 091; CA, 80, 106876g, (分離)  
Thiruvikraman, S.V. et al., Tet. Lett., 1988, 29, 2339, (分離, 合成法)  
Fock, A. et al., Phytochemistry, 1992, 31, 2327, (分離)

§ Cucurbitic acid; 6,7-Diepimer

[化学名・別名] 6-Epi-7-isocucurbit acid

[CAS No.] 120330-52-1

[化合物分類] 脂肪族化合物 (Monocarbocyclic carboxylic acids and lactones)

[構造式]

[分子式]  $C_{12}H_{20}O_3$

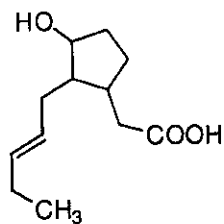
[分子量] 212.288

[正確な分子量] 212.141245

[天然基原] *Vicia faba*. また *Equisetum* sp., *Juglans regia* から分離される

[性状] オイル

[比旋光度]:  $[\alpha]_D^{22} +6.1$  (c, 0.1 in EtOH)



-----文献-----

Fukui, H. et al., Agric. Biol. Chem., 1977, 41, 175, (分離)

Miersch, O. et al., Phytochemistry, 1989, 28, 339; 1999, 50, 517-523, (分離)

Fujita, T. et al., Biosci., Biotechnol., Biochem., 1996, 60, 732-735, (配糖体, H-NMR, C13-NMR)

### § 2,4-Diamino-5,6-dihydroxypyrimidine; 5-O-β-D-Glucopyranoside

[化学名・別名] Vicine †, Vicoside

[CAS No.] 152-93-2

[化合物分類] アルカロイド化合物

(Pyrimidines)

[構造式]

[分子式]  $C_{10}H_{16}N_4O_7$

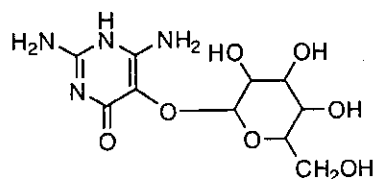
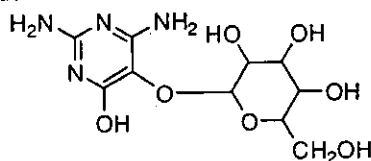
[分子量] 304.259

[正確な分子量] 304.101901

[天然基原] 次の植物から分離: ベッチ (*Vicia sativa*), *Vicia faba*, その他のマメ科植物

[融点] Mp 243-244 °C で分解

[比旋光度]:  $[\alpha]_D^{20} -11.7$  (0.2 M NaOH)



物

-----文献-----

Bendich, A. et al., Biochim. Biophys. Acta, 1953, 12, 462, (分離, 構造決定)

Dutta, P.K. et al., Indian J. Chem., Sect. B, 1981, 20, 669, (分離, H-NMR, C13-NMR)

Kunesch, N. et al., Annalen, 1994, 1059, (合成法, Vicine)

### § Di-4-coumaroylputrescine

[化学名・別名] *N,N'*-1,4-Butanediylbis[3-(4-hydroxyphenyl)-2-propenamamide] (CAS 名). *N,N'*-Bis(4-hydroxycinnamoyl)-1,4-butanediamine

[CAS No.] 37946-59-1

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

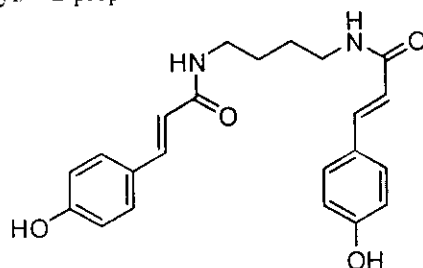
[構造式]

[分子式]  $C_{22}H_{22}N_2O_4$

[分子量] 380.443

[正確な分子量] 380.173608

[天然基原] 次の植物に含まれるアルカロイド: *Dianthus caryophyllus*, *Helianthus annuus*, *Nicotiana tabacum*, *Pyrus communis*, *Rubus idaeus*, *Vicia faba* (ナデシコ科, キク科, ナス科, パラ科, マメ科)



-----文献-----

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

Cabanne, F. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1976, 282, 1959, (UV, 構造決定, Dicafeoylputrescine)

Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927, (生育, 誘導体)

### § Di-4-coumaroylputrescine; 3,3'-Dimethoxy

[化学名・別名] Diferuloylputrescine. *N,N'*-Bis(4-hydroxy-3-methoxycinnamoyl)-1,4-butanediamine

[CAS No.] 42369-86-8

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

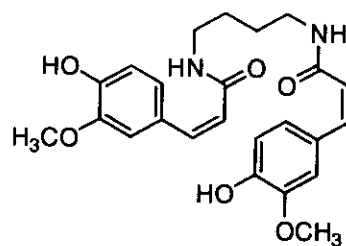
[構造式]

[分子式]  $C_{25}H_{35}N_3O_6$

[分子量] 440.495

[正確な分子量] 440.194738

[天然基原] 次の植物に含まれるアルカロイド: *Ananas comosus*, *Triticum vulgare*, *Gomphrena globosa*, *Dianthus caryophyllus*, *Vicia faba*, *Lycopersicon esculentum*, *Petunia* sp., *Nicotiana tabacum* (パイナップル科, イネ科, ヒユ科, ナデシコ科, マメ科, ナス科)



-----文献-----

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

Cabanne, F. et al., C. R. Hebd. Seances Acad. Sci. Ser. D, 1976, 282, 1959, (UV, 構造決定, Dicafeoylputrescine)

Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927, (生育, 誘導体)

### § $N^1, N^{10}$ -Dicoumaroylspermidine

[化学名・別名]  $N^1, N^{10}$ -Bis(4-hydroxycinnamoyl) spermidine

[CAS No.] 65715-79-9

[関連 CAS No.] 101330-61-4

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

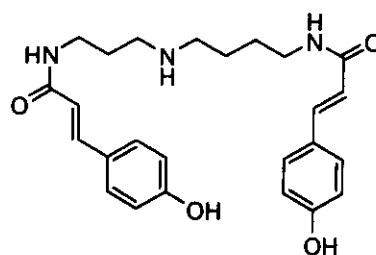
[構造式]

[分子式]  $C_{25}H_{31}N_3O_6$

[分子量] 437.538

[正確な分子量] 437.231457

[天然基原] 次の植物に含まれるアルカロイド: *Dianthus caryophyllus*, *Helianthus annuus*, *Aesculus hippocastanum*, *Vicia faba*, *Pyrus communis* (ナデシコ科, トチノキ科, マメ科, パラ科, ナス科)



-----文献-----

Deleacutetang, J., Ann. Tab., Sect. 2, 1974, 11, 123; CA, 84, 147656m, (UV, H-NMR, 構造決定, Dicafeoylspermidine)

Cabanne, F. et al., Physiol. Veg., 1977, 15, 429; CA, 88, 86095m, (UV, 構造決定)

Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927, (生育)

Meurer, B. et al., Phytochemistry, 1986, 25, 433, (Caffeoylferuloylspermidine, Diferuloylspermidine)

### § $N^1, N^{10}$ -Dicoumaroylspermidine; 3',3''-Dimethoxy

[化学名・別名]  $N^1, N^{10}$ -Diferuloylspermidine

[CAS No.] 70185-61-4

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

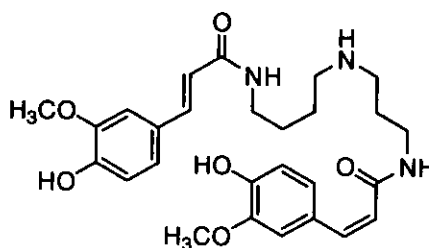
[構造式]

[分子式]  $C_{27}H_{33}N_3O_6$

[分子量] 497.59

[正確な分子量] 497.252587

[天然基原] 次の植物に含まれるアルカロイド: *Corylus avellana* の花粉, また *Ananas comosus*, *Dianthus caryophyllus*, *Vicia faba*, *Lunaria esculentum* (Corylaceae, パイナップル科, ナデシコ科, マメ科, ナス科)  
[その他のデータ] Only the alkaloid from *C. avellana* has been shown to have the exact struct. shown. The other isolates are diferuloylspermidine with undefined regioisomerism (i.e. could be N 5 -substituted)



-----文献-----

Deleacutetang, J., Ann. Tab., Sect. 2, 1974, 11, 123; CA, 84, 147656m, (UV, H-NMR, 構造決定, Dicafeoylspermidine)

Cabanne, F. et al., Physiol. Veg., 1977, 15, 429; CA, 88, 86095m, (UV, 構造決定)

Martin-Tanguy, J. et al., Phytochemistry, 1978, 17, 1927, (生育)

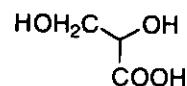
Meurer, B. et al., Phytochemistry, 1986, 25, 433, (Caffeoylferuloylspermidine, Diferuloylspermidine)

### § 2,3-Dihydroxypropanoic acid; (R)-form

[化学名・別名] D-form

[CAS No.] 6000-40-4

[化合物分類] 脂肪酸化合物 (Saturated unbranched carboxylic acids and lactones)



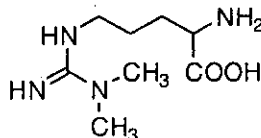
[分子式] C<sub>3</sub>H<sub>7</sub>O<sub>2</sub>  
[分子量] 106.078  
[正確な分子量] 106.02661  
[天然基原] 色々な植物から分離, 例えば, *Vicia faba*, クレソン  
[用途] 植物代謝周期の中間体  
[性状] 厚みのあるガム  
[その他のデータ] Dec. on dist. Laevorotatory

-----文献-----

Sallach, J.A.C.S., 1952, 74, 2415, (合成法, 成書)  
Isherwood, F.A. et al., Biochem. J., 1954, 56, 15, (分離)

### § N<sup>ε</sup>, N<sup>ε</sup>-Dimethylarginine; (S)-form

[化学名・別名] L-form  
[CAS No.] 30315-93-6  
[その他の CAS No.] 65005-57-4  
[化合物分類] アミノ酸とペプチド (Non-protein α-aminoacids)  
[構造式]



[分子式] C<sub>8</sub>H<sub>18</sub>N<sub>4</sub>O<sub>2</sub>  
[分子量] 202.256  
[正確な分子量] 202.142976  
[天然基原] 次の植物から分離: ソラマメの種子 (*Vicia faba*), ヒトの尿  
[性状] 結晶 (EtOH 溶液) (as hydrochloride)  
[融点] Mp 198-201 hydrochloride °C

-----文献-----

Hempel, K. et al., Naturwissenschaften, 1968, 55, 37, (分離)  
Kakimoto, Y. et al., J. Biol. Chem., 1970, 245, 5751, (分離, 合成法)  
Nakajima, T. et al., Biochim. Biophys. Acta, 1971, 230, 212; 243, 31, (分離)  
Kasai, T. et al., Agric. Biol. Chem., 1976, 40, 2449, (分離, 合成法, H-NMR, IR)  
Paik, W.K. et al., Amino Acids, 1993, 4, 267, (レビュー, 生合成, 代謝)

### § Epinine

[化学名・別名] 4-[2-(Methylamino)ethyl]-1,2-benzenediol (CAS 名), 4-[2-(Methylamino)ethyl]pyrocatechol (旧 CAS 名), 4-(β-Methylaminoethyl)catechol, N-Methyl-2-(3,4-dihydroxyphenyl)ethylamine, Deoxyadrenaline, Desoxyepinephrine, N-Methyldopamine

[CAS No.] 501-15-5  
[化合物分類] 薬物: 心正変力剤 (Inotropic agents), 薬物: ドーパミン受容体作用薬 (Dopamine receptor agonists), 薬物: 血管拡張剤 (Vasodilators), アルカロイド化合物 (Simple tyramine alkaloids), 薬物: β-アドレナリン受容体作用薬 (β-Adrenoceptor agonists), 薬物: α-アドレナリン受容体作用薬 (α-Adrenoceptor agonists)

[構造式]

[分子式] C<sub>9</sub>H<sub>13</sub>NO<sub>2</sub>  
[分子量] 167.207  
[正確な分子量] 167.094629

[天然基原] 次の植物に含まれるアルカロイド: *Cytisus scoparius*, *Vicia faba*,  
*Lophora williamsii* (マメ科, サボテン科)

[代謝] Active metab. of DMQ55-G

[用途] ドーパミン D<sub>1</sub>-, D<sub>2</sub>-作用薬, α-, β-アドレナリン受容体作用薬, 明確な心正変力剤, 血管拡張剤

[性状] 結晶 (EtOH)

[融点] Mp 188-189 °C

[Log P 計算値] Log P 0.16 (計算値)



-----文献-----

Path. P.N. et al., J. Pharmacol. Exp. Ther., 1967, 155, 1, (薬理)  
Tocher, R.D. et al., Phytochemistry, 1972, 11, 1161, (分離)  
Giesecke, J., Acta Cryst. B, 1976, 32, 2337, (結晶構造)  
Smith, T.A., Phytochemistry, 1977, 16, 9, (レビュー, 生育)  
Van Woerkens, L.J. et al., Br. J. Pharmacol., 1992, 107, 303, (薬理)  
Ianneli, S. et al., Acta Cryst. C, 1995, 51, 1338, (結晶構造, phosphate)  
Daul, A. et al., Naunyn-Schmiedeberg's Arch. Pharmacol., 1995, 352, 429, (薬理)