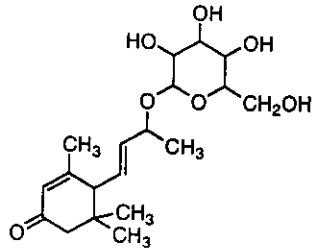
§ 4,7-Megastigmadiene-3,9-diol; (3*S*,7*E*,9*S*)-form, 3-Ketone, 9-*O*-β-D-glucopyranoside
[化合物分類]テルペノイド(Megastigmane norterpenoids)
[構造式]

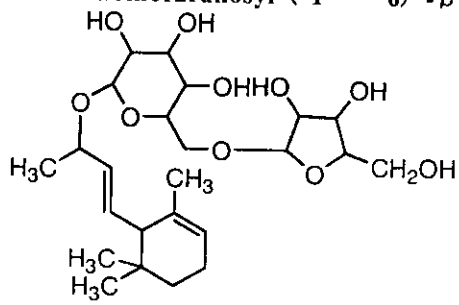


[分子式]$C_{19}H_{30}O_7$
[分子量]370.442
[基原]ブラックベリー(*Rubus idaeus*), ダルメシアンセージ(*Salvia officinalis*)の葉
[性状]無定型の粉末

----------文 献----------

Murakami, T. et al., Chem. Pharm. Bull., 1981, 29, 866-868, (3-ketone 9-glucoside)
De Tommasi, N. et al., J. Nat. Prod., 1992, 55, 1025, (配糖体)
Wang, M. et al., J. Agric. Food Chem., 1998, 46, 2509-2511, (3-ketone glucoside, 分離, NMR)

§ 4,7-Megastigmadien-9-ol; (6*R*,7*E*,9*R*)-form, *O*-[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]
[化合物分類]テルペノイド(Megastigmane norterpenoids)
[構造式]

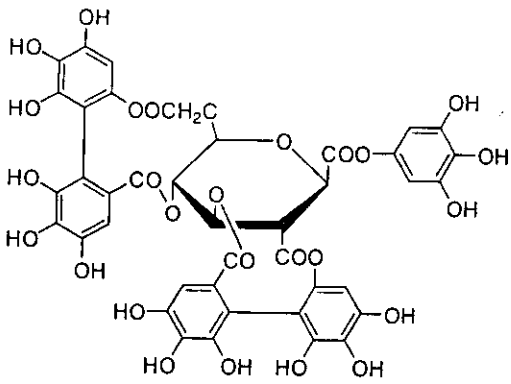


[分子式]$C_{24}H_{40}O_{10}$
[分子量]488.574
[基原]*Rubus idaeus* の果実

----------文 献----------

Aasen, A.J. et al., Acta Chem. Scand., 1973, 27, 2107, (Ac)
Pabst, A. et al., Phytochemistry, 1992, 31, 2043, (分離, H-NMR, C13-NMR, 合成法)

§ Pedunculagin; 1-*O*-(3,4,5-Trihydroxybenzoyl)(1β-)
[化学名・別名]1-*O*-Galloylpedunculagin
[化合物分類]タンニン化合物(Hexahydroxydiphenoyl ester tannins)
[構造式]

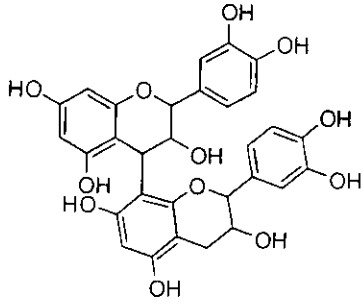


[分子式]$C_{41}H_{28}O_{26}$
[分子量]936.657
[基原]次の植物から得られるタンニン: *Rosa canina*, *Quercus infectoria*, *Rubus fruticosus*, *Rubus idaeus*
[性状]淡褐色の無定型粉末・一水和物
[比旋光度]:$[\alpha]_D^{20}$ +34.9 (c, 0.6 in MeOH)

----------文 献----------

Gupta, R.K. et al., J.C.S. Perkin 1, 1982, 2525, (1-*O*-Galloylpedunculagin)

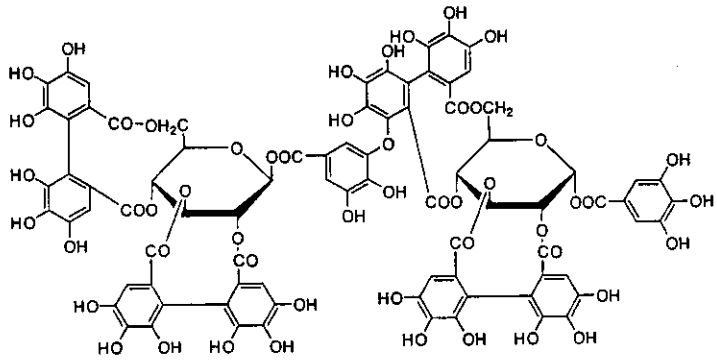
§ 3,3',4',5,7-Pentahydroxyflavan(4→8)-3,3',4',5,7-pentahydroxyflavan; (2*R*,2'*R*,3*S*,3'*R*,4*S*)-form
[化学名・別名]Procyanidin B4. Catechin(4α→8)epicatechin
[CAS No.]29106-51-2
[化合物分類]フラボノイド(Proanthocyanidin flavonoids), フラボノイド(Neoflavonoids)
[構造式]



[分子式]$C_{30}H_{26}O_{12}$
[分子量]578.528
[基原]*Rubus fruticosus* (ブラックベリー), *Rubus idaeus*
[性状]結晶 (EtOH) (as deca-Ac)
[融点]Mp 172-173℃ (deca-Ac)
[比旋光度]:$[\alpha]_D$ -194 (EtOH)

The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Bae, Y.-S. et al., Phytochemistry, 1994, 35, 473, (Procyanidin B_3 3-glucoside)

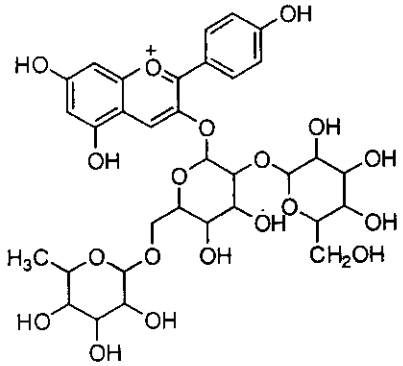
§ Sanguiin H6



[CAS No.]82978-00-5
[化合物分類]タンニン化合物
(Sanguisorbyl ester tannins)
[構造式]
[分子式]$C_{82}H_{54}O_{52}$
[分子量]1871.297
[一般的性質]構造式は 1985 年に改正され
[基原]次の植物から得られるタンニン: *Sanguisorba officinalis, Rubus chingii, Rubus fruticosus, Rubus idaeus*
[性状]褐色の無定型粉末
[比旋光度]:$[\alpha]_D$ +72 (Me_2CO)

文献
Nonaka, G. et al., Chem. Pharm. Bull., 1982, 30, 2255, (分離)
Gupta, R.K. et al., J.C.S. Perkin 1, 1982, 2525, (H-NMR, C13-NMR)
Tanaka, T. et al., J. Chem. Res., Synop., 1985, 176, (構造決定)
Tanaka, T. et al., Chem. Pharm. Bull., 1993, 41, 1214, (Lambertianin A, Lambertianin B)

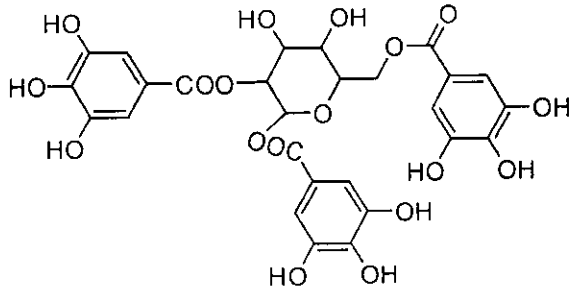
§ 3,4',5,7-Tetrahydroxyflavylium(1+); 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside]



[化学名・別名]Pelargonidin 3-(2^{III}glucosylrutinoside)
[化合物分類]フラボノイド
(Anthocyanidins and anthocyanins; 4 × O-置換基)
[構造式]
[分子式]$C_{33}H_{41}O_{19}^{(+)}$
[分子量]741.675
[基原]次の植物から分離: キイチゴ(*Rubus idaeus*)の果実
[その他のデータ]λ_{max} 275, 508 nm (MeOH/HCl)

文献
Karrer, P. et al., Helv. Chim. Acta, 1927, 10, 67; 1928, 12, 292, (分離, Monardein)
Robertson, A. et al., J.C.S., 1928, 1460; 1533, (分離)
Timberlake, C.F. et al., The Flavonoids, (Eds. Harborne, J.B. et al), Chapman and Hall, London, 1975, 215, (レビュー)
Iacobucci, G.A. et al., Tetrahedron, 1983, 39, 3005, (レビュー)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

§ 1,2,6-Trigalloylglucose; β-D-Pyranose-form



[CAS No.]79886-49-0
[化合物分類]タンニン化合物(Simple gallate ester tannins)
[構造式]
[分子式]$C_{27}H_{24}O_{18}$
[分子量]636.476
[基原]次の植物から分離: *Rubus fruticosus, Rubus idaeus, Rosa canina*
[性状]黄褐色の無定型粉末・一水和物
[比旋光度]:$[\alpha]_D^{20}$ +10.3 (c, 0.5 in Me_2CO)

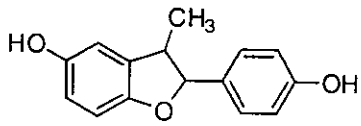
文献
Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515, (分離, 構造決定, H-NMR, C13-NMR)

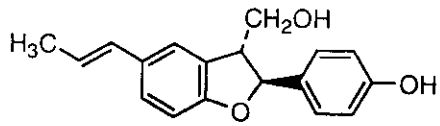
----------文 献----------
Haddock, E.A. et al., J.C.S. Perkin 1, 1982, 2515, (分離, 構造決定, H-NMR, C13-NMR)
Ishimatsu, M. et al., Chem. Pharm. Bull., 1989, 37, 129, (構造決定)
Nishizawa, K. et al., Phytochemistry, 1990, 29, 2491, (UV, IR, H-NMR, C13-NMR)
Nawwar, M.A.M. et al., Phytochemistry, 1994, 36, 793, (分離, H-NMR, C13-NMR)
Amakura, Y. et al., Can. J. Chem., 1997, 75, 727-733, (分離, α-D-glucose)

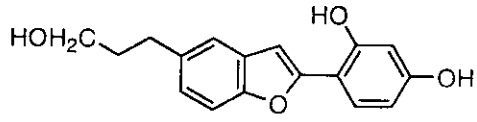
§§バラ科クロミキイチゴ(*Rubus occidentailis* Linne)の果実または葉。
本調査研究では、成分に関する文献はなかった。

**********ラタニア (Rhatany) **********

§§マメ科ラタニア(*Krameria triandra* Ruiz et Pavon)の根。

§ 2,3-Dihydro-5-hydroxy-2-(4-hydroxyphenyl)-3-methylbenzofuran; (2*R*,3*R*)-form
[その他のCAS No.]119322-05-3
[化合物分類]リグナン化合物(Norlignans), ベンゾフラノイド(Benzofurans)
[構造式]

[分子式]$C_{15}H_{14}O_3$
[分子量]242.274
[基原]*Krameria triandra*
[性状]ガラス様の塊
[融点]Mp 50-55 ℃
[比旋光度]:[α]$_D$ +159 (c, 0.1 in $CHCl_3$)
UV: [neutral] λ $_{max}$ 223 (ε 15000); 280 (ε 3500); 298 (ε 4500) (EtOH) [neutral] λ $_{max}$ 223 (ε 15000); 280 (ε 3500); 298 (ε 4500) (EtOH) (Berdy)
----------文 献----------
Arnone, A. et al., Gazz. Chim. Ital., 1988, 118, 675-682

§ 2,3-Dihydro-3-hydroxymethyl-2-(4-hydroxyphenyl)-5-(1-propenyl)benzofuran
[化学名・別名]2,3-Dihydro-2-(4-hydroxyphenyl)-5-(1-propenyl)-3-benzofuranmethanol(CAS名). 4,7'-Epoxy-3,8'-bilignan-4',9'-diol
[CAS No.]119322-04-2
[化合物分類]リグナン化合物(Neolignans)
[構造式]

[分子式]$C_{18}H_{18}O_3$
[分子量]282.338
[基原]*Krameria triandra*
[性状]ガラス様の塊
[融点]Mp 56-58 ℃
[比旋光度]:[α]$_D$ -19.3 (c, 0.2 in $CHCl_3$)
UV: [neutral] λ $_{max}$ 264 (ε 18650); 305 (ε 5500) (EtOH) [neutral] λ $_{max}$ 264 (ε 18650); 305 (ε 5500) (EtOH) (Berdy)
----------文 献----------
Arnone, A. et al., Gazz. Chim. Ital., 1988, 118, 675-682

§ 2-(2,4-Dihydroxyphenyl)-5-benzofuranpropanol
[化学名・別名]2-(2,4-Dihydroxyphenyl)-5-(3-hydroxypropyl)benzofuran
[CAS No.]119321-97-0
[化合物分類]リグナン化合物(Norlignans), リグナン化合物(Neolignans)
[構造式]

[分子式]$C_{17}H_{16}O_4$
[分子量]284.311
[基原]次の植物から分離: Ratanhiae radix (*Krameria triandra*)の根

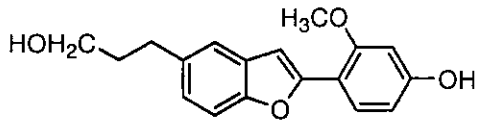
UV: [neutral] λ max 207 (ε 28300); 278 (ε 14200); 284 (ε 13300); 315 (ε 23950); 338 (ε 21100) (溶媒の報告はない) [neutral] λ max 207 (ε 28300); 278 (ε 14200); 284 (ε 13300); 315 (ε 23950); 338 (ε 21100) (EtOH) (Berdy)

----------文献----------

Arnone, A. et al., Gazz. Chim. Ital., 1988, 118, 675-682, (分離, 構造決定, IR, UV, H-NMR, C13-NMR)

§ 2-(2,4-Dihydroxyphenyl)-5-benzofuranpropanol; 2'-Me ether

[化学名・別名]2-(4-Hydroxy-2-methoxyphenyl)-5-benzofuranpropanol (CAS 名)
[CAS No.]119321-96-9
[化合物分類]リグナン化合物(Neolignans), リグナン化合物(Norlignans)
[構造式]
[分子式]$C_{18}H_{18}O_4$
[分子量]298.338
[基原]*Krameria triandra*
[性状]青白い黄色の結晶
[融点]Mp 143-145 ℃



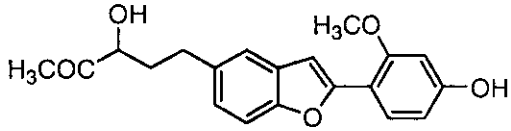
UV: [neutral] λ max 205 (ε 38150); 277 (ε 18160); 287 (ε 19500); 312 (ε 40800); 328 (ε 34750) (溶媒の報告はない)

----------文献----------

Arnone, A. et al., Gazz. Chim. Ital., 1988, 118, 675-682, (分離, 構造決定, IR, UV, H-NMR, C13-NMR)

§ 2-(2,4-Dihydroxyphenyl)-5-benzofuranpropanol; 2'-Me ether, 3''-Ac

[CAS No.]119321-99-2
[化合物分類]リグナン化合物(Neolignans), リグナン化合物(Norlignans)
[構造式]
[分子式]$C_{20}H_{20}O_5$
[分子量]340.375
[基原]次の植物から分離: *Krameria triandra*
[性状]黄色の塊
[融点]Mp 115-118 ℃



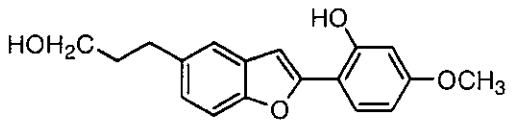
UV: [neutral] λ max 205 (ε 40000); 277 (ε 17150); 288 (ε 18200); 312 (ε 26800); 328 (ε 29300) (溶媒の報告はない) [neutral] λ max 205 (ε 40000); 277 (ε 17150); 288 (ε 18200); 312 (ε 26800); 328 (ε 29300) (EtOH) (Berdy)

----------文献----------

Arnone, A. et al., Gazz. Chim. Ital., 1988, 118, 675-682, (分離, 構造決定, IR, UV, H-NMR, C13-NMR)

§ 2-(2,4-Dihydroxyphenyl)-5-benzofuranpropanol; 4'-Me ether

[化学名・別名]2-(2-Hydroxy-4-methoxyphenyl)-5-benzofuranpropanol (CAS 名)
[CAS No.]119321-98-1
[化合物分類]リグナン化合物(Norlignans), リグナン化合物(Neolignans)
[構造式]
[分子式]$C_{18}H_{18}O_4$
[分子量]298.338
[基原]次の植物から分離: *Krameria triandra*
[性状]黄色の塊
[融点]Mp 80-82 ℃



UV: [neutral] λ max 207 (ε 33000); 278 (ε 17100); 283 (ε 16800); 313 (ε 32950); 329 (ε 28700) (溶媒の報告はない) [neutral] λ max 207 (ε 33000); 278 (ε 17100); 287 (ε 32900); 313 (ε 32950); 329 (ε 28900) (EtOH) (Berdy)

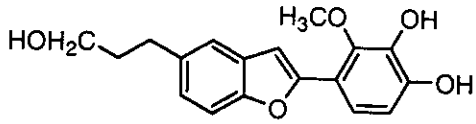
----------文献----------

Arnone, A. et al., Gazz. Chim. Ital., 1988, 118, 675-682, (分離, 構造決定, IR, UV, H-NMR, C13-NMR)

§ 2-(2,4-Dihydroxyphenyl)-5-benzofuranpropanol; 3'-Hydroxy, 2'-Me ether

[化学名・別名]5-(3-Hydroxypropyl)-2-(2-methoxy-3,4-dihydroxyphenyl)benzofuran
[CAS No.]119322-00-8
[化合物分類]リグナン化合物(Norlignans), リグナン化合物(Neolignans)
[構造式]

[化合物分類]リグナン化合物(Norlignans), リグナン化合物(Neolignans)
[構造式]
[分子式]$C_{18}H_{18}O_5$
[分子量]314.337
[基原]*Krameria triandra*
[性状]黄色の結晶
[融点]Mp 140-143 ℃

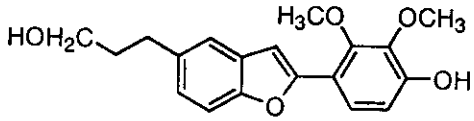


UV: [neutral] λ max 210 (ε 14350); 288 (sh) (ε 10000); 307 (ε 14650); 320 (ε 12500) (溶媒の報告はない) [neutral] λ max 210 (ε 14350); 307 (ε 14650); 320 (ε 12500) (EtOH) (Berdy)
[その他のデータ]Unusual 2,3,4-trihydroxylation pattern

----------文 献----------

Arnone, A. et al., Gazz. Chim. Ital., 1988, 118, 675-682, (分離, 構造決定, IR, UV, H-NMR, C13-NMR)

§ 2-(2,4-Dihydroxyphenyl)-5-benzofuranpropanol; 3'-Methoxy, 2'-Me ether
[化学名・別名]2-(4-Hydroxy-2,3-dimethoxyphenyl)-5-benzofuranpropanol (CAS 名). 5-(3-Hydroxypropyl)-2-(4-hydroxy-2,3-dimethoxyphenyl) benzofuran
[CAS No.]119322-01-9
[化合物分類]リグナン化合物(Norlignans), リグナン化合物(Neolignans)
[構造式]
[分子式]$C_{19}H_{20}O_5$
[分子量]328.364
[基原]*Krameria triandra*
[性状]黄色のガラス状結晶

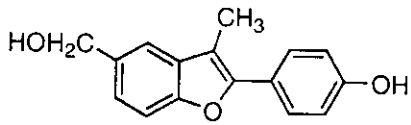


UV: [neutral] λ max 310 (ε 8350); 325 (ε 7130) (EtOH) [neutral] λ max 310 (ε 8350); 325 (ε 7130) (EtOH) (Berdy)

----------文 献----------

Arnone, A. et al., Gazz. Chim. Ital., 1988, 118, 675-682, (分離, 構造決定, IR, UV, H-NMR, C13-NMR)

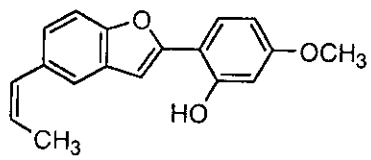
§ 2-(4-Hydroxyphenyl)-3-methyl-5-benzofuranmethanol (CAS 名)
[化学名・別名]5-Hydroxymethyl-2-(4-hydroxyphenyl)-3-methylbenzofuran
[CAS No.]119322-03-1
[化合物分類]ベンゾフラノイド(Benzofurans), リグナン化合物(Norlignans)
[構造式]
[分子式]$C_{16}H_{14}O_3$
[分子量]254.285
[基原]*Krameria triandra*
[性状]粉末
[融点]Mp 187-192 ℃



----------文 献----------

Arnone, A. et al., Gazz. Chim. Ital., 1988, 118, 675-682

§ 2-(4-Hydroxyphenyl)-5-(1-propenyl) benzofuran; 2'-Hydroxy, 4'-Me ether
[化学名・別名]2-(2-Hydroxy-4-methoxyphenyl)-5-(1-propenyl) benzofuran. Ratanhiaphenol I
[CAS No.]79214-54-3
[化合物分類]リグナン化合物(Neolignans)
[構造式]
[分子式]$C_{18}H_{16}O_3$
[分子量]280.323
[基原]*Krameria triandra*, *Krameria cystisoides*
[性状]結晶
[融点]Mp 182-184 ℃



----------文 献----------

Stahl, E. et al., Planta Med., 1981, 42, 144, (分離)
Achenbach, H. et al., Phytochemistry, 1987, 26, 1159; 2041; 1995, 39, 413, (分離, H-NMR, C13-NMR, 誘導体)

*********ラディッシュ（Radish）*********

§§アブラナ科ハツカダイコン(*Raphanus sativus* L.)の根茎。

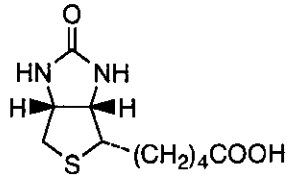
§ Biotin; (+)-form

[CAS No.]58-85-5

[その他の CAS No.]22879-79-4

[化合物分類]アルカロイド化合物(Imidazole alkaloids)

[構造式]



[分子式]$C_{10}H_{16}N_2O_3S$

[分子量]244.314

[基原]酵母, 卵, 肝臓に存在. また数種のその他の微生物から生産され, 数種の高等植物起源から分離される. 例えば, トウモロコシの発芽種子, *Raphanus sativus* の葉

[用途]化粧品や家畜飼料の添加物. Bacterial growth factor for "egg white injury"

[性状]微細長針状結晶（H_2O）

[融点]Mp 232-233 ℃

[比旋光度]:$[\alpha]_D^{20}$ +91（c, 1 in 0.1 *M* NaOH）

[溶解性]水に可溶

[傷害・毒性]研究報告がある

[化学物質毒性データ総覧(RTECS)登録番号]XJ9088200

[販売元]Aldrich:86164-2; Fluka:14400; Sigma:B4639; Supelco:R47-5090

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Marx, M. et al., J.A.C.S., 1977, 99, 6754,（合成法, 成書）

Vasilevskis, J. et al., J.A.C.S., 1978, 100, 7423,（合成法, 成書）

Uskokovic, M.R., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, 24, 41,（レビュー）

Bonjour, J.-P., Handbook of Vitamins,（ed. Machlin, L.J.）, M. Dekker, New York, 1984, 403,（レビュー）

Dakshinamurti, K. et al., Ann. N.Y. Acad. Sci.,（Eds.）, 1985, 447,（専門書）

Bentley, R., Trends Biochem. Sci., 1985, 10, 51,（レビュー, 絶対構造）

Senuma, M. et al., Chem. Pharm. Bull., 1990, 38, 882,（レビュー, 合成法）

Deroose, F.D. et al., J.O.C., 1995, 60, 321,（合成法, 成書）

Nicolaou, K.C. et al., Classics in Total Synthesis, Targets, Strategies, Methods, VCH, 1996, 285,（成書, 合成法）

De Clercq, P.J. et al., Chem. Rev., 1997, 97, 1755-1792,（レビュー, 合成法）

VSU100

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

生殖に関するデータ

〈〈試験方法〉〉最小毒性量(TDLo).

曝露経路　　：皮下投与.

被験動物　　：げっ歯類-ラット.

投与　　：200 mg/kg

雌雄投与期間：雌 14-15 日間(交配後)

毒性影響　　：〔生殖〕[母系影響]子宮, 頸管, 膣.

〔生殖〕[胚または胎仔に対する影響]胚外構造(たとえば胎盤, 臍帯).

〔生殖〕[胚または胎仔に対する影響]胎仔毒性(死亡をのぞく.たとえば胎仔の発育阻害).

参照文献

Journal of Nutritional Science and Vitaminology.(Business Center for Academic Soc. Japan, 2-4-16 Yayoi, Bunkyo-ku, Tokyo 113, Japan) 22,181,1976

参照文献

Current Science.(Current Science Assoc., Sadashivanagar P.O., Bangalore 560 080, India) 42,613,1973

〈〈試験方法〉〉最小毒性量(TDLo).

曝露経路　　：皮下投与.

被験動物　　：げっ歯類-ラット.

投与　　：200 mg/kg

雌雄投与期間：雌 1-2 日間(交配後)

毒性影響　　：〔生殖〕[受精能への影響]着床後死亡率（例えば着床総数当たりの着床の死亡

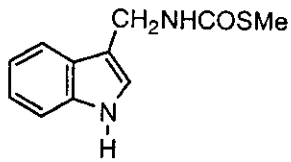
被験動物　　：げっ歯類-ラット.
投与　　：200 mg/kg
雌雄投与期間：雌 1-2 日間(交配後)
毒性影響　　：〔生殖〕[受精能への影響]着床後死亡率（例えば着床総数当たりの着床の死亡および／または吸収)

参照文献

Journal of Nutritional Science and Vitaminology.(Business Center for Academic Soc. Japan, 2-4-16 Yayoi, Bunkyo-ku, Tokyo 113, Japan) 21,89,1975

§ Brassitin

[化学名・別名]*S*-Methyl 1*H*-indole-3-ylmethylcarbamothioate(CAS 名)



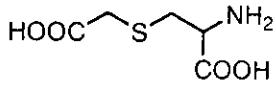
[CAS No.]113866-42-5
[化合物分類]アルカロイド化合物(Simple indole alkaloids)
[構造式]
[分子式]$C_{11}H_{12}N_2OS$
[分子量]220.295
[基原]次の植物のストレス代謝物: 日本ラディッシュのダイコン(*Raphanus sativus* var. *hortensis*, アブラナ科)へ次の菌を接種: *Psudomonas cichorii*
[性状]無定型
UV: [neutral] λ_{max} 218 (ε 36800); 271 (ε 5910); 277 (ε 5910); 287 (ε 4830) (MeOH) (Berdy)

----------文 献----------

Takasugi, M. et al., Bull. Chem. Soc. Jpn., 1988, 61, 285, (Methoxybrassitin)
Monde, K. et al., Phytochemistry, 1995, 39, 581, (Brassitin)
Kutschy, P. et al., Tetrahedron, 1998, 54, 3549-3566, (合成法)

§ *S*-Carboxymethylcysteine; (*R*)-form

[化学名・別名]L-form



[CAS No.]2387-59-9
[化合物分類]アミノ酸とペプチド(Non-protein α-aminoacids)
[構造式]
[分子式]$C_5H_9NO_4S$
[分子量]179.196
[基原]ラディッシュ(*Raphanus sativus*)の発芽種子
[用途]粘液溶解作用, 去痰作用, nasal antiinfective
[融点]Mp 204-207 ℃
[比旋光度]:$[\alpha]_D^{24}$ +0.5 (1 *M* HCl)
[傷害・毒性]治療に用いるとき逆作用効果を示すことがある. 50 %致死量(LD_{50})(マウス, 皮下) 9000 mg/kg
[化学物質毒性データ総覧(RTECS)登録番号]AY4341000

----------文 献----------

Buziassy, C. et al., Biochim. Biophys. Acta, 1964, 86, 185, (分離)
Mighell, A.D. et al., Acta Cryst. B, 1979, 35, 1258, (結晶構造)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 745

RTECS（化学物質毒性データ）

生体影響物質　　：医薬品.

健康障害に関するデータ
急性毒性に関するデータ

<<試験方法>> LD50 試験(50%致死量試験).
曝露経路　　：皮下投与.
被験動物　　：げっ歯類-マウス.
投与量・期間：9 gm/kg
毒性影響　　：致死量以外に毒性影響に関する報告はない.

参照文献

Iyakuhin Kenkyu. Study of Medical Supplies.(Nippon Koteisho Kyokai, 12-15, 2-chome, Shibuya, Shibuya-ku, Tokyo 150, Japan) 12,668,1981

その他の多回投与試験

<<試験方法>> 最小毒性量(TDLo).

〔慢性データ関連〕睾丸重量の変化.

参照文献

Oyo Yakuri. Pharmacometrics. (Oyo Yakuri Kenkyukai, CPO Box 180, Sendai 980-91, Japan) 14,567,1977

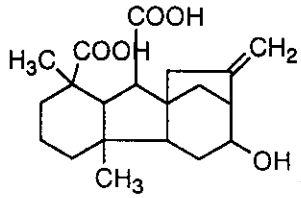
§ Gibberellin A_{12} ; 12 α-Hydroxy

[化学名・別名]Gibberellin A_{111}

[CAS No.]75803-47-3

[化合物分類]テルペノイド(Gibberellins)

[構造式]



[分子式]$C_{20}H_{28}O_5$

[分子量]348.438

[基原]*Raphanus sativus*

----------文献----------

Nakayama, M. et al., Phytochemistry, 1998, 48, 587-593, (GA_{111}, GA_{112})

Toyota, M. et al., J.A.C.S., 2000, 122, 9036-9037; 2001, 123, 1856-1861, (合成法, GA_{12}, GA_{111}:GA_{112})

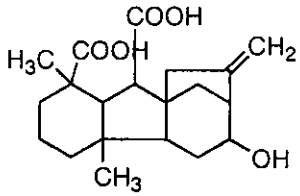
§ Gibberellin A_{12} ; 12 β-Hydroxy

[化学名・別名]Gibberellin A_{112}

[CAS No.]90806-15-8

[化合物分類]テルペノイド(Gibberellins)

[構造式]



[分子式]$C_{20}H_{28}O_5$

[分子量]348.438

[基原]*Matthiola incana*, *Raphanus sativus*

----------文献----------

Hisamatsu, T. et al., Phytochemistry, 1998, 47, 3-6, (GA_{112})

Nakayama, M. et al., Phytochemistry, 1998, 48, 587-593, (GA_{111}, GA_{112})

Toyota, M. et al., J.A.C.S., 2000, 122, 9036-9037; 2001, 123, 1856-1861, (合成法, GA_{12}, GA_{111}:GA_{112})

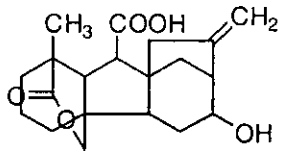
§ Gibberellin A_{15} ; 12 α-Hydroxy

[化学名・別名]Gibberellin A_{113}

[CAS No.]90806-31-8

[化合物分類]テルペノイド(Gibberellins)

[構造式]



[分子式]$C_{20}H_{26}O_5$

[分子量]346.422

[基原]*Raphanus Sativus*

----------文献----------

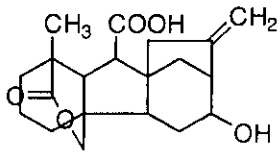
Nakayama, M. et al., Phytochemistry, 1998, 48, 587-593, (GA_{113}, GA_{114})

§ Gibberellin A_{15} ; 12 β-Hydroxy

[化学名・別名]Gibberellin A_{114}

[化合物分類]テルペノイド(Gibberellins)

[構造式]



[分子式]$C_{20}H_{26}O_5$

[分子量]346.422

[基原]*Raphanus sativus*

----------文献----------

Nakayama, M. et al., Phytochemistry, 1998, 48, 587-593, (GA_{113}, GA_{114})

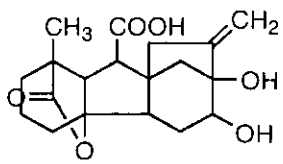
§ Gibberellin A_{20} ; 12 α-Hydroxy

[化学名・別名]Gibberellin A_{77}

[CAS No.]128230-24-0

[化合物分類]テルペノイド(Gibberellins)

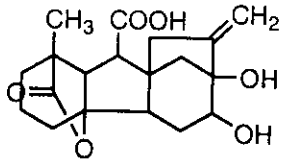
[構造式]



[分子式]$C_{19}H_{24}O_6$

[分子量]348.395

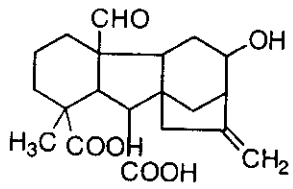
[CAS No.] 128230-24-0
[化合物分類] テルペノイド (Gibberellins)
[構造式]
[分子式] $C_{19}H_{24}O_6$
[分子量] 348.395
[基原] *Raphanus sativus*



文 献

Nakayama, M. et al., Agric. Biol. Chem., 1990, 54, 837, (GA_{77})

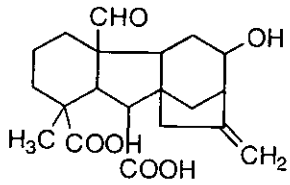
§ Gibberellin A_{24} ; 12 α-Hydroxy
[化学名・別名] Gibberellin Ga_{115}
[CAS No.] 137694-17-8
[化合物分類] テルペノイド (Gibberellins)
[構造式]
[分子式] $C_{20}H_{26}O_6$
[分子量] 362.422
[基原] *Raphanus sativus*



文 献

Nakayama, M. et al., Phytochemistry, 1998, 48, 587-593, (Ga_{115}, GA_{116})

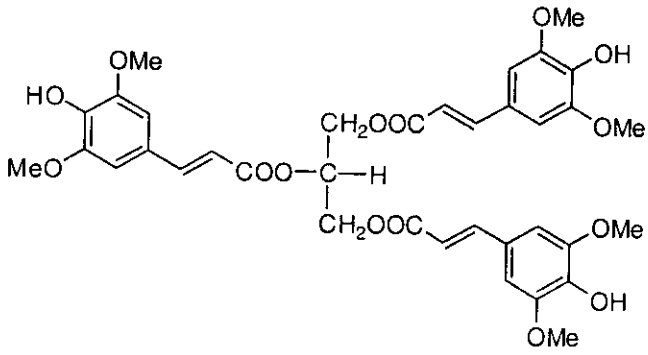
§ Gibberellin A_{24} ; 12 β-Hydroxy
[化学名・別名] Gibberlin GA_{116}
[CAS No.] 90806-27-2
[化合物分類] テルペノイド (Gibberellins)
[構造式]
[分子式] $C_{20}H_{26}O_6$
[分子量] 362.422
[基原] *Raphanus sativus*



文 献

Nakayama, M. et al., Phytochemistry, 1998, 48, 587-593, (Ga_{115}, GA_{116})

§ Glycerol tris (4-hydroxy-3,5-dimethoxyphenyl-2-propenoate)
[化学名・別名] Glycerol trisinapate. Tri-*O*-sinapoylglycerol
[化合物分類] 単環芳香族 (Simple phenylpropanoids), 脂肪族化合物 (Triacylglycerols)
[構造式]



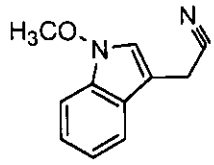
[分子式] $C_{36}H_{38}O_{15}$
[分子量] 710.687
[基原] *Raphanus sativus*. Component of Lai Fu Zi

文 献

Traditional Chinese Medicines, (ed. Milne, G.A.), Ashgate, 1999, 2694

§ Hexyl glucosinolate
[化学名・別名] 1-Thio-β-D-glucopyranose 1-[*N*-(sulfooxy) heptanimidate] (CAS 名)
[CAS No.] 127929-25-3
[化合物分類] 炭水化物 (Glycosinolates)
[構造式] $H_3C(CH_2)_5C(SGlc)=NOSO_3H$
[分子式] $C_{13}H_{25}NO_9S_2$
[分子量] 403.474

§ 1*H*-Indole-3-acetic acid Nitrile, 1-methoxy

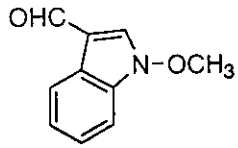


[化学名・別名]1-Methoxy-1*H*-indole-3-acetonitrile(CAS 名)
[CAS No.]30536-48-2
[化合物分類]アルカロイド化合物(Simple indole alkaloids)
[構造式]
[分子式]$C_{11}H_{10}N_2O$
[分子量]186.213
[基原]次の植物のストレス代謝物: 日本ラディッシュのダイコン(*Raphanus sativus* var. *hortensis*)へ次の菌を接種したもの: *Pseudomonas cichorii*, *Plasmodiophora brassicae* に感染した Chinese cabbage (*Brassica pekinensis*)の clubroots

----------文献----------

Henbest, H.B. et al., J.C.S., 1953, 3796, (分離, nitrile)
Stowe, B.B., Prog. Chem. Org. Nat. Prod., 1959, 17, 248, (成書)
Isogai, Y. et al., Chem. Pharm. Bull., 1963, 11, 1217, (分離, amide)
Nomoto, M. et al., Agric. Biol. Chem., 1970, 34, 1590, (分離, 1-Methoxy-3-indoleacetonitrile)
Abe, H. et al., Agric. Biol. Chem., 1972, 36, 2259, (分離, UV, Mass)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 2514; 2515, (成書)
Cardellina, J.H. et al., J. Nat. Prod., 1986, 49, 1065-1067, (分離, amide)
Katayama, N. et al., Plant Cell Physiol., 1987, 28, 383, (分離, Me ester)
Wall, M.E. et al., J. Nat. Prod., 1988, 51, 129, (分離, nitrile)
Monde, K. et al., Phytochemistry, 1995, 39, 581, (分離, 1-Methoxy-3-indoleacetonitrile)

§ 1*H*-Indole-3-carboxaldehyde; 1-Methoxy



[化学名・別名]1-Methoxy-1*H*-indole-3-carboxaldehyde(CAS 名). 1-Methoxy-3-formylindole
[CAS No.]67282-55-7
[化合物分類]アルカロイド化合物(Simple indole alkaloids)
[構造式]
[分子式]$C_{10}H_9NO_2$
[分子量]175.187
[基原]次の植物のストレス代謝物: 日本ラディッシュのダイコン(*Raphanus sativus* var. *hortensis*)へ次の菌を接種したもの: *Pseudomonas cichorii*
[性状]プリズム結晶 + $1/2H_2O$(Et_2O/hexane)
[融点]Mp 50-51 ℃

----------文献----------

Somei, M. et al., Chem. Pharm. Bull., 1986, 34, 677, (合成法, 1-Methoxy-3-indolecarboxaldehyde)
Monde, K. et al., Phytochemistry, 1995, 39, 581, (分離, 1-Methoxy-3-indolecarboxaldehyde)

§ 1-Isothiocyanatohexane(CAS 名)

[化学名・別名]Hexyl isothiocyanate
[CAS No.]4404-45-9
[化合物分類]脂肪族化合物(Simple thiocyanates and isothiocyanates)
[構造式]$H_3C(CH_2)_5NCS$
[分子式]$C_7H_{13}NS$
[分子量]143.252
[基原]次の植物から分離: ラディッシュ(*Raphanus sativus*), その他のアブラナ科の植物
[性状]液体
[沸点]Bp 210 ℃. Bp_{27} 98 ℃. Bp_{15} 100 ℃
[販売元]Fluka:53197

----------文献----------

Kjaer, A. et al., Agric. Biol. Chem., 1978, 42, 1715, (分離)
Yamamoto, T. et al., Org. Prep. Proced. Int., 1992, 24, 346; 1994, 26, 555, (合成法, IR, H-NMR)

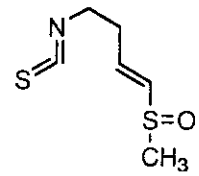
§ 1-Isothiocyanato-4-methylpentane(CAS 名)

[化学名・別名]4-Methylpentyl isothiocyanate. Isohexyl isothiocyanate
[CAS No.]17608-07-0
[化合物分類]脂肪族化合物(Simple thiocyanates and isothiocyanates)

§ 1-Isothiocyanato-4-methylpentane（CAS 名）
[化学名・別名]4-Methylpentyl isothiocyanate. Isohexyl isothiocyanate
[CAS No.]17608-07-0
[化合物分類]脂肪族化合物(Simple thiocyanates and isothiocyanates)
[構造式] $(H_3C)_2CH(CH_2)_3NCS$
[分子式] $C_7H_{13}NS$
[分子量]143.252
[基原]次の植物から分離: ラディッシュ(*Raphanus sativus*)

---文 献---

Kaluza, L., Monatsh. Chem., 1909, 30, 701, (合成法)
Kjaer, A. et al., Agric. Biol. Chem., 1978, 42, 1715, (分離, Mass)



§ 4-Isothiocyanato-1-(methylsulfinyl)-1-butene; (*R*)-(*E*)-form
[CAS No.]2404-46-8
[化合物分類]脂肪族化合物(Simple thiocyanates and isothiocyanates)
[構造式]
[分子式] $C_6H_9NOS_2$
[分子量]175.275
[基原]次の植物から得られるマスタードオイル: ラディッシュの種子(*Raphanus sativus* var. *alba*)と *Matthiola bicornis* の Glucoraphenin (4-(Methylthio)-3-butenyl glucosinolate 参照)
[沸点] $Bp_{0.015}$ 125-130 ℃
[比旋光度]: $[\alpha]_D$ -108 (c, 1.427 in $CHCl_3$)
[溶解性]BERDY SOL: メタノール, クロロホルム, 水に可溶; エーテルに易溶; ヘキサンに難溶
UV: [neutral] λ_{max} 226 (ε 2951) (H_2O) (Berdy)
[傷害・毒性]BERDY HAZD : 50 %致死量(LD_{50}) (マウス, 静脈内) 10 mg/kg

---文 献---

Kjaer, A. et al., Acta Chem. Scand., Ser. B, 1974, 28, 418, (分離)
Spencer, G.F. et al., J. Sci. Food Agric., 1980, 31, 359, (Mass)

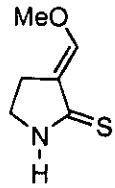
§ 4-Isothiocyanato-1-(methylthio)-1-butene; (*E*)-form
[CAS No.]13028-50-7
[化合物分類]脂肪族化合物(Simple thiocyanates and isothiocyanates)
[構造式]
[分子式] $C_6H_9NS_2$
[分子量]159.276
[基原]ラディッシュの根(*Raphanus sativus*)の刺激成分の主成分. Formed by hydrolysis of 4-(Methylthio)-3-butenyl glucosinolate
[性状]オイル
[溶解性]BERDY SOL: ヘキサンに難溶
[屈折率] n^{25}_D 1.5815

---文 献---

Früs, P. et al., Acta Chem. Scand., 1966, 20, 698, (分離)
Brandsma, L. et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.), 1972, 91, 729, (合成法)
Spencer, G.F. et al., J. Sci. Food Agric., 1980, 31, 359, (Mass)
Kosemura, S. et al., Tet. Lett., 1993, 34, 481, (分離)

§ 1-Isothiocyanatopentane（CAS 名）
[化学名・別名]Pentyl isothiocyanate. n -Amyl isothiocyanate
[CAS No.]629-12-9
[化合物分類]脂肪族化合物(Simple thiocyanates and isothiocyanates)
[構造式] $H_3C(CH_2)_4NCS$
[分子式] $C_6H_{11}NS$
[分子量]129.226
[基原]次の植物から分離: ラディッシュ(*Raphanus sativus*)
[性状]液体
[沸点]Bp 191 ℃

§ 3-(Methoxymethylene)-2-pyrrolidinethione



[化学名・別名]Raphanusamide
[CAS No.]104730-65-6
[化合物分類]アルカロイド化合物(Simple pyrrolidine alkaloids)
[構造式]
[分子式]C_6H_9NOS
[分子量]143.209
[一般的性質]Originally assigned a 1,3-oxazepin-2-one struct. The 1997 *CA* Index Guide retains the erroneous nomencl.
[基原]次の植物から分離: *Raphanus sativus* var. *hortensis* f. *gigantissimus* (アブラナ科)
[用途]Growth inhibitor involved in phototropism of radish hypocotyls
[性状]プリズム結晶 (EtOAc/hexane)
[融点]Mp 150-151 ℃
UV: [neutral] λ_{max} 270 (ε 15800); 307 (ε 8200) (MeOH) (Derep)

----------文献----------

Hasegawa, K. et al., Plant Physiol., 1986, 81, 976, (分離)
Harada, N. et al., Tet. Lett., 1991, 32, 6761, (UV, IR, H-NMR, C13-NMR, Mass, 結晶構造, 成書)

§ 3-Methylpentyl glucosinolate

[化学名・別名]1-Thio-β-D-glucopyranose 1-[4-methyl-*N*-(sulfooxy)hexanimidate]
[化合物分類]炭水化物(Glycosinolates)
[構造式]$H_3CCH_2CH(CH_3)CH_2CH_2C(SGlc)=NOSO_3H$
[分子式]$C_{13}H_{25}NO_9S_2$
[分子量]403.474
[基原]*Raphanus sativus, Wasabi japonica*

----------文献----------

Fahey, J.W. et al., Phytochemistry, 2001, 56, 5-51, (レビュー)

§ 4-Methylpentyl glucosinolate

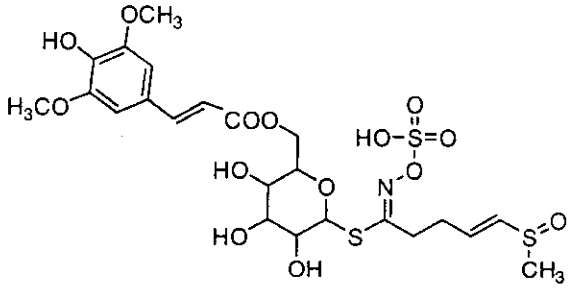
[化合物分類]炭水化物(Glycosinolates), AF9600
[構造式]$(H_3C)_2CHCH_2CH_2CH_2C(SGlc)=NOSO_3H$
[分子式]$C_{13}H_{25}NO_9S_2$
[分子量]403.474
[基原]ラディッシュ(*Raphanus sativus*)に存在

----------文献----------

Kjaer, A. et al., Agric. Biol. Chem., 1978, 42, 1715, (生育)

§ 4-(Methylthio)-3-butenyl glucosinolate; *S*-Oxide, 6'-(4-hydroxy-3,5-dimethoxycinnamoyl)

[化学名・別名]6-Sinapoylglucoraphenin
[CAS No.]76653-80-0
[化合物分類]炭水化物(Glycosinolates)
[構造式]



[分子式]$C_{23}H_{31}NO_{14}S_3$
[分子量]641.694
[基原]次の植物から分離: ラディッシュ(*Raphanus sativus*)

----------文献----------

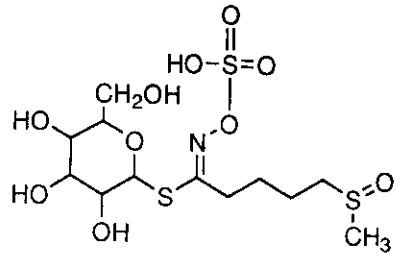
Schultz, O.E. et al., Arch. Pharm. (Weinheim, Ger.), 1955, 288, 525, (分離)
Kjaer, A., Acta Chem. Scand., 1959, 13, 851, (分離)
Gmelin, R. et al., Phytochemistry, 1970, 9, 569, (分離)
Wendisch, D. et al., Z. Naturforsch., C, 1980, 35, 907, (分離)

§ 4-(Methylthio)butyl glucosinolate; *S*-Oxide

[化学名・別名]4-(Methylsulfinyl)butyl glucosinolate. Glucoraphanin

Gmelin, R. et al., Phytochemistry, 1970, 9, 569, (分離)
Wendisch, D. et al., Z. Naturforsch., C, 1980, 35, 907, (分離)

§ 4-(Methylthio)butyl glucosinolate; *S*-Oxide
[化学名・別名]4-(Methylsulfinyl)butyl glucosinolate. Glucoraphanin
[CAS No.]21414-41-5
[化合物分類]AF9600, 炭水化物(Glycosinolates)
[構造式]



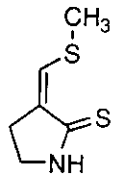
[分子式]$C_{12}H_{23}NO_{10}S_3$
[分子量]437.512
[基原]次の植物から分離: ラディッシュ(*Raphanus sativus*), その他のアブラナ科の植物

----------文 献----------
Schmidt, H. et al., Helv. Chim. Acta, 1948, 31, 1017, (Glucoraphanin)
Gmelin, R. et al., Acta Chem. Scand., 1968, 22, 2875, (Glucoerysolin)
Fenwick, G.R. et al., Biomed. Mass Spectrom., 1980, 7, 410; 1981, 8, 265, (Mass)
Cox, I.J. et al., Carbohydr. Res., 1984, 132, 323, (C13-NMR)

§ Pentyl glucosinolate
[化学名・別名]1-Thio-β-D-glucopyranose 1-[*N*-(sulfooxy)hexanimidate](CAS 名)
[CAS No.]127929-24-2
[化合物分類]AF9600, 炭水化物(Glycosinolates)
[構造式]$H_3C(CH_2)_4C(SGlc)=NOSO_3H$
[分子式]$C_{12}H_{23}NO_9S_2$
[分子量]389.447
[基原]ラディッシュ(*Raphanus sativus*), カブタマナに存在

----------文 献----------
Kjaer, A. et al., Agric. Biol. Chem., 1978, 42, 1715, (生育)
Macleod, G. et al., Phytochemistry, 1990, 29, 1183, (生育)

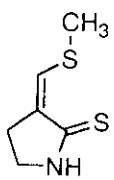
§ Raphanusanin; (*E*)-form
[CAS No.]128463-44-5
[その他の CAS No.]104760-73-8
[化合物分類]アルカロイド化合物(Simple pyrrolidine alkaloids)
[構造式]



[分子式]$C_6H_9NS_2$
[分子量]159.276
[基原]次の植物から分離: *Raphanus sativus* var. *hortensis* f. *gigantissimus* (アブラナ科)
[用途]Growth inhibitor involved in phototropism of hypocotyls
[性状]針状結晶(MeOH)

----------文 献----------
Sakoda, M. et al., Phytochemistry, 1990, 29, 1031, (分離)
Harada, N. et al., Tet. Lett., 1991, 32, 6757, (UV, IR, H-NMR, C13-NMR, Mass, 成書)
Kosemura, S. et al., Tet. Lett., 1993, 34, 481-484, (構造決定)
Matsuoka, H. et al., Phytochemistry, 1998, 47, 975-977, (分離)
Hasegawa, T. et al., Phytochemistry, 2000, 54, 275-279, (生合成)

§ Raphanusanin; (*Z*)-form
[CAS No.]148225-27-8
[その他の CAS No.]104760-72-7
[化合物分類]アルカロイド化合物(Simple pyrrolidine alkaloids)
[構造式]



[分子式]$C_6H_9NS_2$
[分子量]159.276
[基原]*Raphanus sativus* var. *hortensis* f. *gigantissimus* (アブラナ科)

Kosemura, S. et al., Tet. Lett., 1993, 34, 481-484, (構造決定)
Matsuoka, H. et al., Phytochemistry, 1998, 47, 975-977, (分離)
Hasegawa, T. et al., Phytochemistry, 2000, 54, 275-279, (生合成)

§ Raphanusol A
[化学名・別名] 6-*O*-β -D-Glucopyranosyl-β -D-glucopyranose-1,4-bis[3-(4-hydroxy-3,5-dimethoxyphenyl) -2-propenoate] (CAS 名). 1,4-Di-*O*-sinapoylgentiobiose
[CAS No.] 74565-72-3
[化合物分類] 炭水化物(Disaccharides)
[構造式]
[分子式] $C_{34}H_{42}O_{19}$
[分子量] 754.694
[基原] 次の植物から分離: *Raphanus sativus* (桜島ダイコン) の発芽種子
[用途] Endogenous hypocotyl growth inhibitor
[性状] 粉末 (Me_2CO/C_6H_6)
[融点] Mp 137-138 ℃
[比旋光度]: $[\alpha]_D^{22}$ +79.4 (c, 0.23 in MeOH)
[溶解性] BERDY SOL: メタノールに可溶; ヘキサンに難溶
UV: [neutral] λ_{max} 204 (ε 27400); 241 (ε 23300); 333 (ε 27300) (EtOH) (Berdy)
----------文献----------
Hase, T. et al., Phytochemistry, 1982, 21, 1021, (分離, 構造決定)
Hase, T. et al., CA, 1985, 103, 138518b

§ Spirobrassinin; (*S*)-form
[化合物分類] アルカロイド化合物(Miscellaneous polycyclic alkaloids)
[構造式]
[分子式] $C_{11}H_{10}N_2OS_2$
[分子量] 250.345
[基原] *Raphanus sativus* var. *hortensis* のファイトアレキシン
[性状] 結晶
[比旋光度]: $[\alpha]_D$ -69.5 (c, 1.14 in $CHCl_3$) (natural). $[\alpha]_D$ -143.6 (opt. pure)
UV: [neutral] λ_{max} 215 (ε 23500); 250 (ε 8200); 300 (ε 1900) (MeOH)
[その他のデータ] 天然物は部分的にラセミ体. Undergoes strong enantiomeric enrichment in achiral chromatographic phase
----------文献----------
Takasugi, M. et al., Chem. Lett., 1987, 1631, (分離, 構造決定)
Monde, K. et al., J.A.C.S., 1994, 116, 6650-6657, (合成法)
Gross, D. et al., Z. Naturforsch., C, 1994, 49, 281-285, (1-Methoxyspirobrassinin)
Monde, K. et al., Chem. Lett., 2000, 886-887, (絶対構造)
Monde, K. et al., J. Nat. Prod., 2000, 63, 1312-1314, (opt purity)
Pedras, M.S.C. et al., Phytochemistry, 2000, 53, 161-176, (レビュー)

§ Spirobrassinol; *N*-Methoxy
[化学名・別名] *N*-Methoxyspirobrassinol
[その他の CAS No.] 165746-57-6, 166020-09-3
[化合物分類] アルカロイド化合物(Miscellaneous polycyclic alkaloids)
[構造式]

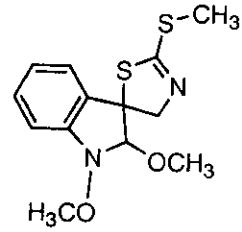
[分子式] $C_{12}H_{14}N_2O_2S_2$
[分子量] 282.387
[基原] 次の植物のストレス代謝物: 日本ラディッシュのダイコン(*Raphanus sativus* var. *hortensis*) (アブラナ科) へ次の菌を接種: *Pseudomonas cichorii*
[性状] ガム
[比旋光度]: $[\alpha]_D^{20}$ 0 (c, 0.52 in $CHCl_3$)
UV: [neutral] λ_{max} 211 (ε 27300); 246 (ε 15500); 292 (ε 3630) (EtOH) (Berdy)

[分子量]282.387
[基原]次の植物のストレス代謝物: 日本ラディッシュのダイコン(*Raphanus sativus* var. *hortensis*)(アブラナ科)へ次の菌を接種: *Pseudomonas cichorii*
[性状]ガム
[比旋光度]:[α]$_D^{20}$ 0 (c, 0.52 in $CHCl_3$)
UV: [neutral] λ $_{max}$ 211 (ε 27300); 246 (ε 15500); 292 (ε 3630) (EtOH) (Berdy)
[その他のデータ]Unusual hemi-aminal struct. Occurs as a mixt. of diastereoisomers; ratio α- OH : β- OH estimated as 2.5:1

----------文 献----------

Monde, K. et al., Phytochemistry, 1995, 39, 581, (分離, H-NMR, C13-NMR, Mass)

§ Spirobrassinol; *N*-Methoxy, Me ether

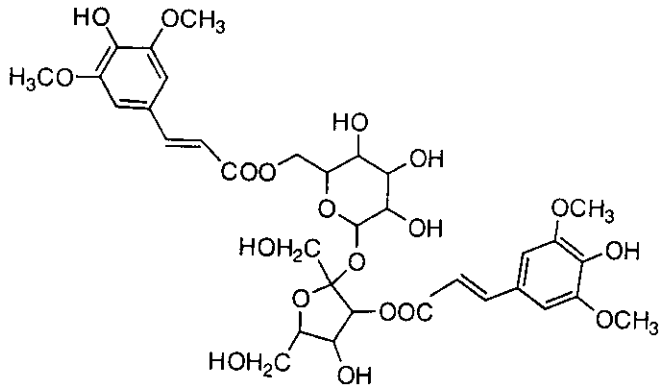


[化学名・別名]*N*-Methoxyspirobrassinol methyl ether
[CAS No.]113866-41-4
[化合物分類]アルカロイド化合物(Miscellaneous polycyclic alkaloids)
[構造式]
[分子式]$C_{13}H_{16}N_2O_2S_2$
[分子量]296.414
[基原]次の植物のストレス代謝物: *Raphanus sativus* var. *hortensis* (アブラナ科)へ次の菌を接種: *Pseudomonas cichorii*
[性状]ガム
[比旋光度]:[α]$_D^{18}$ -1.9 (c, 1.57 in $CHCl_3$)
UV: [neutral] λ $_{max}$ 210 (ε 26400); 291 (ε 2880) (EtOH) (Berdy)
[その他のデータ]Has 2 β-OMe config. 絶対構造は未知

----------文 献----------

Monde, K. et al., Phytochemistry, 1995, 39, 581, (分離, H-NMR, C13-NMR, Mass)

§ Sucrose; 3',6-Bis-*O*-(4-hydroxy-3,5-dimethoxycinnamoyl)

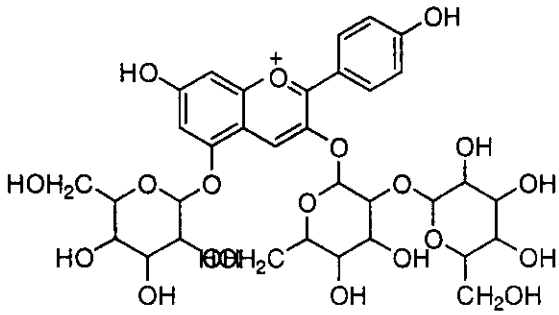


[化学名・別名]3',6-Disinapoylsucrose
[CAS No.]139891-98-8
[化合物分類]炭水化物(Disaccharides), 単環芳香族(Simple phenylpropanoids)
[構造式]
[分子式]$C_{34}H_{42}O_{19}$
[分子量]754.694
[基原]*Polygala virgata*, *Polygala reinii*, *Polygala tenuifolia*, *Raphanus sativus*, *Securidaca longipedunculata*
[性状]黄色の粉末
[融点]Mp 138-141 ℃
[比旋光度]:[α]$_D$ -94 (c, 0.2 in MeOH)

----------文 献----------

Tollens, B. et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth, 1935, 477, (レビュー)
Kollonitsch, V., Sucrose Chemicals, Kline, The International Sugar Research Foundation, Washington, D.C., 1970, (レビュー)
Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 654, (生育)
Khan, R., Adv. Carbohydr. Chem. Biochem., 1976, 33, 235, (レビュー)
Sucrochemistry, (Ed. Hickson, J.L.), ACS Symp. Series, 1977, 41, (レビュー)
Opdyke, D.L.J., Food Chem. Toxicol., 1982, 20, 827, (レビュー, 毒性, octa-Ac)
James, C.E. et al., Prog. Chem. Org. Nat. Prod., 1989, 55, 117, (レビュー)
Rathbone, E.B., Carbohydr. Res., 1990, 205, 402, (合成法, 成書, acetates)
Mathlouthi, M. et al., Sucrose, Blackie, 1995, (専門書)

§ 3,4',5,7-Tetrahydroxyflavylium(1+); 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside

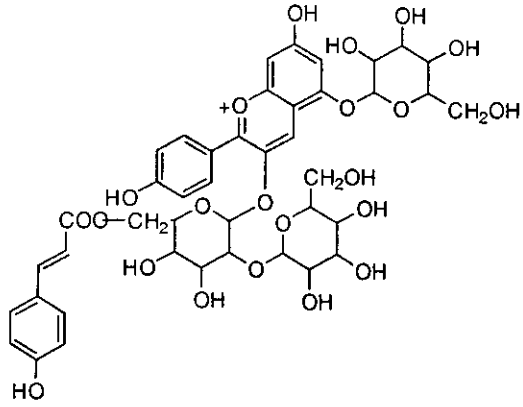


[化学名・別名]Rubrobrassicin
[CAS No.]75093-88-8
[化合物分類]フラボノイド(Anthocyanidins and antho cyanins; 4 × O-置換基)
[構造式]
[分子式]$C_{33}H_{41}O_{20}^{(+)}$
[分子量]757.675
[基原]ラディッシュ(*Raphanus sativus*)の根, *Matt hiola incana*, *Brassica oleracea*
[性状]結晶・四水和物
[その他のデータ]Apparently present as acylated derivs. in *R. sativus*, known as Raphanusins

文献

Robertson, A. et al., J.C.S., 1928, 1460; 1533, (分離)
Ishikura, N. et al., CA, 1965, 64, 2411, (Raphanusins, Rubrobrassicins)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

§ 3,4',5,7-Tetrahydroxyflavylium(1+); 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-[4-hydroxycinnamoyl-(→ 6)]-β-D-glucopyranoside] (*E*-), 5-*O*-β-D-glucopyranoside

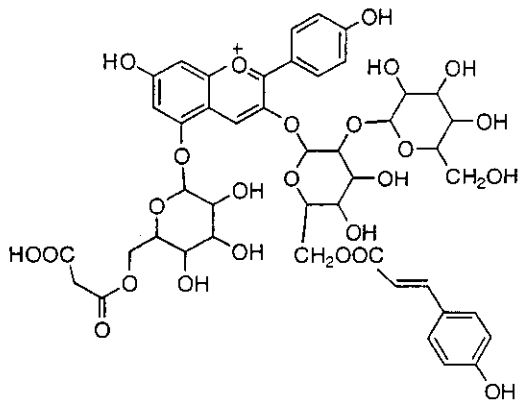


[CAS No.]218963-78-1
[化合物分類]フラボノイド(Anthocyanidins and antho cyanins; 4 × O-置換基)
[構造式]
[分子式]$C_{42}H_{47}O_{22}^{(+)}$
[分子量]903.82
[基原]*Raphanus sativus*

文献

Ishikura, N. et al., CA, 1965, 64, 2411, (Raphanusins, Rubrobrassicins)
Timberlake, C.F. et al., The Flavonoids, (Eds. Harborne, J.B. et al), Chapman and Hall, London, 1975, 215,
Iacobucci, G.A. et al., Tetrahedron, 1983, 39, 3005, (レビュー)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Giusti, M.M. et al., J. Agric. Food Chem., 1998, 46, 4858-4863, (*Raphanus sativus* anthocyanins)

§ 3,4',5,7-Tetrahydroxyflavylium(1+); 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-[4-hydroxycinnamoyl-(→ 6)]-β-D-glucopyranoside] (*E*-), 5-*O*-(6-*O*-malonyl-β-D-glucopyranoside)



[CAS No.]218963-76-9
[化合物分類]フラボノイド(Anthocyanidins and antho cyanins; 4 × O-置換基)
[構造式]
[分子式]$C_{45}H_{49}O_{25}^{(+)}$
[分子量]989.867
[基原]*Raphanus sativus*

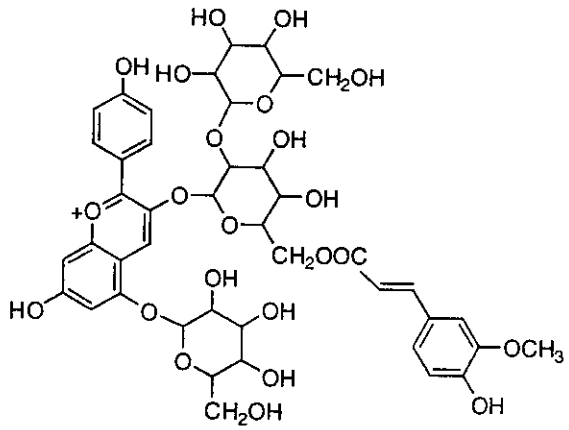
文献

Karrer, P. et al., Helv. Chim. Acta, 1927, 10, 67; 1928, 12, 292, (分離, Monardein)

Karrer, P. et al., Helv. Chim. Acta, 1927, 10, 67; 1928, 12, 292, (分離, Monardein)
Timberlake, C.F. et al., The Flavonoids, (Eds. Harborne, J.B. et al), Chapman and Hall, London, 1975, 215, (レビュー)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Giusti, M.M. et al., J. Agric. Food Chem., 1998, 46, 4858-4863, (*Raphanus sativus* anthocyanins)

§ 3,4',5,7-Tetrahydroxyflavylium(1+) ; 3-*O*-[β -D-Glucopyranosyl-(1 → 2) -[4-hydroxy-3-methoxycinnamoyl-(→ 6)]-β-D-glucopyranoside] (*E*-), 5-*O*-β-D-glucopyranoside

[CAS No.]185027-87-6
[化合物分類]フラボノイド(Anthocyanidins and anthocyanins; 4 × O-置換基)
[構造式]

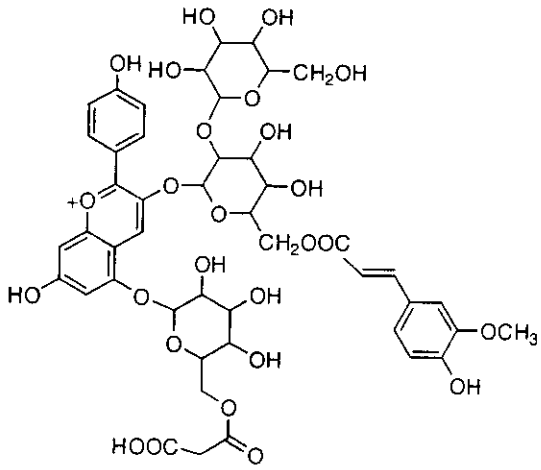


[分子式]$C_{43}H_{49}O_{23}^{(+)}$
[分子量]933.846
[基原]*Raphanus sativus*

文献
Karrer, P. et al., Helv. Chim. Acta, 1927, 10, 67; 1928, 12, 292, (分離, Monardein)
Timberlake, C.F. et al., The Flavonoids, (Eds. Harborne, J.B. et al), Chapman and Hall, London, 1975, 215, (レビュー)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Giusti, M.M. et al., J. Agric. Food Chem., 1998, 46, 4858-4863, (*Raphanus sativus* anthocyanins)

§ 3,4',5,7-Tetrahydroxyflavylium(1+) ; 3-*O*-[β -D-Glucopyranosyl-(1 → 2) -[4-hydroxy-3-methoxycinnamoyl-(→ 6)]-β-D-glucopyranoside] (*E*-), 5-*O*-(6-*O*-malonyl-β-D-glucopyranoside)

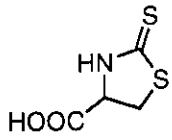
[CAS No.]218963-77-0
[化合物分類]フラボノイド(Anthocyanidins and anthocyanins; 4 × O-置換基)
[構造式]



[分子式]$C_{46}H_{51}O_{26}^{(+)}$
[分子量]1019.893
[基原]*Raphanus sativus*

文献
Karrer, P. et al., Helv. Chim. Acta, 1927, 10, 67; 1928, 12, 292, (分離, Monardein)
Timberlake, C.F. et al., The Flavonoids, (Eds. Harborne, J.B. et al), Chapman and Hall, London, 1975, 215, (レビュー)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988
Giusti, M.M. et al., J. Agric. Food Chem., 1998, 46, 4858-4863, (*Raphanus sativus* anthocyanins)

§ 2-Thioxo-4-thiazolidinecarboxylic acid; (*R*)-form

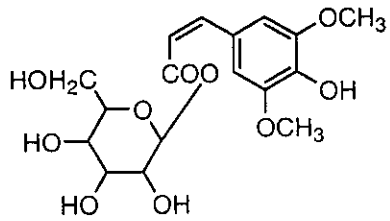


[化学名・別名]Raphanusamic acid
[CAS No.]98169-56-3
[化合物分類]アルカロイド化合物(Simple thiazole and benzothiazole alkaloids)
[構造式]
[分子式]$C_4H_5NO_2S_2$
[分子量]163.221
[基原]次の植物から分離: *Raphanus sativus* var. *hortensis* の黄化した発芽種子
[用途]植物成長阻害因子
[比旋光度]:$[\alpha]_D^{29}$ -86 (c, 2.5 in 0.5 *M* HCl)
[販売元]Aldrich:27344-9; Fluka:89113

----------文献----------

Calo, V. et al., Tetrahedron, 1994, 50, 7283, (合成法, ester, H-NMR)
Dobson, A.J. et al., Acta Cryst. C, 1998, 54, 1634-1637, (R-form, 結晶構造)

§ 3-(3,4,5-Trihydroxyphenyl)-2-propenoic acid; (*E*)-form, 3,5-Di-Me ether, β-D-glucopyranosyl ester

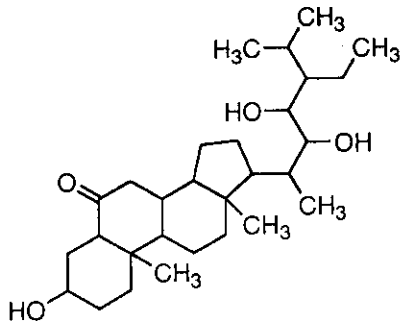


[化学名・別名]Raphanusol B. 1-Sinapoylglucose
[CAS No.]78185-48-5
[化合物分類]単環芳香族(Simple phenylpropanoids)
[構造式]
[分子式]$C_{17}H_{22}O_{10}$
[分子量]386.355
[基原]次の植物から分離: *Raphanus sativus* の発芽種子; also identified in *Brassica oleracea*, *Pelargonium zonale*, *Lilium speciosum*
[用途]ラディッシュの黄化した発芽種子の成長を阻害
[性状]青白い黄色の針状結晶
[融点]Mp 123-124 ℃

----------文献----------

Hasegawa, K. et al., Plant Cell Physiol., 1980, 21, 363; 1981, 22, 303, (Raphanusol B)
Hashimoto, K. et al., Planta Med., 1994, 60, 124, (Sinapic acid 4-glucoside)
Pauli, G.F. et al., Phytochemistry, 1995, 38, 1245, (Raphanusol B)

§ 3,22,23-Trihydroxystigmastan-6-one; (3 β,22*R*,23*R*,24*S*)-form

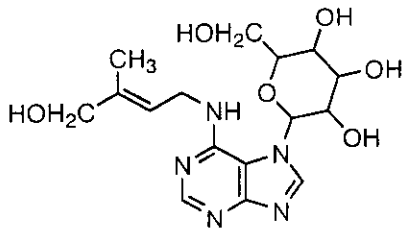


[化学名・別名]28-Homoteasterone
[CAS No.]90524-90-6
[化合物分類]ステロイド(Stigmastane steroids). (C29).
[構造式]
[分子式]$C_{29}H_{50}O_4$
[分子量]462.712
[基原]*Raphanus sativus*
[性状]結晶 (EtOAc/hexane)
[融点]Mp 206-209 ℃

----------文献----------

Takatsuto, S. et al., J.C.S. Perkin 1, 1984, 439, (合成法, H-NMR)
Schmidt, J. et al., Phytochemistry, 1993, 34, 391, (分離, 28-Homoteasterone)
Abe, H. et al., Biosci., Biotechnol., Biochem., 1995, 59, 176, (28-Homotyphasterol, Mass)

§ Zeatin; (*E*)-form, 7-β-D-Glucopyranosyl (7*H*-form)



[化学名・別名]Raphanatin
[CAS No.]38165-56-9
[化合物分類]アルカロイド化合物(Purines)
[構造式]
[分子式]$C_{16}H_{23}N_5O_6$
[分子量]381.388
[基原]*Raphanus sativus*, *Vinca rosea* のクラウンゴール
[用途]サイトカイニン
[性状]結晶 (MeOH)

[融点]Mp 266-271 ℃ (分解)
[比旋光度]:[α]$_D^{25}$ -14.8 (c, 3.5 in DMSO)

----------文 献----------

Cowley, D.E. et al., Aust. J. Chem., 1978, 31, 1095, (Raphanatin)

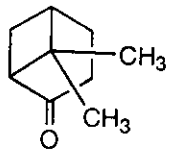
*********ラブダナム (Labdanum, Ciste) *********

§§ハンニチバナ科システ(*Cistus ladaniferus* L.)の葉または枝からの樹脂。
本調査研究では、成分に関する文献はなかった。

*********ラベンダー (Lavender) *********

§§シソ科トゥルーラベンダー(*Lavandula officinalis* Chaix)の花または茎葉。

§ **6,6-Dimethylbicyclo[3.1.1]heptan-2-one; (-)-form**



[CAS No.]77982-63-9
[化合物分類]テルペノイド(Pinane monoterpenoids)
[構造式]
[分子式]$C_9H_{14}O$
[分子量]138.209
[基原]次の植物から分離: *Lavandula officinalis* のオイル
[沸点]Bp$_{11}$ 85 ℃
[比旋光度]:[α]$_D$ -18.35 (semisynthetic)
[屈折率]n$^{25}_D$ 1.4772

----------文 献----------

Stadler, P.A., Helv. Chim. Acta, 1960, 43, 1601, (分離)
Ferreira, J.T.B., Chem. Eng. News, Dec. 10, 1990, 4, (haz)

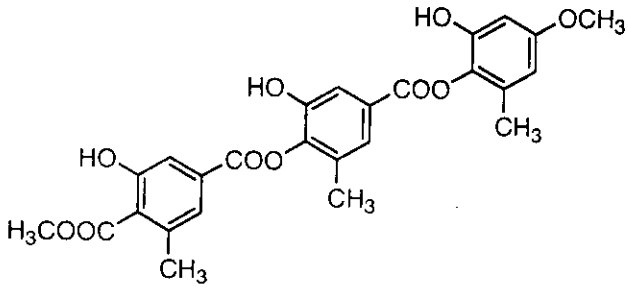
*********ラングウォルト (Lungwort) *********

§§ムラサキ科ヤクヨウヒメムラサキ(*Pulmonaria officinalia* L.)の茎葉。
本調査研究では、成分に関する文献はなかった。

*********ラングモス (Lungmoss) *********

§§地位類のラングモス(*Lobaria pulmonaria* (L.) Hoffmann)の葉状体。

§ **Gyrophoric acid; 4-Me ether, Me ester**



[化学名・別名]Tenuiorin. Peltigerin
[CAS No.]570-07-0
[化合物分類]単環芳香族
(Trimeric unchlorinated depsides)
[構造式]
[分子式]$C_{28}H_{24}O_{10}$
[分子量]496.47
[基原]次の植物から分離: *Peltigera polydactyla*, *Peltigera opthosa*, *Lobaria pulmonaria*, *Lobaria linita*, *Pseudocyphellaria* spp.
[性状]板状結晶 (Me_2CO/C_6H_6)
[融点]Mp 178-180 ℃ (cloudy melt). Mp 238 ℃で分解

----------文 献----------

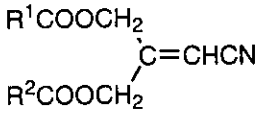
Huneck, S. et al., Annalen, 1965, 685; 128, (Tenuiorin, 成書)

*********ランブータン (Ramboutan) *********

§§ムクロジ科ランブータン(*Nephelium lappaceum* L.)の果実および種子。

§ *Nephelium lappaceum* **Type II cyanolipids**

[構造式]



N-IIb $R^1 = R^2 = -(CH_2)_7CH{=}CH(CH_2)_7CH_3(Z)$

[基原] *Nephelium lappaceum* の種子 N-IIc $R^1 = -(CH_2)_7CH{=}CH(CH_2)_7CH_3(Z)$, $R^2 = -(CH_2)_9CH{=}CH(CH_2)_7CH_3(Z)$ *lapp*

N-IId $R^1 = -(CH_2)_7CH{=}CH(CH_2)_7CH_3(Z)$, $R^2 = -(CH_2)_{18}CH_3$

[用途]殺虫作用を示す

----------文献----------

Nishizawa, M. et al., Phytochemistry, 1983, 22, 2853-2855, (分離, H-NMR, Mass)
Nishizawa, M. et al., Tet. Lett., 1983, 24, 4447-4450, (合成法)

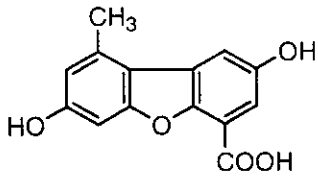
**********リキュール (Liqueur) **********

§§ベルモット，コアントロー，アブサン，スロージン，キュラソーなどのリキュール。(その他) 通常分別蒸留を行って最も香気の強い留分を採取する。

**********リーク (Leek) **********

§§ユリ科ニラネギ(*Allium porrum* L.)の茎葉。

§ **2,7-Dihydroxy-9-methyl-4-dibenzofurancarboxylic acid (CAS 名)**



[化学名・別名]Porric acid C

[CAS No.]207285-04-9

[化合物分類]単環芳香族(Dibenzofurans)

[構造式]

[分子式]$C_{14}H_{10}O_5$

[分子量]258.23

[基原]*Allium porrum* の球根

[用途]抗カビ剤

[性状]青白い黄色の結晶

[融点]Mp 230-232 ℃

UV: [neutral] λ max 238 ; 256 ; 288 ; 298 ; 334 (MeOH) [neutral] λ max 238 ; 256 ; 288 ; 298 ; 334 (MeOH) (Berdy)

----------文献----------

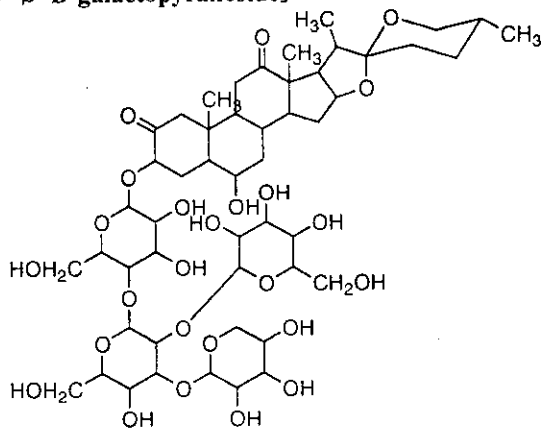
Carotenuto, A. et al., Eur. J. Org. Chem., 1998, 661-663, (分離, UV, H-NMR, C13-NMR)

§ **3,6-Dihydroxyspirostane-2,12-dione; (3 β,5 α,6 β,25*R*)-form, 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside]**

[CAS No.]289690-77-3

[化合物分類]ステロイド(Spirostane steroids). (C27).

[構造式]



[分子式]$C_{50}H_{78}O_{23}$

[分子量]1079.151

[基原]*Allium porrum*

[比旋光度]:$[\alpha]_D^{25}$ -13 (c, 0.003 in MeOH)

----------文献----------