

[化学名・別名] Ohchinolide B

[CAS No.] 71902-49-3

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)

[構造式]

[分子式] $C_{35}H_{44}O_{10}$

[分子量] 624.727

[正確な分子量] 624.29345

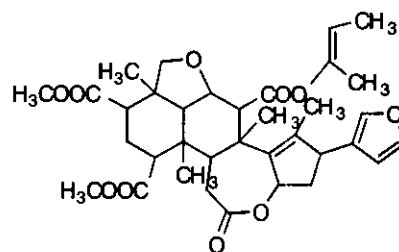
[基原] *Melia azedarach*, *Azadirachta indica*

[用途] Antifeedant against *Spodoptera littoralis*

[性状] 結晶 (MeOH)

[融点] Mp 211-212 °C

[比旋光度]: $[\alpha]_D^{20} -46.5$ (c, 1 in $CHCl_3$)



-----文献-----

Kraus, W. et al., Chem. Ber., 1981, 114, 267, (Ohchinolide B)

Kraus, W., The Neem Tree, (ed. Schmutterer, H.), VCH, 1995, 35, (レビュー)

§ Nimbolinin B

[CAS No.] 76689-93-5

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)

[構造式]

[分子式] $C_{35}H_{46}O_{10}$

[分子量] 626.742

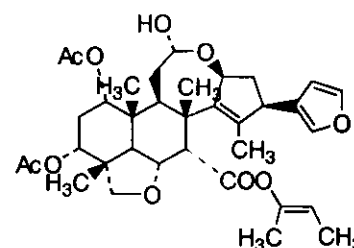
[正確な分子量] 626.3091

[基原] *Melia azedarach*

[性状] 無定型

[比旋光度]: $[\alpha]_D^{20} -55.5$ (c, 0.91 in $CHCl_3$)

[UV]: [neutral] λ_{max} 217 (ϵ 11000) (MeOH)



-----文献-----

Nakatani, M. et al., Heterocycles, 2000, 53, 689, (Nimbolinin)

§ Nimbolinin B; 1-De-Ac

[化学名・別名] 1-Deacetylnimbolinin B

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)

[構造式]

[分子式] $C_{33}H_{44}O_9$

[分子量] 584.705

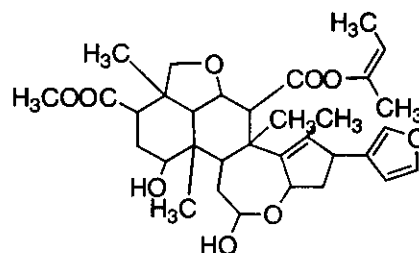
[正確な分子量] 584.298535

[基原] *Melia azedarach*

[性状] 無定型

[比旋光度]: $[\alpha]_D^{20} -42.8$ (c, 0.74 in $CHCl_3$)

[UV]: [neutral] λ_{max} 217 (ϵ 11000) (MeOH)



-----文献-----

Nakatani, M. et al., Phytochemistry, 1999, 52, 707, (1-Deacetylnimbolinin A)

Nakatani, M. et al., Heterocycles, 2000, 53, 689, (Nimbolinin)

§ Nimbolinin B; O⁷-Detigloyl, O⁷-benzoyl

[化学名・別名] Nimbolinin A

[CAS No.] 220698-26-0

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)

[構造式]

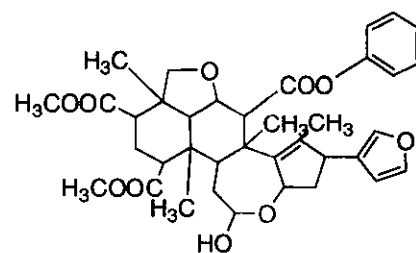
[分子式] $C_{37}H_{44}O_{10}$

[分子量] 648.749

[正確な分子量] 648.29345

[基原] 次の植物から分離: *Melia azedarach*, *Melia toosendan*

[性状] 無定型の粉末



[比旋光度]: $[\alpha]_D -35$ (c, 0.075 in MeOH)
[UV]: [neutral] λ_{max} 217 (ϵ 20000); 228 (ϵ 13000) (MeOH)

-----文献-----

Nakatani, M. et al., *Phytochemistry*, 1999, 52, 707, (1-Deacetylnimbolinin A)
Nakatani, M. et al., *Heterocycles*, 2000, 53, 689, (Nimbolinin)

§ Nimbolinin B; *O*⁷-Detigloyl, *O*⁷-benzoyl, *O*¹-de-Ac

[化学名・別名] 1-Deacetylnimbolinin A
[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)

[構造式]

[分子式] $C_{35}H_{42}O_9$

[分子量] 606.711

[正確な分子量] 606.28285

[基原] 次の植物から分離: *Melia azedarach*

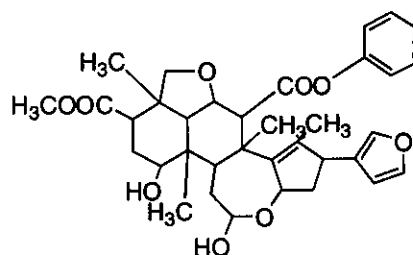
[性状] 無定形の粉末

[比旋光度]: $[\alpha]_D -7$ (c, 0.15 in MeOH)

[UV]: [neutral] λ_{max} 207 (ϵ 12000); 225 (ϵ 11000) (MeOH)

-----文献-----

Nakatani, M. et al., *Phytochemistry*, 1999, 52, 707, (1-Deacetylnimbolinin A)
Nakatani, M. et al., *Heterocycles*, 2000, 53, 689, (Nimbolinin)



§ Ohchinal

[CAS No.] 67023-79-4

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)

[構造式]

[分子式] $C_{35}H_{40}O_8$

[分子量] 588.696

[正確な分子量] 588.27232

[基原] *Melia azedarach*

[性状] 結晶

[融点] Mp 265-270 °C

[比旋光度]: $[\alpha]_D^{27} +107$ (c, 0.1 in $CHCl_3$)

-----文献-----

Ochi, M. et al., *Chem. Lett.*, 1978, 331

§ Ohchinin

[CAS No.] 67023-80-7

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)

[構造式]

[分子式] $C_{36}H_{42}O_8$

[分子量] 602.723

[正確な分子量] 602.28797

[基原] *Melia azedarach*

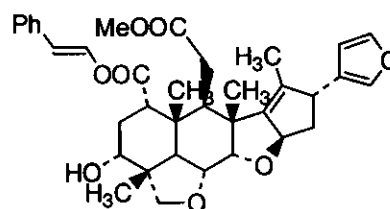
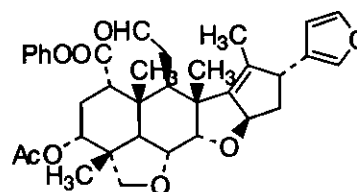
[性状] 結晶 (MeOH)

[融点] Mp 184-185 °C

[比旋光度]: $[\alpha]_D^{23} +64$ (c, 0.17 in EtOH)

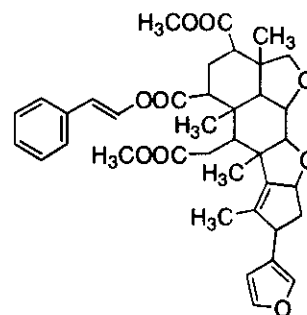
-----文献-----

Fukuyama, Y. et al., *Bull. Chem. Soc. Jpn.*, 1983, 56, 1139
Kraus, W., *Stud. Org. Chem. (Amsterdam)*, 1986, 26, 237, (tigloyl)



§ Ohchinin; Ac

[化学名・別名] Ohchinin acetate
[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)
[構造式]
[分子式] $C_{38}H_{44}O_9$
[分子量] 644.76
[正確な分子量] 644.298535
[基原] *Melia azedarach*
[性状] 結晶 (Et₂O/CH₂Cl₂)
[融点] Mp 223-226 °C
[比旋光度]: $[\alpha]_D^{23} +227$ (c, 0.23 in EtOH)



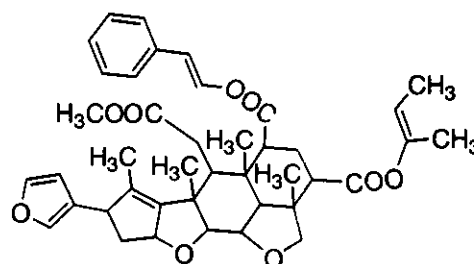
-----文献-----

Fukuyama, Y. et al., Bull. Chem. Soc. Jpn., 1983, 56, 1139
Kraus, W., Stud. Org. Chem. (Amsterdam), 1986, 26, 237, (tigloyl)

§ Ohchinin; 3-O-Tigloyl

[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)
[構造式]

[分子式] $C_{41}H_{48}O_9$
[分子量] 684.825
[正確な分子量] 684.329835
[基原] 次の植物の果実から分離: *Melia azedarach*

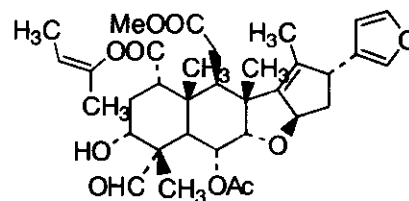


-----文献-----

Fukuyama, Y. et al., Bull. Chem. Soc. Jpn., 1983, 56, 1139
Kraus, W., Stud. Org. Chem. (Amsterdam), 1986, 26, 237, (tigloyl)

§ Ohchinolal

[化学名・別名] Salannal
[CAS No.] 86160-86-3
[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)
[構造式]
[分子式] $C_{34}H_{44}O_{10}$
[分子量] 612.716
[正確な分子量] 612.29345
[基原] *Melia azedarach*
[性状] 結晶 (Et₂O)
[融点] Mp 163-164.5 °C
[比旋光度]: $[\alpha]_D^{23} +52$ (c, 0.22 in EtOH). $[\alpha]_D^{20} +67$ (c, 0.05 in MeOH)

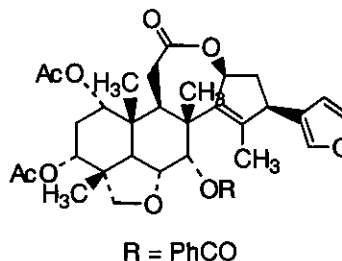


-----文献-----

Fukuyama, Y. et al., Bull. Chem. Soc. Jpn., 1983, 56, 1139
Nakatani, M. et al., Chem. Lett., 1995, 995, (分離, H-NMR, C13-NMR)
Huang, R.C. et al., Phytochemistry, 1996, 43, 581, (Salannal, 分離, H-NMR)
Zhou, J.-B. et al., Phytochemistry, 1997, 46, 911, (3-Ac)

§ Ohchinolide A

[CAS No.] 71902-48-2
[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)
[構造式]
[分子式] $C_{37}H_{42}O_{10}$
[分子量] 646.733
[正確な分子量] 646.2778
[基原] *Melia azedarach*
[性状] 結晶 (MeOH)
[融点] Mp 230-231 °C
[比旋光度]: $[\alpha]_D^{20} -42.5$ (c, 1 in $CHCl_3$)

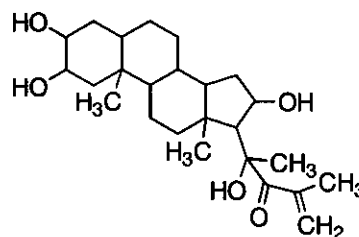


-----文献-----

Kraus, W. et al., Chem. Ber., 1981, 114, 267

§ Pregnane-2,3,16,20-tetrol; (2 α ,3 α ,5 α ,16 β ,20R)-form, 20-(2-Methylpropenoyl)

[化学名・別名] Azedarachol
[化合物分類] ステロイド (Pregnane steroid). (C21)
[構造式]
[分子式] $C_{25}H_{40}O_5$
[分子量] 420.588
[正確な分子量] 420.287575
[基原] Antifeedant from *Melia azedarach*
[性状] 結晶 (MeOH)
[融点] Mp 231-232 °C
[比旋光度]: $[\alpha]_D^{24} +20$ ($CHCl_3$)

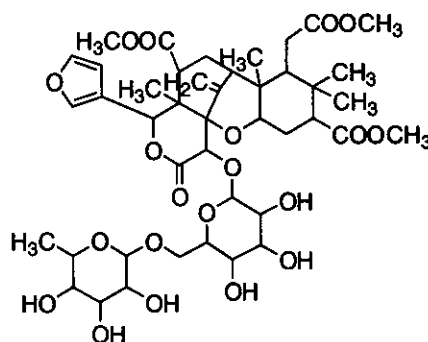


-----文献-----

Nakatani, M. et al., Phytochemistry, 1985, 24, 1945

§ Sandoricin; 15-O-[α -L-Rhamnopyranosyl (1 \rightarrow 6) - β -D-glucopyranoside]

[化学名・別名] Azecin 1
[CAS No.] 182565-73-7
[化合物分類] テルペノイド (Ring cleaved tetranortriterpenoid)
[構造式]
[分子式] $C_{43}H_{60}O_{20}$
[分子量] 896.935
[正確な分子量] 896.3678
[基原] *Melia azedarach*
[性状] 結晶
[融点] Mp 180-182 °C



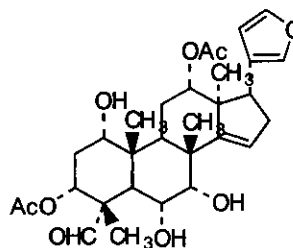
-----文献-----

Powell, R.G. et al., J. Nat. Prod., 1991, 54, 241, (分離, H-NMR, C13-NMR, 結晶構造)

Srivastava, S.D. et al., J. Indian Chem. Soc., 1996, 73, 467, (Azecin 1)

§ Sendandal

[CAS No.] 67721-74-8
[化合物分類] テルペノイド (Intact tetranortriterpenoid)
[構造式]
[分子式] $C_{30}H_{40}O_9$
[分子量] 544.641
[正確な分子量] 544.267235
[基原] *Melia azedarach*
[性状] 結晶
[融点] Mp 276-277 °C
[比旋光度]: $[\alpha]_D^{12} -14$ (c, 0.1 in EtOH)



Ochi, M. et al., Chem. Lett., 1978, 621

§ 1,3,5,8-Tetrahydroxy-2-methylantraquinone; 8-Me ether, 3-O- α -L-rhamnopyranoside

[CAS No.] 99624-38-1

[化合物分類] 多環芳香族 (9,10-Anthraquinone; 4 × O-置換基)

[構造式]

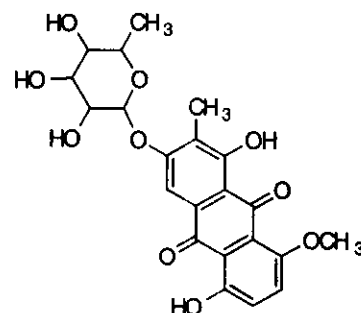
[分子式] C₂₂H₂₂O₁₀

[分子量] 446.41

[正確な分子量] 446.1213

[基原] 次の植物から分離: *Acacia leucophloea* の根, *Melia azedarach* の茎皮

[性状] 橙-黄色の結晶 (MeOH)



Tiwari, R.D. et al., Planta Med., 1971, 19, 299, (8-Me ether glucoside)

Srivastava, S.K. et al., Indian J. Chem., Sect. B, 1985, 24, 793, (8-Me ether rhamnoside)

Saxena, M. et al., J. Nat. Prod., 1986, 49, 205, (5-Me ether, 8-Me ether rhamnoside)

Singh, J. et al., Phytochemistry, 1987, 26, 507, (3-glucoside)

Tripathi, A.K. et al., Fitoterapia, 1993, 64, 63, (3-galactoside)

Courchesne, M. et al., J. Nat. Prod., 1993, 56, 722, (合成法, H-NMR, C13-NMR, 成書, 構造決定)

§ 2,3,5,6-Tetramethylxanthone

[化学名・別名] 2,3,5,6-Tetramethyl-9H-xanthen-9-one (CAS 名). Melianxanthone

[CAS No.] 224964-10-7

[化合物分類] 単環芳香族 (Xanthone; no O-置換基)

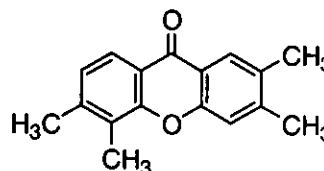
[構造式]

[分子式] C₁₇H₁₆O₂

[分子量] 252.312

[正確な分子量] 252.11503

[基原] *Melia azedarach* の樹皮



Yang, G. et al., CA, 1999, 130, 356986b

§ Trichilin B; 12-Ac

[化学名・別名] 12-O-Acetyltrichilin B

[化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

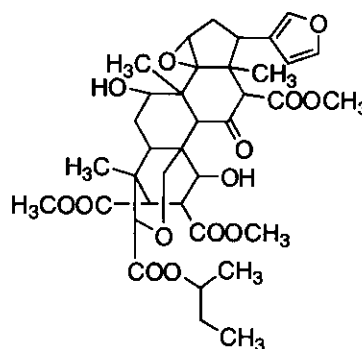
[分子式] C₃₇H₄₈O₁₄

[分子量] 716.778

[正確な分子量] 716.30441

[基原] *Melia azedarach*

[比旋光度]: [α]_D²² -2.5 (c, 0.16 in MeOH)



Nakatani, M. et al., Heterocycles, 1993, 36, 725, (Trichilins A, F, G)

Nakatani, M. et al., Heterocycles, 1994, 38, 2407, (Trichilin)

Zhou, J.-B. et al., Phytochemistry, 1996, 41, 117, (Trichilins K and L)

Gunatikala, A.A.L. et al., J. Nat. Prod., 1998, 61, 179, (Trichilin A, H-NMR, C13-NMR)

§ Trichilin B; 1,12-Di-Ac

[化学名・別名] 1,12-Di-O-acetyltrichilin B

[化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

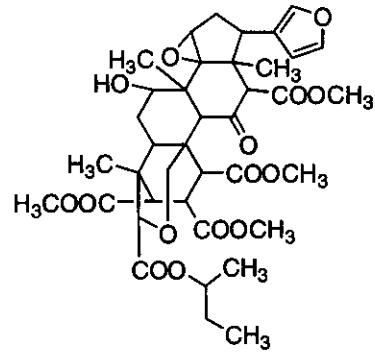
[分子式] $C_{39}H_{50}O_{15}$

[分子量] 758.815

[正確な分子量] 758.314975

[基原] *Melia azedarach*

[比旋光度]: $[\alpha]_D^{22} +0.8$ (c, 0.08 in MeOH)



-----文献-----

Nakatani, M. et al., *Phytochemistry*, 1985, 24, 195; 1994, 36, 39, (誘導體)

Nakatani, M. et al., *Heterocycles*, 1993, 36, 725, (Trichilins A, F, G)

Huang, R.C. et al., *Bull. Chem. Soc. Jpn.*, 1994, 67, 2468, (誘導體, H-NMR, C13-NMR)

Nakatani, M. et al., *Heterocycles*, 1994, 38, 2407, (Trichilin)

Takeya, K. et al., *Bioorg. Med. Chem.*, 1996, 4, 1355, (誘導體, H-NMR, C13-NMR)

Zhou, J.-B. et al., *Phytochemistry*, 1996, 41, 117, (Trichilins K and L)

Gunatikala, A.A.L. et al., *J. Nat. Prod.*, 1998, 61, 179, (Trichilin A, H-NMR, C13-NMR)

§ Trichilin B; 2-O-De-Ac

[化学名・別名] 12-Deacetyltrichilin I

[化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

[分子式] $C_{33}H_{44}O_{12}$

[分子量] 632.703

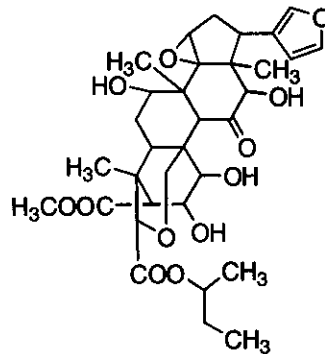
[正確な分子量] 632.28328

[基原] *Melia azedarach*

[性状] 粉末 (MeOH)

[融点] Mp 175-176 °C

[比旋光度]: $[\alpha]_D -32.4$ (c, 0.12 in MeOH)



-----文献-----

Nakatani, M. et al., *Heterocycles*, 1993, 36, 725, (Trichilins A, F, G)

Huang, R.C. et al., *Bull. Chem. Soc. Jpn.*, 1994, 67, 2468, (誘導體, H-NMR, C13-NMR)

Nakatani, M. et al., *Heterocycles*, 1994, 38, 2407, (Trichilin)

Takeya, K. et al., *Bioorg. Med. Chem.*, 1996, 4, 1355, (誘導體, H-NMR, C13-NMR)

Gunatikala, A.A.L. et al., *J. Nat. Prod.*, 1998, 61, 179, (Trichilin A, H-NMR, C13-NMR)

§ Trichilin B; 29-Deacyl, 29-(2-methylpropanoyl), 12-Ac

[化学名・別名] Trichilin H

[CAS No.] 156250-68-9

[化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

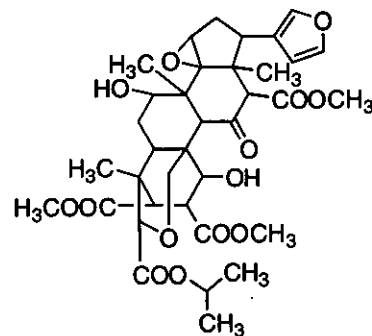
[分子式] $C_{36}H_{46}O_{14}$

[分子量] 702.751

[正確な分子量] 702.28876

[基原] *Melia azedarach*

[比旋光度]: $[\alpha]_D^{22} -20.2$ (c, 0.12 in MeOH)



-----文献-----

Nakatani, M. et al., *Heterocycles*, 1993, 36, 725, (Trichilins A, F, G)

Huang, R.C. et al., *Bull. Chem. Soc. Jpn.*, 1994, 67, 2468, (誘導體, H-NMR, C13-NMR)

Nakatani, M. et al., *Heterocycles*, 1994, 38, 2407, (Trichilin)

Takeya, K. et al., *Bioorg. Med. Chem.*, 1996, 4, 1355, (誘導體, H-NMR, C13-NMR)

Zhou, J.-B. et al., *Phytochemistry*, 1996, 41, 117, (Trichilins K and L)

Gunatikala, A.A.L. et al., *J. Nat. Prod.*, 1998, 61, 179, (Trichilin A, H-NMR, C13-NMR)

§ Trichilin B; 29-Deacyl, 29-(2-methylpropanoyl), 1,12-di-Ac

[化学名・別名] 1-Acetyltrichilin H

[化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

[分子式] $C_{38}H_{48}O_{13}$

[分子量] 744.788

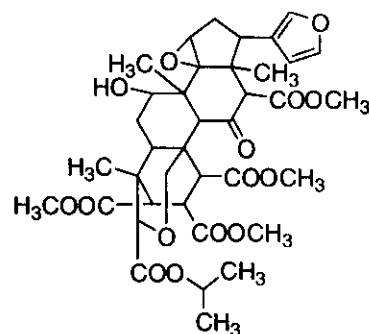
[正確な分子量] 744.299325

[基原] *Melia azedarach*

[性状] 粉末 (CHCl₃)

[融点] Mp 170-172 °C

[比旋光度]: $[\alpha]_D -19.7$ (c, 0.6 in CHCl₃)



-----文献-----

Huang, R.C. et al., Bull. Chem. Soc. Jpn., 1994, 67, 2468, (誘導体, H-NMR, C13-NMR)

Nakatani, M. et al., Heterocycles, 1994, 38, 2407, (Trichilin)

Takeya, K. et al., Bioorg. Med. Chem., 1996, 4, 1355, (誘導体, H-NMR, C13-NMR)

Zhou, J.-B. et al., Phytochemistry, 1996, 41, 117, (Trichilins K and L)

Gunatikala, A.A.L. et al., J. Nat. Prod., 1998, 61, 179, (Trichilin A, H-NMR, C13-NMR)

§ Trichilin B; 29-Deacyl, 29-(2-methylpropanoyl), 2-O-de-Ac, 1,12-di-Ac

[化学名・別名] 1-Acetyl-2-deacetyltrichilin H

[化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

[分子式] $C_{36}H_{46}O_{14}$

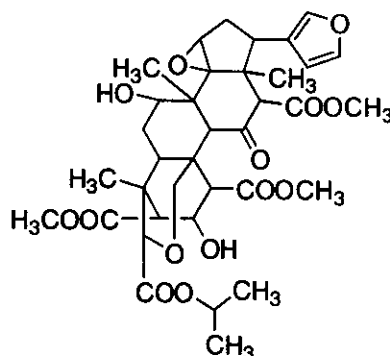
[分子量] 702.751

[正確な分子量] 702.28876

[基原] *Melia azedarach*

[性状] 粉末 (CHCl₃)

[融点] Mp 218-220 °C



-----文献-----

Nakatani, M. et al., Heterocycles, 1993, 36, 725, (Trichilins A, F, G)

Huang, R.C. et al., Bull. Chem. Soc. Jpn., 1994, 67, 2468, (誘導体, H-NMR, C13-NMR)

Nakatani, M. et al., Heterocycles, 1994, 38, 2407, (Trichilin)

Takeya, K. et al., Bioorg. Med. Chem., 1996, 4, 1355, (誘導体, H-NMR, C13-NMR)

Zhou, J.-B. et al., Phytochemistry, 1996, 41, 117, (Trichilins K and L)

Gunatikala, A.A.L. et al., J. Nat. Prod., 1998, 61, 179, (Trichilin A, H-NMR, C13-NMR)

§ Trichilin B; 29-Deacyl, 29-(2-methylpropanoyl), 3-O-de-Ac, 12-Ac

[化学名・別名] 3-Deacetyltrichilin H

[化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

[分子式] $C_{34}H_{44}O_{13}$

[分子量] 660.714

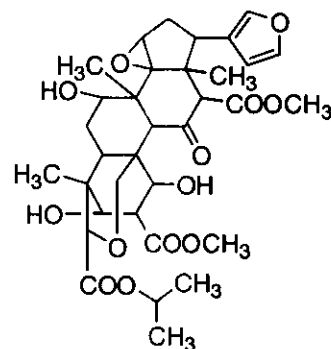
[正確な分子量] 660.278195

[基原] *Melia azedarach*

[性状] 粉末 (CHCl₃)

[融点] Mp 162-164 °C

[比旋光度]: $[\alpha]_D -4$ (c, 0.2 in CHCl₃)



-----文献-----

Nakatani, M. et al., Heterocycles, 1993, 36, 725, (Trichilins A, F, G)

Huang, R.C. et al., Bull. Chem. Soc. Jpn., 1994, 67, 2468, (誘導体, H-NMR, C13-NMR)

Nakatani, M. et al., Heterocycles, 1994, 38, 2407, (Trichilin)

Takeya, K. et al., *Bioorg. Med. Chem.*, 1996, 4, 1355, (誘導体, H-NMR, C13-NMR)
 Zhou, J.-B. et al., *Phytochemistry*, 1996, 41, 117, (Trichilins K and L)
 Gunatikala, A.A.L. et al., *J. Nat. Prod.*, 1998, 61, 179, (Trichilin A, H-NMR, C13-NMR)

§ **Trichilin B; 29-Deacyl, 29-(2-methylpropanoyl), 3-O-de-Ac, 1,12-di-Ac**

[化学名・別名] 1-Acetyl-3-deacetyltrichilin H
 [化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

[分子式] $C_{36}H_{46}O_{14}$

[分子量] 702.751

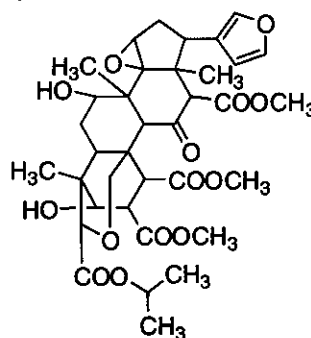
[正確な分子量] 702.28876

[基原] *Melia azedarach*

[性状] 粉末 (CHCl₃)

[融点] Mp 162-164 °C

[比旋光度]: $[\alpha]_D^{25} -11.7$ (c, 0.2 in CHCl₃)



-----文献-----

Nakatani, M. et al., *Heterocycles*, 1993, 36, 725, (Trichilins A, F, G)
 Huang, R.C. et al., *Bull. Chem. Soc. Jpn.*, 1994, 67, 2468, (誘導体, H-NMR, C13-NMR)
 Nakatani, M. et al., *Heterocycles*, 1994, 38, 2407, (Trichilin)
 Takeya, K. et al., *Bioorg. Med. Chem.*, 1996, 4, 1355, (誘導体, H-NMR, C13-NMR)
 Zhou, J.-B. et al., *Phytochemistry*, 1996, 41, 117, (Trichilins K and L)
 Gunatikala, A.A.L. et al., *J. Nat. Prod.*, 1998, 61, 179, (Trichilin A, H-NMR, C13-NMR)

§ **Trichilin B; 12-Deoxy**

[化学名・別名] Trichilin D. Meliatoxin A₁

[CAS No.] 77196-03-3

[化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

[分子式] $C_{35}H_{46}O_{12}$

[分子量] 658.741

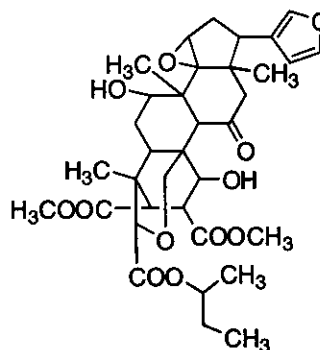
[正確な分子量] 658.29893

[基原] 次の植物から分離: *Trichilia roka*, *Melia azedarach*

[用途] *Spodoptera eridania* に対して活性を有する

[性状] オイル

[融点] Mp 148-154 °C で分解



-----文献-----

Oelrichs, P.B. et al., *Phytochemistry*, 1983, 22, 531, (Meliatoxin A₁)

§ **3,12,16-Trihydroxyeupha-7,24-dien-21-oic acid; (3 β, 12 β, 16 β)-form**

[CAS No.] 245072-64-4

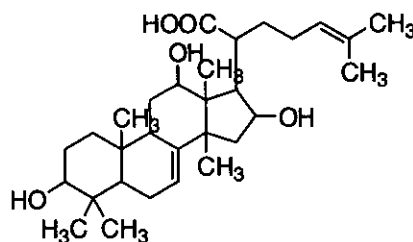
[化合物分類] テルペノイド (Tirucallane/euphane triterpenoid)

[構造式]

[基原] *Melia azedarach*

[性状] ガム

[比旋光度]: $[\alpha]_D^{22} -127.5$ (c, 0.02 in CHCl₃)



-----文献-----

Zhao, W.M. et al., *Chin. Chem. Lett.*, 1999, 10, 289, (分離, H-NMR, C13-NMR)

§ 4',5,7-Trihydroxyflavone; 5-O-β-D-Galactopyranoside

[CAS No.] 84268-41-7

[化合物分類] フラボノイド (Flavone; 3 × O-置換基)

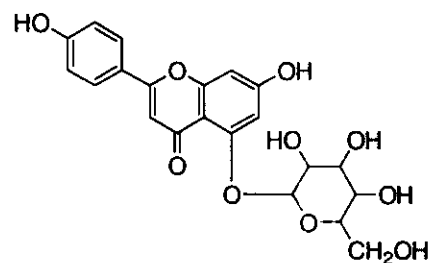
[構造式]

[分子式] C₂₁H₂₀O₁₀

[分子量] 432.383

[正確な分子量] 432.10565

[基原] 次の植物から分離: *Ixora arborea*, *Melia azedarach*



-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhauser Verlag, Basel, 1972, 1449, (生育)

Matsuura, S. et al., *Chem. Pharm. Bull.*, 1978, 26, 305, (合成法, 4',5,7-Trimethoxyflavone)

Chauhan, J.S. et al., *Curr. Sci.*, 1982, 51, 1069; 1985, 54, 570, (5-galactoside)

Jaipetch, T. et al., *Phytochemistry*, 1983, 22, 625, (4',5,7-Trimethoxyflavone)

Besson, E. et al., *Phytochemistry*, 1984, 23, 159, (分離, 成書)

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

§ 4',5,7-Trihydroxyflavone; 7-O-[α-L-Rhamnopyranosyl-(1 → 4)-β-D-glucopyranoside]

[CAS No.] 93053-01-1

[化合物分類] フラボノイド (Flavone; 3 × O-置換基)

[構造式]

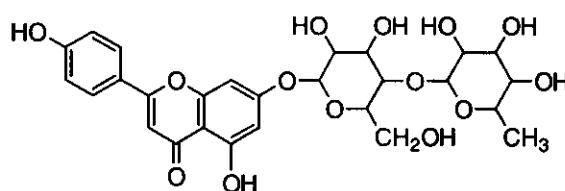
[分子式] C₂₇H₃₀O₁₄

[分子量] 578.526

[正確な分子量] 578.16356

[基原] *Melia azedarach* の茎皮

[融点] Mp 208-210 °C



-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhauser Verlag, Basel, 1972, 1449, (生育)

Wollenweber, E., *Phytochemistry*, 1974, 13, 2318; 1975, 15, 438; 2013; 1977, 16, 295, (生育)

Matsuura, S. et al., *Chem. Pharm. Bull.*, 1978, 26, 305, (合成法, 4',5,7-Trimethoxyflavone)

Jaipetch, T. et al., *Phytochemistry*, 1983, 22, 625, (4',5,7-Trimethoxyflavone)

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

Ahmed, A.A. et al., *Phytochemistry*, 1989, 28, 1751, (7-rhamnosylgalacturonoside)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, CDH250

§ Vilasinin; 7-Cinnamoyl, 1,3-di-Ac

[化学名・別名] Nimbolin A

[CAS No.] 24480-41-9

[化合物分類] テルペノイド (Intact tetranortriterpenoid)

[構造式]

[分子式] C₃₉H₄₆O₉

[分子量] 642.788

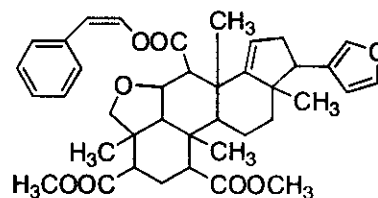
[正確な分子量] 642.31927

[基原] *Azadirachta indica*, *Melia azedarach*

[性状] 結晶

[融点] Mp 180-183 °C

[比旋光度]: [α]_D -38.6



-----文献-----

Ekong, D.E.U. et al., *Chem. Comm.*, 1969, 1166, (Nimbolin A)

Okogun, J.I. et al., *J.C.S. Perkin 1*, 1975, 1352, (Nimbolin A)

*****セントジョーンズウォルト (St. John's wort) *****

§ § オトギリソウ科セイヨウトドリ (*Hypericum perforatum* L.) の全草または果実。

§ Furohyperforin

[CAS No.] 219793-20-1

[化合物分類] テルペノイド (Meroterpenoid)

[構造式]

[分子式] $C_{35}H_{52}O_5$

[分子量] 552.793

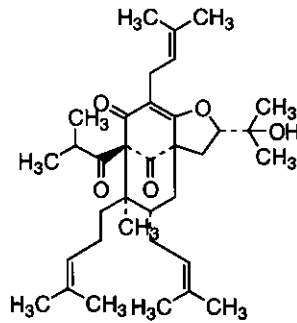
[正確な分子量] 552.381475

[基原] *Hypericum perforatum*

[性状] オイル

[比旋光度]: $[\alpha]_D^{20} +62.4$ (c, 0.9 in $CHCl_3$)

[UV]: [neutral] λ_{max} 272 (log ϵ 4.06) (EtOH)



-----文献-----

Verotta, L. et al., J. Nat. Prod., 1999, 62, 770, (分離, H-NMR, C13-NMR, UV, IR, CD, Mas)

§ 8-Hydroxyhyperforin 8,1-hemiacetal

[CAS No.] 262857-89-6

[化合物分類] テルペノイド (Meroterpenoid), 単環芳香族

(Acylphloroglucinol)

[構造式]

[分子式] $C_{35}H_{52}O_5$

[分子量] 552.793

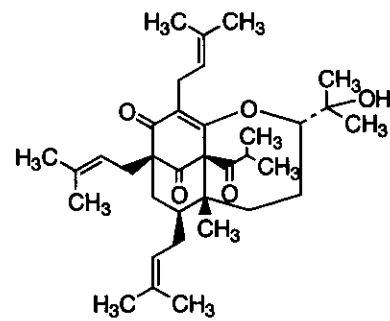
[正確な分子量] 552.381475

[基原] *Hypericum perforatum*

[性状] 粘着性オイル

[比旋光度]: $[\alpha]_D^{20} +34$ (c, 1 in $CHCl_3$)

[UV]: [neutral] λ_{max} 270 (log ϵ 3.21); 380 (log ϵ 1.66) ($CHCl_3$)



-----文献-----

Verotta, L. et al., J. Nat. Prod., 2000, 63, 412

§ Hyperforin

[CAS No.] 11079-53-1

[化合物分類] 単環芳香族 (Acylphloroglucinol), 薬物: 抗うつ薬

(Antidepressant)

[構造式]

[分子式] $C_{35}H_{52}O_4$

[分子量] 536.793

[正確な分子量] 536.38656

[基原] *Hypericum perforatum* (St John's Wort)

[用途] グラム陽性・陰性菌に対して抗菌性を有する. 抗うつ薬

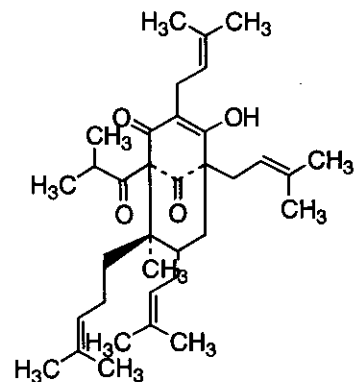
[性状] 結晶

[融点] Mp 79-80 °C

[比旋光度]: $[\alpha]_D^{18} +41$ (EtOH)

[溶解性] BERDY SOL: ベンゼンに可溶

[UV]: [acid] λ_{max} 278 (ϵ 8400) (EtOH/HCl) [base] λ_{max} 298 (ϵ 12000) (EtOH/NaOH) [neutral] λ_{max} 278 (ϵ 8400) (EtOH/HCl) [neutral] λ_{max} 278 (ϵ 8200); 298 (ϵ 11000) (EtOH) [acid] λ_{max} 278 (ϵ 8400) (EtOH-HCl) [base] λ_{max} 298 (ϵ 12000) (EtOH-NaOH)



-----文献-----

Gurevich, A.I. et al., Antibiotiki (Moscow), 1971, 16, 510; CA, 75, 95625, (分離, 性質)

Bystrov, N.S. et al., Bioorg. Khim., 1978, 4, 791, (構造決定)

Brondz, I. et al., Tet. Lett., 1982, 23, 1299, (結晶構造)

Schempp, C.M. et al., Lancet, 1999, i, 2129, (活性)

Moore, L.B. et al., Proc. Natl. Acad. Sci. U.S.A., 2000, 97, 7500, (薬理)

§ Hypericin

[化学名・別名] 1,3,4,6,8,13-Hexahydroxy-10,11-dimethylphenanthro[1,10,9,8-*opqra*] perylene-7,14-dione (CAS 名). Mycoporphyrin. Hypericum red

[CAS No.] 548-04-9

[化合物分類] 多環芳香族 (Extended quinone), 多環芳香族 (Miscellaneous polycyclic aromatic), 薬物: 抗うつ薬 (Antidepressant), 薬物: 抗ウイルス物質 (Antiviral agent), 薬物: トランキライザ (Tranquilliser)

[構造式]

[分子式] $C_{30}H_{16}O_8$

[分子量] 504.452

[正確な分子量] 504.08452

[基原] 次の植物から分離: the mealy bug *Nipaecoccus aurilanatus*. Widespread in *Hypericum* spp. esp. *Hypericum perforatum* (St. John's wort) which is used as a folk remedy for treating depression and other nervous disturbances

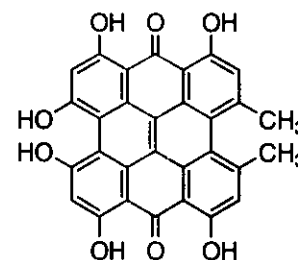
[用途] 抗うつ薬, トランキライザ; shows potent antiretroviral activity

[性状] blue-black needles

[融点] Mp 300 °C (分解)

[Log P 計算値] Log P 4.55 (計算値)

[UV]: [acid] λ_{max} 290 (ϵ 34000); 340 (ϵ 26000); 465 (ϵ 11500); 600 (ϵ 18500); 640 (ϵ 22500) (DMSO as potassium salt) [base] λ_{max} 384 (ϵ 12100); 446 (ϵ 12900); 472 (ϵ 13800); 509 (ϵ 10000); 546 (ϵ 24700); 589 (ϵ 43600) (MeOH as potassium salt) [neutral] λ_{max} 292 (ϵ 34000); 340 (ϵ 26500); 377 (ϵ 12000); 475 (ϵ 13500); 509 (ϵ 10000); 560 (ϵ 24000); 607 (ϵ 44000) (DMSO) [neutral] λ_{max} 508 (); 548 (); 590 () (MeOH) [neutral] λ_{max} 520 (); 559 (); 603 () (Py)



-----文献-----

Pace, N. et al., J.A.C.S., 1941, 63, 2570, (構造決定)

Banks, H.J. et al., Aust. J. Chem., 1976, 29, 1509, (分離)

Rodewald, G. et al., Angew. Chem., Int. Ed., 1977, 16, 46, (合成法, 成書)

Duran, N. et al., Photochem. Photobiol., 1986, 43, 677, (レビュー, 性質)

Meruelo, D., Proc. Natl. Acad. Sci. U.S.A., 1988, 85, 5230, (anti-HIV activity)

Etzistorfer, C. et al., Monatsh. Chem., 1993, 124, 923, (互変異性)

Freeman, D. et al., Chem. Comm., 1994, 891, (結晶構造, IR)

Gutman, I. et al., Monatsh. Chem., 1998, 129, 481; 1999, 130, 827, (互変異性)

Gruszecka-Kowalik, E. et al., Org. Prep. Proced. Int., 2000, 32, 57, (合成法, H-NMR)

§ Hyperin (旧 CAS 名)

[化学名・別名] 3-O- β -D-Galactopyranosyloxy-3',4',5,7-tetrahydroxyflavone. Quercetin 3-galactoside.

Hyperoside

[CAS No.] 482-36-0

[関連 CAS No.] 30113-33-8, 56508-10-2, 77133-40-5, 124086-76-6

[化合物分類] 薬物: 抗高血圧薬 (Antihypertensive agent), 薬物: 心正変力剤 (Inotropic agent), 薬物: 血管拡張剤 (Vasodilator), フラボノイド (Flavonol; 5 × O-置換基)

[構造式]

[分子式] $C_{27}H_{20}O_{12}$

[分子量] 464.382

[正確な分子量] 464.09548

[基原] 植物界に広く存在する, 例えば, リンゴの皮, *Crataegus laevigata* (hawthorn), *Hypericum perforatum*, *Betula*, *Juglans*, その他多くの属. Present in almost all of 60 investigated spp. in the タデ科 (Haumlnsel et al, 1954)

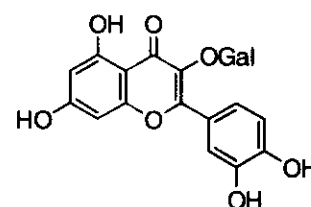
[用途] 抗高血圧薬.

[性状] 黄色の針状結晶 (EtOH)

[融点] Mp 232-233 °C で分解

[比旋光度]: $[\alpha]_D^{20}$ -83 (c, 0.2 in Py)

[Log P 計算値] Log P -2.92 (計算値)



[化学物質毒性データ総覧(RTEC)登録番号]DJ3009200

-----文献-----

Karrer, W. et al., *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhaumluser Verlag, Basel, 1972, no. 1531, (生育)

***RTECS (化学物質毒性データ) ***

生体影響物質 : 変異原物質

健康障害に関するデータ

変異原性に関するデータ

<<試験方法>> 微生物を用いた突然変異試験.

試験系 : 大腸菌 *Salmonella typhimurium*.

投与量・期間: 20 ug/plate

参考文献

ENMUDM *Environmental Mutagenesis* (New York, NY) V.1-9, 1979-87. For publisher information, see EMMUEG. [Vol.,頁,年(19-)]3,401,1981

§ 2-(Methoxycarbonyl)-5-methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone

[化合物分類] 単環芳香族 (Acylphloroglucinol), テルペノイド (Meroterpenoid)

[構造式]

[分子式] $C_{29}H_{46}O_4$

[分子量] 458.68

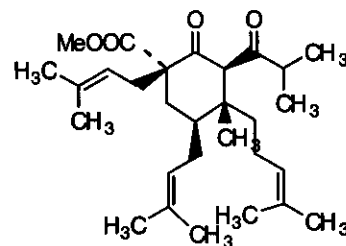
[正確な分子量] 458.33961

[基原] *Hypericum perforatum*

[性状] 粘調性のオイル

[比旋光度]: $[\alpha]_D^{26} +95.5$ (c, 1.1 in $CHCl_3$)

[UV]: [neutral] λ_{max} 245 (log ϵ 2.83); 274 (log ϵ 2.7) ($CHCl_3$)



-----文献-----

Shan, M.D. et al., *J. Nat. Prod.*, 2001, 64, 127-130

§ 2-(Methoxycarbonyl)-5-methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone; De (methoxycarbonyl)

[化合物分類] 単環芳香族 (Acylphloroglucinol), テルペノイド (Meroterpenoid)

[構造式]

[分子式] $C_{27}H_{44}O_6$

[分子量] 400.643

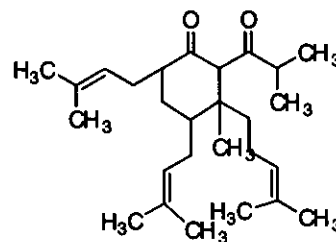
[正確な分子量] 400.33413

[基原] *Hypericum perforatum*

[性状] 粘調性のオイル

[比旋光度]: $[\alpha]_D^{26} +18.3$ (c, 1.8 in $CHCl_3$)

[UV]: [neutral] λ_{max} 245 (log ϵ 3.02); 265 (log ϵ 2.96) ($CHCl_3$)



-----文献-----

Shan, M.D. et al., *J. Nat. Prod.*, 2001, 64, 127-130

§ 2-Methyloctane (CAS 名)

[化学名・別名] Isononane

[CAS No.] 3221-61-2

[化合物分類] 脂肪族化合物 (Branched aliphatic hydrocarbon)

[構造式] $H_3C(CH_2)_5CH(CH_3)_2$

[分子式] C_9H_{20}

[分子量] 128.257

[正確な分子量] 128.1565

[基原] Found in petroleum. *Hypericum perforatum* のオイルの主成分

[融点] Mp -80.1 °C

[沸点] Bp 142.8 °C

[濃度] d^{20}_4 0.713

[屈折率] n_D^{20}

[傷害・毒性] 自然発火温度: 220 °C

-----文献-----

Whitmore, F. et al., J.A.C.S., 1938, 60, 2571, (合成法)

Mathis, C. et al., Phytochemistry, 1964, 3, 115; 133, (分離)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, MNC250

§ Oxepahyperforin

[CAS No.] 59014-02-7

[化合物分類] テルペノイド (Meroterpenoid), 単環芳香族

(Acylphloroglucinol)

[構造式]

[分子式] $C_{35}H_{52}O_5$

[分子量] 552.793

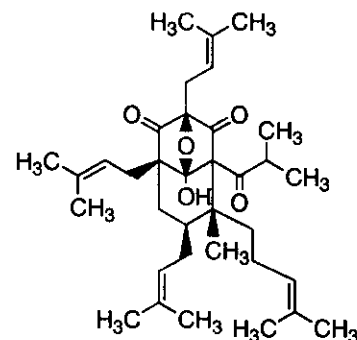
[正確な分子量] 552.381475

[基原] *Hypericum perforatum*

[性状] 粘調性のオイル

[比旋光度]: $[\alpha]_D^{20}$ -73.7 (c, 0.8 in $CHCl_3$)

[UV]: [neutral] λ_{max} 272 (log ϵ 3.83) ($CHCl_3$)



-----文献-----

Verotta, L. et al., J. Nat. Prod., 2000, 63, 412-415

§ Protohypericin

[CAS No.] 548-03-8

[化合物分類] 多環芳香族 (Miscellaneous polycyclic aromatic)

[構造式]

[分子式] $C_{30}H_{18}O_8$

[分子量] 506.467

[正確な分子量] 506.10017

[基原] 次の植物から分離: *Hypericum hirsutum*, *Hypericum montanum*,

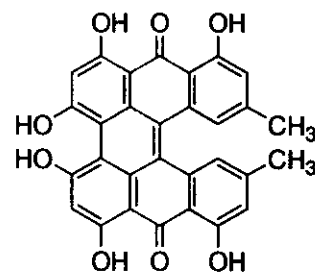
Hypericum perforatum and the mealy bugs *Pseudococcus albizziae*, *Nipaecoccus aurilantus*

[性状] 深い紫色の塊

[融点] Mp 300 °C

[UV]: [acid] λ_{max} 290 (ϵ 34000); 340 (ϵ 26000); 465 (ϵ 11500); 600 (ϵ 18500); 640 (ϵ 22500)

(DMSO as potassium salt) [base] λ_{max} 384 (ϵ 12100); 446 (ϵ 12900); 472 (ϵ 13800); 509 (ϵ 10000); 546 (ϵ 24700); 589 (ϵ 43600) (MeOH as potassium salt) [neutral] λ_{max} 292 (ϵ 34000); 340 (ϵ 26500); 377 (ϵ 12000); 475 (ϵ 13500); 509 (ϵ 10000); 560 (ϵ 24000); 607 (ϵ 44000) (DMSO)



-----文献-----

Brockmann, H. et al., Chem. Ber., 1958, 91, 547, (分離)

Banks, H.J. et al., Aust. J. Chem., 1976, 29, 1509, (分離, H-NMR, 合成法)

Cameron, D.W. et al., Aust. J. Chem., 1976, 29, 1535, (合成法)

Spitzner, D. et al., Angew. Chem., Int. Ed., 1977, 16, 46, (合成法)

§ Pyrano[7,28-b]hyperforin

[化合物分類] 単環芳香族 (Acylphloroglucinol), テルペノイド

(Meroterpenoid)

[構造式]

[分子式] $C_{35}H_{50}O_4$

[分子量] 534.778

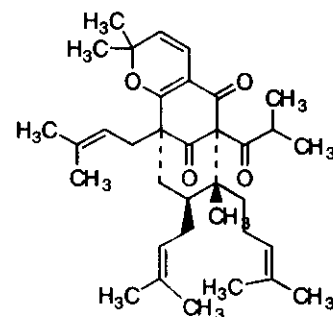
[正確な分子量] 534.37091

[基原] *Hypericum perforatum*

[性状] 粘調性のオイル

[比旋光度]: $[\alpha]_D^{27}$ +83.5 (c, 0.3 in $CHCl_3$)

[UV]: [neutral] λ_{max} 254 (log ϵ 3.77); 315 (log ϵ 3.53) ($CHCl_3$)



-----文献-----

Shan, M.D. et al., J. Nat. Prod., 2001, 64, 127-130

§ Pyrohyperforin

[CAS No.] 303115-46-0

[化合物分類] 単環芳香族 (Acylphloroglucinol), テルペノイド (Meroterpenoid)

[構造式]

[分子式] $C_{35}H_{50}O_4$

[分子量] 534.778

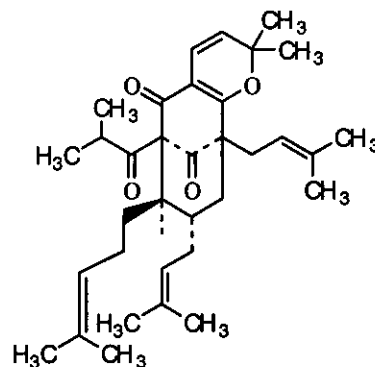
[正確な分子量] 534.37091

[基原] *Hypericum perforatum*

[性状] オイル

[比旋光度]: $[\alpha]_D +83.5$ (c, 0.28 in $CHCl_3$)

[UV]: [neutral] λ_{max} 254 (log ϵ 3.77); 315 (log ϵ 3.53) ($CHCl_3$)



-----文献-----

Shan, M.D. et al., Chin. Chem. Lett., 2000, 11, 701-704

§ Skyrin; (R)-form, 2-O- α -Arabinopyranoside

[化合物分類] 多環芳香族 (9,10-Anthraquinone; 3 \times O-置換基)

[構造式]

[分子式] $C_{35}H_{26}O_{14}$

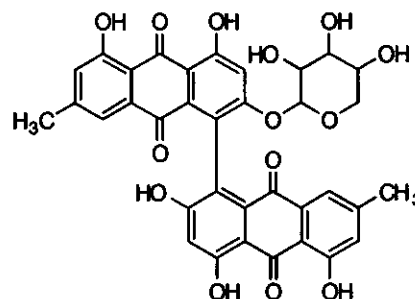
[分子量] 670.582

[正確な分子量] 670.13226

[基原] *Hypericum perforatum*

[性状] 橙-赤色の粉末

[UV]: [neutral] λ_{max} 219 (log ϵ 4.44); 258 (log ϵ 4.39); 294 (log ϵ 4.15); 459 (log ϵ 3.92) (MeOH)



-----文献-----

Shibita, Y. et al., Pharm. Bull., 1955, 3, 274; 278; 286, (分離)

Natori, S. et al., Chem. Pharm. Bull., 1965, 13, 385, (分離)

Briggs, L.H. et al., J.C.S., 1965, 2290, (分離)

Ogihara, Y. et al., Tet. Lett., 1968, 1881, (Auroskyrin)

Santesson, J. et al., Acta Chem. Scand., 1970, 24, 3331, (分離)

Yosioka, I. et al., Chem. Pharm. Bull., 1971, 19, 2420, (分離)

Huneck, S. et al., Phytochemistry, 1974, 13, 2315, (分離)

Cameron, D.W. et al., Aust. J. Chem., 1976, 29, 1509, (分離, 合成法)

Fujitake, N. et al., J. Nat. Prod., 1998, 61, 189-192, (Hinakurin)

Wirz, A. et al., Phytochemistry, 2000, 55, 941-947, (*Hypericum glycoside*)

Cole, R.J. et al., Handbook of Toxic Fungal Metabolites, Academic Press, New York, 1981, 690

§ Skyrin; (R)-form, 2-O- β -D-Xylopyranoside

[化合物分類] 多環芳香族 (9,10-Anthraquinone; 3 \times O-置換基)

[構造式]

[分子式] $C_{35}H_{26}O_{14}$

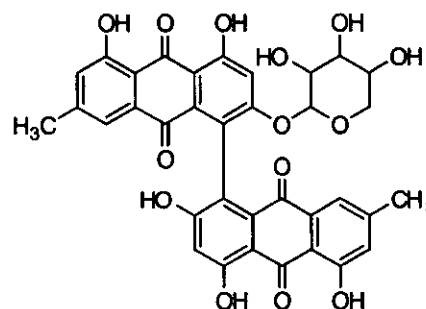
[分子量] 670.582

[正確な分子量] 670.13226

[基原] *Hypericum perforatum*

[性状] 橙-赤色の粉末

[UV]: [neutral] λ_{max} 219 (log ϵ 4.41); 258 (log ϵ 4.37); 294 (log ϵ 4.1); 456 (log ϵ 3.87) (MeOH)



-----文献-----

Shibita, Y. et al., Pharm. Bull., 1955, 3, 274; 278; 286, (分離)

Natori, S. et al., Chem. Pharm. Bull., 1965, 13, 385, (分離)

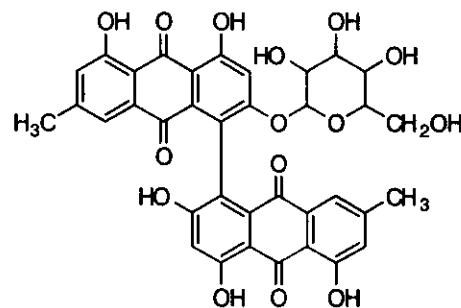
Briggs, L.H. et al., J.C.S., 1965, 2290, (分離)

Ogihara, Y. et al., Tet. Lett., 1968, 1881, (Auroskyrin)
 Santesson, J. et al., Acta Chem. Scand., 1970, 24, 3331, (分離)
 Yosioka, I. et al., Chem. Pharm. Bull., 1971, 19, 2420, (分離)
 Huneck, S. et al., Phytochemistry, 1974, 13, 2315, (分離)
 Cameron, D.W. et al., Aust. J. Chem., 1976, 29, 1509, (分離, 合成法)
 Fujitake, N. et al., J. Nat. Prod., 1998, 61, 189-192, (Hinakurin)
 Wirz, A. et al., Phytochemistry, 2000, 55, 941-947, (Hypericum glycoside)
 Cole, R.J. et al., Handbook of Toxic Fungal Metabolites, Academic Press, New York, 1981, 690

§ Skyrin; (R)-form, 2-O-β-D-Glucopyranoside

[化合物分類] 多環芳香族(9,10-Anthraquinone; 3 × O-置換基)

[構造式]



[分子式] C₃₆H₂₈O₁₅

[分子量] 700.608

[正確な分子量] 700.142825

[基原] *Hypericum perforatum*

[性状] 橙-赤色の粉末

[UV]: [neutral] λ_{max} 222 (log ε 4.59); 258 (log ε 4.54); 296 (log ε 4.28); 455 (log ε 4.14) (MeOH)

[その他のデータ] 融点: Mp >300 °C

-----文献-----

Shibita, Y. et al., Pharm. Bull., 1955, 3, 274; 278; 286, (分離)
 Natori, S. et al., Chem. Pharm. Bull., 1965, 13, 385, (分離)
 Briggs, L.H. et al., J.C.S., 1965, 2290, (分離)
 Ogihara, Y. et al., Tet. Lett., 1968, 1881, (Auroskyrin)
 Santesson, J. et al., Acta Chem. Scand., 1970, 24, 3331, (分離)
 Yosioka, I. et al., Chem. Pharm. Bull., 1971, 19, 2420, (分離)
 Huneck, S. et al., Phytochemistry, 1974, 13, 2315, (分離)
 Cameron, D.W. et al., Aust. J. Chem., 1976, 29, 1509, (分離, 合成法)
 Fujitake, N. et al., J. Nat. Prod., 1998, 61, 189-192, (Hinakurin)
 Wirz, A. et al., Phytochemistry, 2000, 55, 941-947, (Hypericum glycoside)
 Cole, R.J. et al., Handbook of Toxic Fungal Metabolites, Academic Press, New York, 1981, 690

§ Skyrin; (S)-form, 2-O-β-D-Glucopyranoside

[化合物分類] 多環芳香族(9,10-Anthraquinone; 3 × O-置換基)

[構造式]

[分子式] C₃₆H₂₈O₁₅

[分子量] 700.608

[正確な分子量] 700.142825

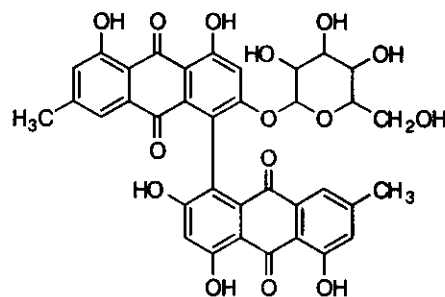
[基原] *Hypericum perforatum*

[性状] 橙-赤色の粉末

[UV]: [neutral] λ_{max} 219 (log ε 4.53); 258 (log ε 4.49); 298

(log ε 4.21); 455 (log ε 4.03) (MeOH)

[その他のデータ] 融点: Mp >300 °C



-----文献-----

Shibita, Y. et al., Pharm. Bull., 1955, 3, 274; 278; 286, (分離)
 Natori, S. et al., Chem. Pharm. Bull., 1965, 13, 385, (分離)
 Briggs, L.H. et al., J.C.S., 1965, 2290, (分離)
 Ogihara, Y. et al., Tet. Lett., 1968, 1881, (Auroskyrin)
 Santesson, J. et al., Acta Chem. Scand., 1970, 24, 3331, (分離)
 Yosioka, I. et al., Chem. Pharm. Bull., 1971, 19, 2420, (分離)
 Huneck, S. et al., Phytochemistry, 1974, 13, 2315, (分離)
 Franck, B. et al., Angew. Chem., Int. Ed., 1975, 14, 819, (合成法)
 Cameron, D.W. et al., Aust. J. Chem., 1976, 29, 1509, (分離, 合成法)
 Fujitake, N. et al., J. Nat. Prod., 1998, 61, 189-192, (Hinakurin)

Wirz, A. et al., *Phytochemistry*, 2000, 55, 941-947, (Hypericum glycoside)
Cole, R.J. et al., *Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 690

§ 1,3,8,9-Tetrahydroxy-6-methylanthracene

[化学名・別名] 1,3,8-Trihydroxy-6-methyl-9(10H)-anthracenone. 6-Methyl-1,3,8,9-anthracenetetrol.
Emodinanthranol. Emodinol. Protophyscihydrone. Frangulaemodinanthrone. Emodinanthrone.
Frangulaemodinanthranol. Emodin anthrone

[CAS No.] 491-60-1

[化合物分類] 多環芳香族 (Anthracene)

[構造式]

[分子式] $C_{15}H_{12}O_4$

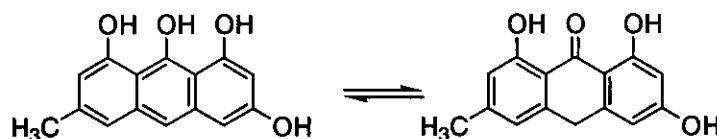
[分子量] 256.257

[正確な分子量] 256.07356

[基原] 次の植物から分離: *Rhamnus* spp., *Hypericum perforatum*, その他の植物物質

[性状] 黄色の板状結晶

[融点] Mp 250-258 °C で分解 (236 °C)



-----文献-----

Perkin, A.G., *J.C.S.*, 1894, 65, 937, (分離)

Tutin, F. et al., *J.C.S.*, 1912, 101, 290, (分離, 構造決定)

Brockmann, H. et al., *Naturwissenschaften*, 1953, 40, 509, (分離)

Lemli, J. et al., *Phytochemistry*, 1975, 14, 1397, (配糖体)

Amonkar, A. et al., *Experientia*, 1981, 37, 1138, (Geranyloxydihydroxymethylanthrone)

Abegaz, B. et al., *Bull. Chem. Soc. Ethiop.*, 1988, 2, 15; *CA*, 110, 92025c, (Prinoidin)

Abegaz, B.M. et al., *Phytochemistry*, 1995, 39, 1411, (Prinoidin)

§ 3',4',5,7-Tetrahydroxy-6-prenylflavone

[化学名・別名] 2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one
(CAS 名). Gancaonin O

[CAS No.] 129145-53-5

[化合物分類] フラボノイド (Flavone; 4 × O-置換基)

[構造式]

[分子式] $C_{20}H_{18}O_6$

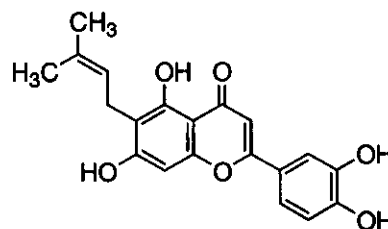
[分子量] 354.359

[正確な分子量] 354.11034

[基原] *Glycyrrhiza uralensis*, *Hypericum perforatum*

[性状] 黄色の針状結晶 (Me₂CO/hexane)

[融点] Mp 245-248 °C



-----文献-----

Crombie, L. et al., *J.C.S. Perkin 1*, 1982, 1455

Fukai, T. et al., *Heterocycles*, 1990, 31, 373, (分離, H-NMR, C13-NMR)

Ngadjui, B.T. et al., *Phytochemistry*, 1998, 48, 349, (分離, UV, H-NMR, C13-NMR)

Dias, A.C.P. et al., *Phytochemistry*, 1998, 48, 1165, (分離, UV, H-NMR, C13-NMR, Mas)

§ § オトギリソウ科オトギリソウ (*Hypericum erectum* Thunberg) の全草または果実。

§ 2-Methyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-propanone; 4-O-(3,7-dimethyl-2E,6E-octadienyl)

[化学名・別名] Otogirin

[CAS No.] 137251-97-9

[化合物分類] テルペノイド (Meroterpenoid)

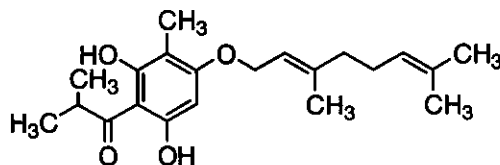
[構造式]

[分子式] $C_{21}H_{30}O_4$

[分子量] 346.466

[正確な分子量] 346.21441

[基原] *Hypericum erectum*



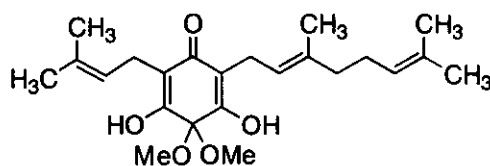
[性状] 結晶
[融点] Mp 66-68 °C

-----文献-----

Tada, M. et al., *Phytochemistry*, 1991, 30, 2559, (分離, H-NMR, C13-NMR)

§ Otogirone

[CAS No.] 137201-18-4
[化合物分類] テルペノイド (Meroterpenoid)
[構造式]
[分子式] C₂₃H₃₄O₅
[分子量] 390.519
[正確な分子量] 390.240625
[基原] *Hypericum erectum*



[性状] オイル
[UV]: [neutral] λ_{max} 252 (ε 11800); 313 (ε 2100) (EtOH)

-----文献-----

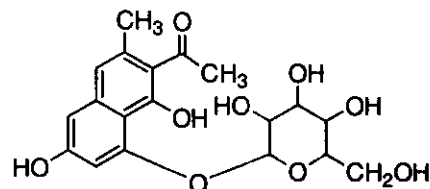
Tada, M. et al., *Phytochemistry*, 1991, 30, 2559, (分離, H-NMR, C13-NMR)

*****センナ (Senna) *****

§ § マメ科センナ (*Cassia senna* Linne) の果実または葉。

§ 2-Acetyl-1,6,8-trihydroxy-3-methylnaphthalene; 8-O-β-D-Glucopyranoside

[CAS No.] 23566-96-3
[化合物分類] 多環芳香族 (Naphthalene)
[構造式]
[分子式] C₁₉H₂₂O₉
[分子量] 394.377
[正確な分子量] 394.126385
[基原] 次の植物から分離: アブラムシ *Aphis nerii*, *Cassia senna* と
ダイオウ *Rhei rhizoma* のさや
[性状] 針状結晶 (EtOAc)
[融点] Mp 214-215 °C (207 °C)



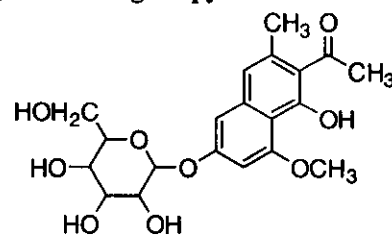
-----文献-----

Shibata, S. et al., *Chem. Pharm. Bull.*, 1969, 17, 454, (Torachryson)
Brown, K.S. et al., *Tet. Lett.*, 1969, 471, (分離, UV, H-NMR)
Tsuboi, M. et al., *Chem. Pharm. Bull.*, 1977, 25, 2708, (分離, H-NMR, C13-NMR, IR, UV, Mas)
Yamasaki, K. et al., *Tet. Lett.*, 1977, 1231, (C13-NMR, 配糖体)
Lin, C.-N. et al., *J. Nat. Prod.*, 1995, 58, 1934, (Isotorachryson)
Hatano, T. et al., *Chem. Pharm. Bull.*, 1999, 47, 1121, (Torachryson glycoside)

§ § マメ科ホソバセンナ (*Cassia angustifolia* Vahl) の果実または葉。

§ 2-Acetyl-1,6,8-trihydroxy-3-methylnaphthalene; 8-Me ether, 6-O-β-D-glucopyranoside

[CAS No.] 80358-06-1
[化合物分類] 多環芳香族 (Naphthalene)
[構造式]
[分子式] C₂₀H₂₄O₉
[分子量] 408.404
[正確な分子量] 408.142035
[基原] 次の植物の葉から分離: *Cassia angustifolia*
[性状] 青白い黄色の粉末
[融点] Mp 175 °C



-----文献-----

- Brown, K.S. et al., Tet. Lett., 1969, 471, (分離, UV, H-NMR)
 Tsuboi, M. et al., Chem. Pharm. Bull., 1977, 25, 2708, (分離, H-NMR, C13-NMR, IR, UV, Mas)
 Yamasaki, K. et al., Tet. Lett., 1977, 1231, (C13-NMR, 配糖体)
 Lemli, J. et al., Planta Med., 1981, 43, 11, (Tinnevellin glucoside)
 Wei, B.-L. et al., J. Nat. Prod., 1992, 55, 967, (Nakahalene)
 Lin, C.-N. et al., Phytochemistry, 1993, 33, 905, (6-Me ether, 8-xylosylglucoside)
 Lin, C.-N. et al., J. Nat. Prod., 1995, 58, 1934, (Isotorachryson)
 Hatano, T. et al., Chem. Pharm. Bull., 1999, 47, 1121, (Torachryson glycoside)

§ Aloemodin dianthrone

[化学名・別名] 4,4',5,5'-Tetrahydroxy-2,2'-bis(hydroxymethyl)-[9,9'-bianthracene]-10,10'-(9H,9'H)-dione
 (CAS名). Aloemodin bianthrone

[CAS No.] 4461-75-0

[化合物分類] 多環芳香族 (Anthracene)

[構造式]

[分子式] C₃₀H₂₂O₈

[分子量] 510.499

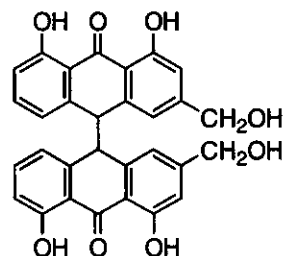
[正確な分子量] 510.13147

[基原] 次の植物から分離: *Cassia angustifolia* の葉, *Frangula alnus* の果実

[性状] 暗褐色の塊

[融点] Mp 260 °C で分解

[その他のデータ] λ_{max} 220, 270 nm



-----文献-----

- Auterhoff, H. et al., Arch. Pharm. (Weinheim, Ger.), 1960, 293, 918, (合成法, IR, UV)
 Lemli, J. et al., Pharm. Weekbl., 1964, 99, 589, (分離)
 Lemli, J., J. Nat. Prod., 1965, 28, 63, (分離)
 Kinjo, J. et al., Phytochemistry, 1994, 37, 1685, (diglucoside)

§ Aloemodin dianthrone; 5,5'-Di-O-D-glucopyranoside

[CAS No.] 99571-23-0

[化合物分類] 多環芳香族 (Anthracene)

[構造式]

[分子式] C₄₂H₄₂O₁₈

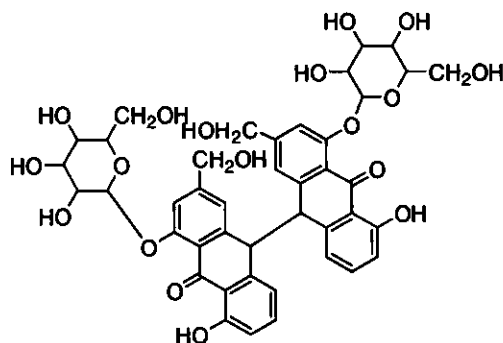
[分子量] 834.783

[正確な分子量] 834.23712

[基原] *Cassia angustifolia*

[性状] 無定型の粉末

[比旋光度]: [α]_D -186.4 (c, 0.49 in DMSO)



-----文献-----

- Auterhoff, H. et al., Arch. Pharm. (Weinheim, Ger.), 1960, 293, 918, (合成法, IR, UV)
 Lemli, J. et al., Pharm. Weekbl., 1964, 99, 589, (分離)
 Lemli, J., J. Nat. Prod., 1965, 28, 63, (分離)
 Kinjo, J. et al., Phytochemistry, 1994, 37, 1685, (diglucoside)

§ 9,10-Dihydro-4,5-dihydroxy-10-oxo-2-anthracenecarboxylic acid; O-Glucoside

[CAS No.] 54003-18-8

[化合物分類] 多環芳香族 (Anthracene)

[構造式] 有効な構造式はない

[分子式] C₂₁H₂₀O₁₀

[分子量] 432.383

[正確な分子量] 432.10565

[基原] *Cassia angustifolia*

-----文献-----

- Lemli, J. et al., Phytochemistry, 1975, 14, 1397, (配糖体)

Evans, F.J. et al., Biomed. Mass Spectrom., 1979, 6, 374, (Mas)
De Witte, P. et al., Pharmacology, suppl. 1, 1988, 36, 152, (代謝)

§ 9,10-Dihydro-4,5-dihydroxy-10-oxo-2-anthracenecarboxylic acid; O-Diglucoside

[CAS No.] 57077-57-3

[化合物分類] 多環芳香族 (Anthracene)

[構造式] 有効な構造式はない

[分子式] $C_{27}H_{30}O_{15}$

[分子量] 594.525

[正確な分子量] 594.158475

[基原] *Cassia angustifolia*

-----文献-----

Lemli, J. et al., Phytochemistry, 1975, 14, 1397, (配糖体)
Evans, F.J. et al., Biomed. Mass Spectrom., 1979, 6, 374, (Mas)
De Witte, P. et al., Pharmacology, suppl. 1, 1988, 36, 152, (代謝)

§ 1,8-Dihydroxy-3-(hydroxymethyl)-9(10H)-anthracenone; O-Glucoside

[CAS No.] 54003-19-9

[化合物分類] 多環芳香族 (Anthracene)

[構造式] 有効な構造式はない

[分子式] $C_{21}H_{22}O_9$

[分子量] 418.399

[正確な分子量] 418.126385

[基原] *Cassia angustifolia*

-----文献-----

Murty, V.K. et al., Tetrahedron, 1967, 23, 515, (合成法)
Lemli, J. et al., Phytochemistry, 1975, 14, 1397, (配糖体)

§ 1,8-Dihydroxy-3-(hydroxymethyl)-9(10H)-anthracenone; O-Diglucoside

[CAS No.] 57077-59-5

[化合物分類] 多環芳香族 (Anthracene)

[構造式] 有効な構造式はない

[分子式] $C_{27}H_{32}O_{14}$

[分子量] 580.541

[正確な分子量] 580.17921

[基原] *Cassia angustifolia*

-----文献-----

Murty, V.K. et al., Tetrahedron, 1967, 23, 515, (合成法)
Lemli, J. et al., Phytochemistry, 1975, 14, 1397, (配糖体)

§ 1,8-Dihydroxy-3-methyl-9(10H)-anthracenone; O-Diglucoside

[CAS No.] 57077-58-4

[化合物分類] 多環芳香族 (Anthracene)

[構造式] 有効な構造式はない

[分子式] $C_{27}H_{32}O_{13}$

[分子量] 564.542

[正確な分子量] 564.184295

[基原] *Cassia angustifolia*

-----文献-----

Howard, B.H. et al., Biochem. J., 1950, 46, 49; 1954, 56, 56, (分離)
Grundon, M.F. et al., J.C.S., 1952, 4580, (分離)
Khan, A.A., Can. J. Chem., 1963, 41, 1622, (分離)
Lemli, J. et al., Phytochemistry, 1975, 14, 1397, (配糖体)
Harris, C.M. et al., J.A.C.S., 1976, 98, 6065, (合成法)
Sax, N.I., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold, 1979, 506

§ Palmidin D

[化合物分類] 構造未知の天然物

[構造式] 不明

[一般的性質] 構造式は未知。

[基原] カルス培養 from cotyledons of *Cassia angustifolia*, *Rheum palmatum* の根

-----文献-----

Lemli, J. et al., *Planta Med.*, 1964, 12, 107, (分離)

Friedrich, H. et al., *Phytochemistry*, 1973, 12, 1459, (分離)

§ 1,2,3,6,8-Pentahydroxy-7-isopropylantraquinone; 1,2,3,6-Tetra-Me ether

[化学名・別名] 1-Hydroxy-2-isopropyl-3,6,7,8-tetramethoxyanthraquinone

[CAS No.] 214038-62-7

[化合物分類] 多環芳香族(9,10-Anthraquinone; 5 × O-置換基)

[構造式]

[分子式] $C_{21}H_{22}O_7$

[分子量] 386.401

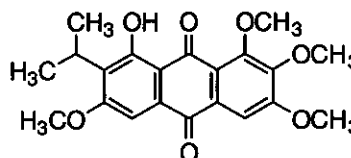
[正確な分子量] 386.136555

[基原] *Cassia angustifolia* の種子

[性状] 黄色の粉末

[融点] Mp 159 °C

[UV]:[neutral] λ_{max} 300 (); 320 (); 330 (); 360 () (EtOH)



-----文献-----

Gupta, A. et al., *Indian J. Chem., Sect. B*, 1998, 37, 615

§ Sennidin; (*R*,R**)-form, 5,5'-Di-O-β-D-glucopyranoside

[化学名・別名] Sennoside A. Amyran. Exprep. Glaxenna. Moivat. Senan. Tisasen A. Many other names

[CAS No.] 81-27-6

[化合物分類] 薬物: 緩下剤(Laxative), 多環芳香族

(Anthracene)

[構造式]

[分子式] $C_{42}H_{38}O_{20}$

[分子量] 862.75

[正確な分子量] 862.19565

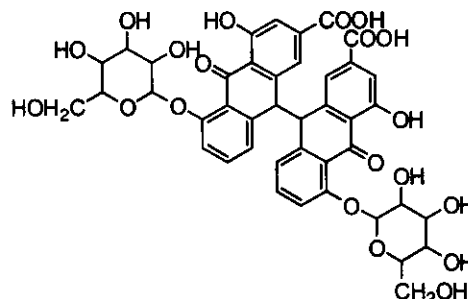
[基原] Cathartic principle from senna (*Cassia angustifolia*) and rhubarb

[性状] 黄色の板状結晶 (Me₂CO 溶液)

[融点] Mp 220-243 °C で分解

[比旋光度]: $[\alpha]_D^{20}$ -164 (c, 0.1 in 60% Me₂CO 溶液)

[Log P 計算値] Log P -1.38 (未確認値) (計算値)



-----文献-----

Stoll, A. et al., *Helv. Chim. Acta*, 1949, 32, 1892; 1950, 33, 313, (構造決定, 分離)

Lemmens, L., *Pharm. Weekbl.*, 1979, 1, 178, (代謝)

Tanaka, H. et al., *Chem. Pharm. Bull.*, 1982, 30, 1550, (分離)

Pharmacology, Suppl. 1, 1988, 36, (薬理, 代謝, 用途, レビュー)

Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, 1993, 903

Pharmacology, Suppl. 1, 1993, 47, (薬理, 代謝, 用途, レビュー)

Negwer, M., *Organic-Chemical Drug and their Synonyms*, 7th edn., Akademie-Verlag, 1994, 11693, (シノニム)

§ Sennidin; (*S*,S**)-form, 5,5'-Di-O-β-D-glucopyranoside

[化学名・別名] Sennoside G. Sennoside A'

[CAS No.] 66575-30-2

[化合物分類] 多環芳香族(Anthracene)

[構造式]