

Bader, G. et al., *Phytochemistry*, 1992, 31, 621, (Virgaureasaponin)

§ § アカテツ科マーマレードブラム (*Calocarpum sapota* Merrill) の果実。

§ 2-Hydroxy-2-phenylacetamide; (*R*)-form, *O*-[ $\beta$ -D-Xylopyranosyl-(1  $\rightarrow$  6)- $\beta$ -D-glucopyranoside]

[化学名・別名] Lucuminamide

[化合物分類] アルカロイド化合物 (Miscellaneous simple amide alkaloid)

[構造式]

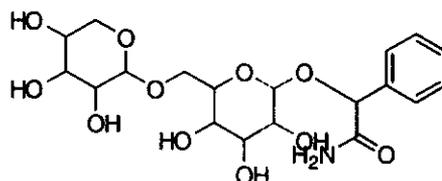
[分子式]  $C_{19}H_{27}NO_{11}$

[分子量] 445.422

[正確な分子量] 445.158414

[基原] *Calocarpum sapota*

[性状] 粉末



-----文献-----

Freudenberg, K. et al., *Annalen*, 1933, 501, 199, (合成法, 絶対構造)

Takeda, T. et al., *Chem. Pharm. Bull.*, 1997, 45, 697, (Lucuminamide)

§ Mandelic acid; (*R*)-form, *O*-[ $\beta$ -D-Xylopyranosyl-(1  $\rightarrow$  6)- $\beta$ -D-glucopyranoside]

[化学名・別名] Lucuminic acid

[化合物分類] 単環芳香族 (Phenylacetic acid derivative)

[構造式]

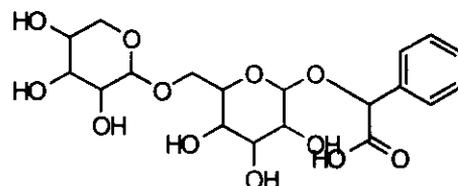
[分子式]  $C_{19}H_{26}O_{12}$

[分子量] 446.407

[正確な分子量] 446.14243

[基原] *Calocarpum sapota*

[性状] 粉末



-----文献-----

Welcher, F.J., *Organic Analytical Reagents*, Van Nostrand, New York, 1947, 2, 112, (合成法, 用途)

Takeda, T. et al., *Chem. Pharm. Bull.*, 1997, 45, 697, (Lucuminic acid)

\*\*\*\*\*サボテン (Cactus) \*\*\*\*\*

§ § サボテン科ウチワサボテン属のサボテン (*Opuntia megacantha* Salm-Dyck) の果実または茎節。  
本調査研究では研究報告ない。

§ § サボテン科ハシラサボテン属のベンケイチュウ (*Cereus gigantea* (Engelm.) Britton et Rose  
(*Cactus gigantea* Engelmann)) の果実または茎節。  
本調査研究では研究報告ない。

\*\*\*\*\*サラシナショウマ (Sarashinashoma) \*\*\*\*\*

§ § キンボウゲ科サラシナショウマ (*Cimicifuga simplex* Wormskjold) の根茎。

§ Acteol; 7,8-Didehydro, 12-Ac, 3-O- $\beta$

-D-xylopyranoside

[化学名・別名] Cimicifugoside

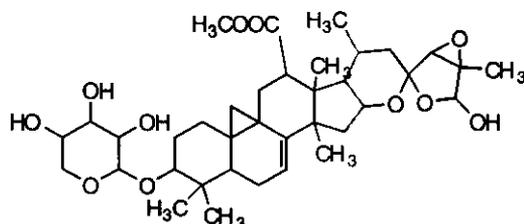
[CAS No.] 66176-93-0

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

[構造式]

[分子式]  $C_{37}H_{54}O_{11}$

[分子量] 674.827



[正確な分子量] 674.366615

[基原] *Cimicifuga simplex*

[性状] 結晶 (EtOH)

[融点] Mp 237-238 °C

-----文献-----

Kusano, G. et al., Chem. Pharm. Bull., 1977, 25, 3182

Wang, D. et al., CA, 1995, 123, 193603p, (27-Deoxyactein, Actein, C13-NMR)

Kadota, S. et al., Tetrahedron, 1995, 51, 1143, (arabinoside)

Kusano, A. et al., Chem. Pharm. Bull., 1998, 46, 467, (絶対構造)

Kusano, A. et al., Chem. Pharm. Bull., 1999, 47, 511, (26-Deoxycimicifugoside, 2'-O-Malonylcimicifugoside)

§ Acteol; 7,8-Didehydro, 12-Ac, 3-O-(2-O-malonyl-β-D-xylopyranoside)

[化学名・別名] 2'-O-Malonylcimicifugoside

[CAS No.] 245513-55-7

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

[構造式]

[分子式] C<sub>40</sub>H<sub>56</sub>O<sub>14</sub>

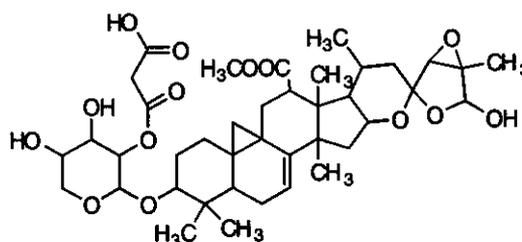
[分子量] 760.874

[正確な分子量] 760.36701

[基原] *Cimicifuga simplex*

[性状] 粉末

[比旋光度]: [α]<sub>D</sub> -55.9 (c, 0.88 in MeOH)



-----文献-----

Kusano, A. et al., Chem. Pharm. Bull., 1999, 47, 511, (26-Deoxycimicifugoside, 2'-O-Malonylcimicifugoside)

Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* const.)

§ Acteol; 26-Deoxy, 7,8-didehydro, 12-Ac

[化学名・別名] 26-Deoxycimicifugenin

[CAS No.] 228251-35-2

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

[構造式]

[分子式] C<sub>32</sub>H<sub>46</sub>O<sub>6</sub>

[分子量] 526.712

[正確な分子量] 526.32944

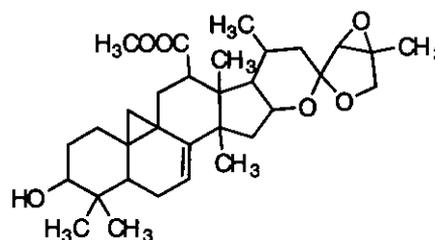
[基原] Aglycone from *Cimicifuga simplex*

[性状] 粉末 (MeOH)

[融点] Mp 300 °C

[比旋光度]: [α]<sub>D</sub> -135.5 (c, 0.73 in MeOH)

[その他のデータ] Mp > 300 °C



-----文献-----

Kusano, A. et al., Chem. Pharm. Bull., 1999, 47, 511, (26-Deoxycimicifugoside, 2'-O-Malonylcimicifugoside)

Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* const.)

§ Acteol; 26-Deoxy, 7,8-didehydro, 3-O-β-D-xylopyranoside, 12-Ac

[化学名・別名] 26-Deoxycimicifugoside

[CAS No.] 214146-75-5

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

[構造式]

[分子式] C<sub>37</sub>H<sub>54</sub>O<sub>10</sub>

[分子量] 658.828

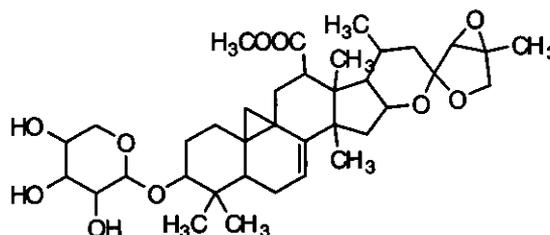
[正確な分子量] 658.3717

[基原] *Cimicifuga simplex*, *Actaea asiatica*

[性状] 針状結晶 (MeOH)

[融点] Mp 285-286 °C

[比旋光度]: [α]<sub>D</sub> -121 (c, 0.57 in MeOH)

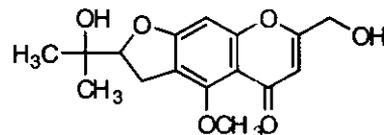


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- Kusano, A. et al., Chem. Pharm. Bull., 1998, 46, 467, (絶対構造)  
 Kusano, A. et al., Chem. Pharm. Bull., 1999, 47, 511, (26-Deoxycimifugoside, 2'-O-Malonylcimifugoside)  
 Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* constit.)

§ Angelicain; (S)-form, 4-Me ether

[化学名・別名] Cimifugin  
 [CAS No.] 37921-38-3  
 [化合物分類] ベンゾピラノイド (Furo-1-benzopyran)  
 [構造式]



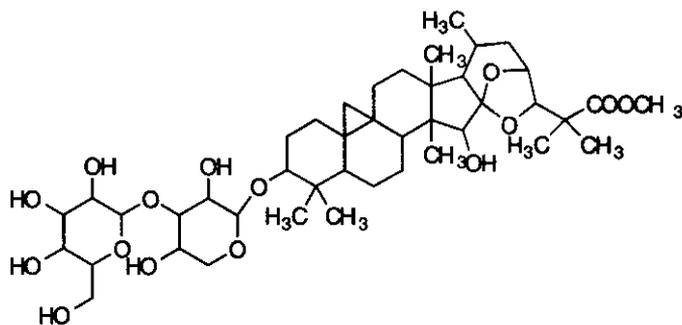
[分子式]  $C_{16}H_{18}O_6$   
 [分子量] 306.315  
 [正確な分子量] 306.11034  
 [基原] *Cimicifuga simplex* の根茎から得られる苦味成分  
 [性状] 針状結晶 (MeOH)  
 [融点] Mp 107-109 °C  
 [比旋光度]:  $[\alpha]_D +79.2$  (c, 0.8 in  $CHCl_3$ )

-----文献-----

- Kondo, Y. et al., Chem. Pharm. Bull., 1972, 20, 1940, (分離, 絶対構造, Cimicifugin)  
 Baba, K. et al., Chem. Pharm. Bull., 1981, 29, 2565, (分離, Cimifugin)  
 Kopp, B. et al., Helv. Chim. Acta, 1991, 74, 611, (Cimifugin glucoside)  
 Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* constit.)

§ Cimigenol; 3-O- $[\beta$ -D-Glucopyranosyl-(1→3)-xylopyranoside] 25-Ac

[CAS No.] 163894-56-2  
 [化合物分類] テルペノイド (Cycloartane triterpenoid)  
 [構造式]



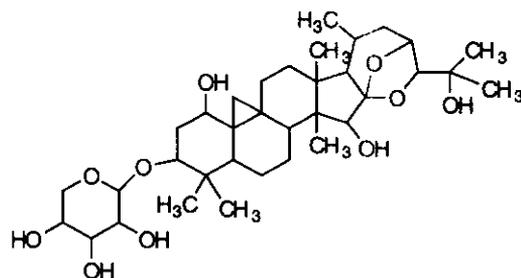
[分子式]  $C_{53}H_{88}O_{15}$   
 [分子量] 825.001  
 [正確な分子量] 824.455825  
 [基原] *Cimicifuga simplex*  
 [性状] 針状結晶  
 [融点] Mp 285-286 °C  
 [比旋光度]:  $[\alpha]_D +11.6$  (c, 0.3 in MeOH)

-----文献-----

- Corsano, S. et al., Chem. Comm., 1965, 185, (構造決定)  
 Takemoto, T. et al., Yakugaku Zasshi, 1968, 88, 623; 1969, 89, 954; 1970, 90, 64, (誘導體)  
 Corsano, S. et al., Gazz. Chim. Ital., 1969, 99, 1140, (構造)  
 Kusano, G. et al., Yakugaku Zasshi, 1975, 95, 1133  
 Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
 Li, C.J. et al., Yaoxue Xuebao, 1993, 28, 777; CA, 120, 143804x, (Cimiside)  
 Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* constit.)

§ Cimigenol; 1  $\alpha$ -Hydroxy, 3-O- $\alpha$ -L-arabinopyranoside

[CAS No.] 228256-76-6  
 [化合物分類] テルペノイド (Cycloartane triterpenoid)  
 [構造式]



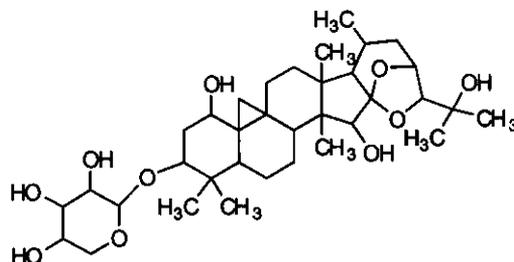
[分子式]  $C_{53}H_{86}O_{10}$   
 [分子量] 630.774  
 [正確な分子量] 630.3404  
 [基原] *Cimicifuga simplex*  
 [性状] 粉末 (MeOH/diisopropyl ether)  
 [融点] Mp 186-187 °C  
 [比旋光度]:  $[\alpha]_D +33.6$  (c, 0.98 in MeOH)

-----文献-----

- Corsano, S. et al., Gazz. Chim. Ital., 1969, 99, 1140, (構造)  
 Kusano, G. et al., Yakugaku Zasshi, 1975, 95, 1133  
 Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
 Li, C.J. et al., Yaoxue Xuebao, 1993, 28, 777; CA, 120, 143804x, (Cimicide)  
 Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* const.)  
 Kusano, A. et al., Chem. Pharm. Bull., 1999, 47, 511, (1  $\alpha$ -Hydroxycimigenol deriv)

§ Cimigenol; 1  $\alpha$ -Hydroxy, 3-O-xylopyranoside

- [CAS No.] 162897-45-2  
 [化合物分類]テルペノイド (Cycloartane triterpenoid)  
 [構造式]  
 [分子式] C<sub>35</sub>H<sub>56</sub>O<sub>10</sub>  
 [分子量] 636.821  
 [正確な分子量] 636.38735  
 [基原] *Cimicifuga simplex*  
 [性状] 針状結晶  
 [融点] Mp 187-188 °C  
 [比旋光度]: [ $\alpha$ ]<sub>D</sub><sup>20</sup> +24.6 (c, 0.68 in MeOH)

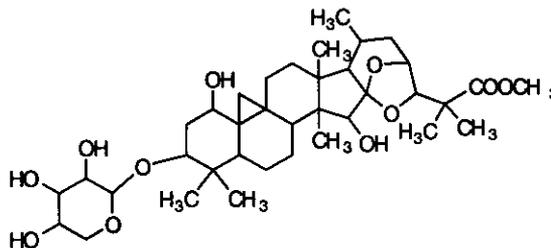


-----文献-----

- Takemoto, T. et al., Yakugaku Zasshi, 1968, 88, 623; 1969, 89, 954; 1970, 90, 64, (誘導體)  
 Kusano, G. et al., Yakugaku Zasshi, 1975, 95, 1133  
 Li, C.J. et al., Yaoxue Xuebao, 1993, 28, 777; CA, 120, 143804x, (Cimicide)  
 Kusano, A. et al., Chem. Pharm. Bull., 1999, 47, 511, (1  $\alpha$ -Hydroxycimigenol deriv)  
 Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* const.)

§ Cimigenol; 1  $\alpha$ -Hydroxy, 3-O-xylopyranoside, 25-Ac

- [CAS No.] 162897-44-1  
 [化合物分類]テルペノイド (Cycloartane triterpenoid)  
 [構造式]  
 [分子式] C<sub>37</sub>H<sub>58</sub>O<sub>11</sub>  
 [分子量] 678.859  
 [正確な分子量] 678.397915  
 [基原] *Cimicifuga simplex*  
 [性状] 針状結晶  
 [融点] Mp 175-176 °C  
 [比旋光度]: [ $\alpha$ ]<sub>D</sub><sup>20</sup> +26.2 (c, 0.97 in MeOH)

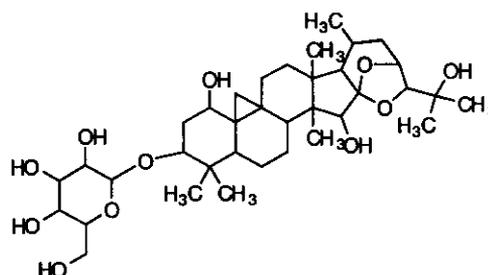


-----文献-----

- Kadota, S. et al., Tetrahedron, 1995, 51, 1143, (25-Acetylcimigenol xyloside, H-NMR, C13-NMR)  
 Kusano, A. et al., Chem. Pharm. Bull., 1999, 47, 511, (1  $\alpha$ -Hydroxycimigenol deriv)  
 Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* const.)

§ Cimigenol; 1  $\alpha$ -Hydroxy, 3-O- $\beta$ -D-galactopyranoside

- [CAS No.] 228251-32-9  
 [化合物分類]テルペノイド (Cycloartane triterpenoid)  
 [構造式]  
 [分子式] C<sub>36</sub>H<sub>58</sub>O<sub>11</sub>  
 [分子量] 666.848  
 [正確な分子量] 666.397915  
 [基原] *Cimicifuga simplex*  
 [性状] 粉末 (MeOH/diisopropyl ether)  
 [融点] Mp 185-186 °C  
 [比旋光度]: [ $\alpha$ ]<sub>D</sub> +25.7 (c, 0.47 in MeOH)



-----文献-----

- Kusano, A. et al., Chem. Pharm. Bull., 1999, 47, 511, (1  $\alpha$ -Hydroxycimigenol deriv)

Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* constit.)

§ Cimigenol; 7  $\beta$ -Hydroxy, 3-O- $\beta$ -D-xylopyranoside

[CAS No.] 168288-00-4

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

[構造式]

[分子式]  $C_{35}H_{56}O_{10}$

[分子量] 636.821

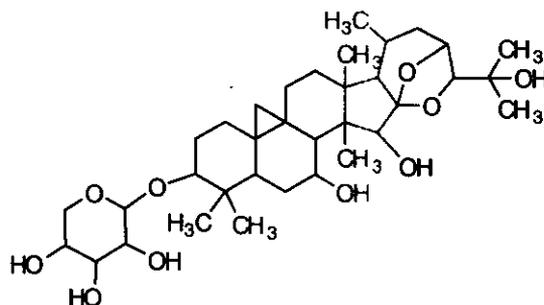
[正確な分子量] 636.38735

[基原] *Cimicifuga simplex*

[性状] 針状結晶 (MeCN/MeOH)

[融点] Mp 310 °C

[比旋光度]:  $[\alpha]_D +14.7$  (c, 1.2 in MeOH)



-----文献-----

Corsano, S. et al., Chem. Comm., 1965, 185, (構造決定)

Takemoto, T. et al., Yakugaku Zasshi, 1968, 88, 623; 1969, 89, 954; 1970, 90, 64, (誘導體)

Corsano, S. et al., Gazz. Chim. Ital., 1969, 99, 1140, (構造)

Kusano, G. et al., Yakugaku Zasshi, 1975, 95, 1133

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)

Li, C.J. et al., Yaoxue Xuebao, 1993, 28, 777; CA, 120, 143804x, (Cimicide)

Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* constit.)

§ Cimigenol; 7  $\beta$ -Hydroxy, 3-O- $\beta$ -D-xylopyranoside, 25-Ac

[CAS No.] 168288-01-5

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

[構造式]

[分子式]  $C_{37}H_{58}O_{11}$

[分子量] 678.859

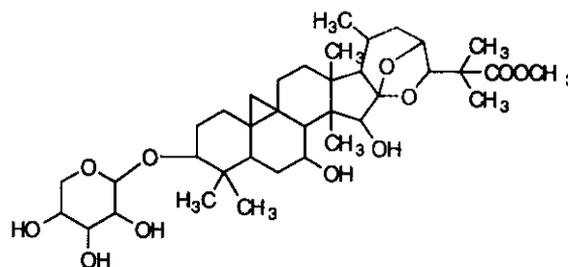
[正確な分子量] 678.397915

[基原] *Cimicifuga simplex*

[性状] 結晶 (MeCN/MeOH)

[融点] Mp 252-253 °C

[比旋光度]:  $[\alpha]_D +14$  (c, 0.4 in MeOH)



-----文献-----

Corsano, S. et al., Chem. Comm., 1965, 185, (構造決定)

Takemoto, T. et al., Yakugaku Zasshi, 1968, 88, 623; 1969, 89, 954; 1970, 90, 64, (誘導體)

Corsano, S. et al., Gazz. Chim. Ital., 1969, 99, 1140, (構造)

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)

Li, C.J. et al., Yaoxue Xuebao, 1993, 28, 777; CA, 120, 143804x, (Cimicide)

Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* constit.)

Kadota, S. et al., Tetrahedron, 1995, 51, 1143, (25-Acetylcimigenol xyloside, H-NMR, C13-NMR)

§ Cimigenol; 12  $\beta$ -Hydroxy, 3-O- $\beta$ -D-xylopyranoside

[化学名・別名] Cimicide A

[CAS No.] 152685-90-0

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

[構造式]

[分子式]  $C_{35}H_{56}O_{10}$

[分子量] 636.821

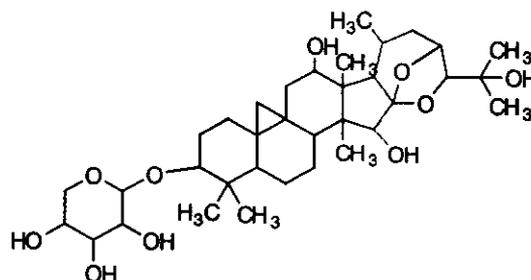
[正確な分子量] 636.38735

[基原] *Cimicifuga simplex*, *Cimicifuga dahurica*

[性状] 結晶 (MeOH)

[融点] Mp 286-287 °C

[比旋光度]:  $[\alpha]_D +6.4$  (c, 0.44 in MeOH)



-----文献-----

- Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
 Li, C.J. et al., Yaoxue Xuebao, 1993, 28, 777; CA, 120, 143804x, (Cimicide)  
 Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* const.)

§ **Cimigenol; 12 β-Hydroxy, 3-O-α-L-arabinopyranoside**

[CAS No.] 168287-99-8

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

[構造式]

[分子式] C<sub>35</sub>H<sub>56</sub>O<sub>10</sub>

[分子量] 636.821

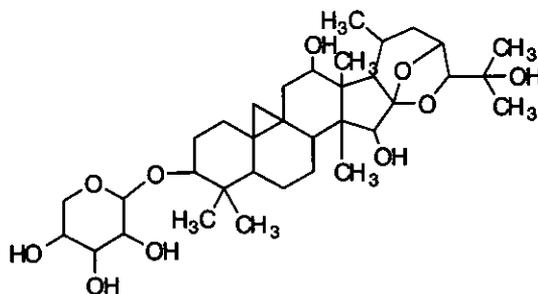
[正確な分子量] 636.38735

[基原] *Cimicifuga simplex*

[性状] 針状結晶 (MeOH)

[融点] Mp 267-268 °C

[比旋光度]: [α]<sub>D</sub> +15.3 (c, 0.4 in MeOH)



-----文献-----

- Corsano, S. et al., Chem. Comm., 1965, 185, (構造決定)  
 Takemoto, T. et al., Yakugaku Zasshi, 1968, 88, 623; 1969, 89, 954; 1970, 90, 64, (誘導体)  
 Corsano, S. et al., Gazz. Chim. Ital., 1969, 99, 1140, (構造)  
 Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
 Li, C.J. et al., Yaoxue Xuebao, 1993, 28, 777; CA, 120, 143804x, (Cimicide)  
 Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1167, (*Cimicifuga simplex* const.)

§ **Cycloarta-16,24-dien-3-ol; 3 β-form**

[化学名・別名] Cimicifugenol

[CAS No.] 28282-48-6

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

[構造式]

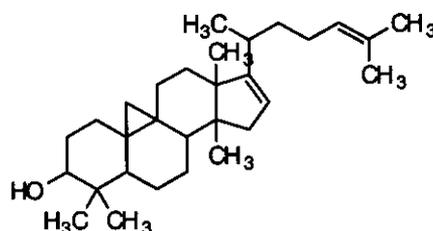
[基原] *Cimicifuga acerina*, *Cimicifuga simplex*, *Cimicifuga japonica*

[性状] 結晶

[融点] Mp 112-113 °C

[比旋光度]: [α]<sub>D</sub><sup>19</sup> +21.4 (c, 4.33 in CHCl<sub>3</sub>)

[その他のデータ] 構造式は 1999 年に改正された。Formerly thought to be Cycloarta-7,24-dien-3-ol



-----文献-----

- Akihisa, T. et al., Chem. Pharm. Bull., 1999, 47, 1157

§ **16,23:16,24-Diepoxy-cycloart-7-ene-3,15,25-triol; (3 β,15 α,23R,24S)-form, 3-O-α-L-Arabinopyranoside**

[CAS No.] 228251-29-4

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

[構造式]

[分子式] C<sub>35</sub>H<sub>54</sub>O<sub>9</sub>

[分子量] 618.806

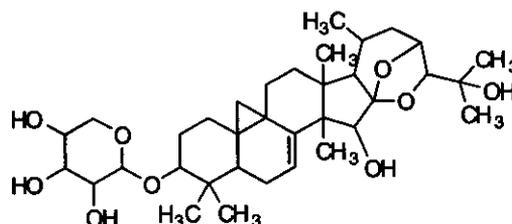
[正確な分子量] 618.376785

[基原] *Cimicifuga simplex*

[性状] 針状結晶 (MeOH/CHCl<sub>3</sub>)

[融点] Mp 272-273 °C

[比旋光度]: [α]<sub>D</sub> -3.64 (c, 1.17 in MeOH)



-----文献-----

- Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR, 結晶構造)  
 Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511, (分離, H-NMR, C13-NMR)

§ **16,23:16,24-Diepoxy-cycloart-7-ene-3,15,25-triol; (3 β,15 α,23R,24S)-form, 3-O-β-D-Xylopyranoside**  
 [CAS No.] 228251-28-3

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

[構造式]

[分子式]  $C_{35}H_{54}O_9$

[分子量] 618.806

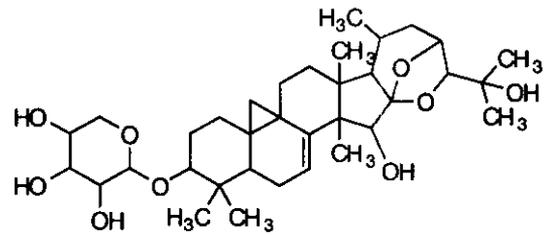
[正確な分子量] 618.376785

[基原] *Cimicifuga simplex*

[性状] 針状結晶 (MeOH)

[融点] Mp 291-292 °C

[比旋光度]:  $[\alpha]_D -14.8$  (c, 0.88 in MeOH)



-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR, 結晶構造)

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511, (分離, H-NMR, C13-NMR)

§ 16,23:16,24-Diepoxy-3,15,25-triol; (3  $\beta$ , 15  $\alpha$ , 23R, 24S)-form, 3-O- $\beta$

-D-Galactopyranoside

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

[構造式]

[分子式]  $C_{36}H_{56}O_{10}$

[分子量] 648.832

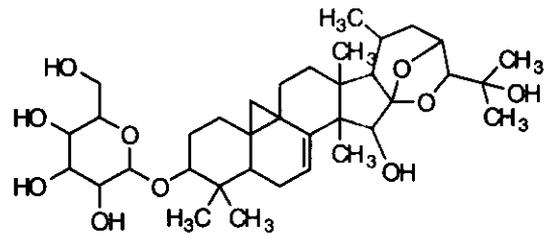
[正確な分子量] 648.38735

[基原] *Cimicifuga simplex*

[性状] 針状結晶

[融点] Mp 229-230 °C

[比旋光度]:  $[\alpha]_D +22.9$  (c, 0.6 in MeOH)



-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR, 結晶構造)

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511, (分離, H-NMR, C13-NMR)

§ 16,23:16,24-Diepoxy-3,15,25-triol; (3  $\beta$ , 15  $\alpha$ , 23R, 24S)-form, 25-Ac, 3-O- $\alpha$

-L-arabinopyranoside

[CAS No.] 228251-31-8

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

[構造式]

[分子式]  $C_{37}H_{56}O_{10}$

[分子量] 660.843

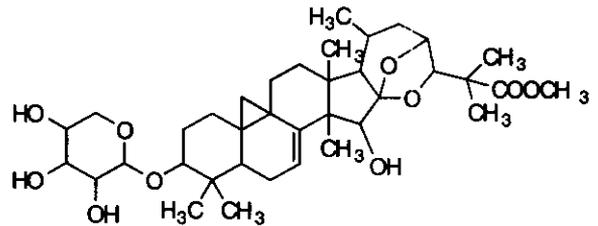
[正確な分子量] 660.38735

[基原] *Cimicifuga simplex*

[性状] 粉末 (MeOH)

[融点] Mp 167-168 °C

[比旋光度]:  $[\alpha]_D -4.7$  (c, 0.7 in MeOH)



-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR, 結晶構造)

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511, (分離, H-NMR, C13-NMR)

§ 16,23:16,24-Diepoxy-3,15,25-triol; (3  $\beta$ , 15  $\alpha$ , 23R, 24S)-form, 25-Ac,

3-O- $\beta$ -D-xylopyranoside

[CAS No.] 228251-30-7

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

[構造式]

[分子式]  $C_{37}H_{56}O_{10}$

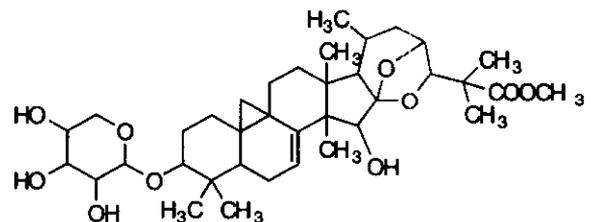
[分子量] 660.843

[正確な分子量] 660.38735

[基原] *Cimicifuga simplex*

[性状] 針状結晶 (MeOH)

[融点] Mp 255-256 °C



[比旋光度]:  $[\alpha]_D -14.9$  (c, 0.74 in MeOH)

-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR, 結晶構造)

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511, (分離, H-NMR, C13-NMR)

§ 16,23:16,24-Diepoxyart-7-ene-3,15,25-triol; (3  $\beta$ , 15  $\alpha$ , 23R, 24S)-form, 25-Ac,

3-O- $\beta$ -D-glucopyranoside

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

[構造式]

[分子式]  $C_{38}H_{58}O_{11}$

[分子量] 690.87

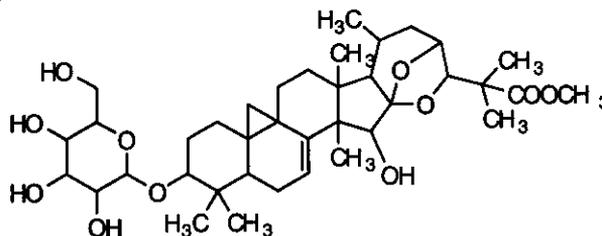
[正確な分子量] 690.397915

[基原] *Cimicifuga simplex*

[性状] 針状結晶

[融点] Mp 216-217 °C

[比旋光度]:  $[\alpha]_D +20.6$  (c, 0.7 in MeOH)



-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR, 結晶構造)

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511, (分離, H-NMR, C13-NMR)

§ 16,23:16,24-Diepoxyart-7-ene-3,15,25-triol; (3  $\beta$ , 15  $\alpha$ , 23R, 24S)-form, 25-Ac,

3-O- $\beta$ -D-galactopyranoside

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

[構造式]

[分子式]  $C_{38}H_{58}O_{11}$

[分子量] 690.87

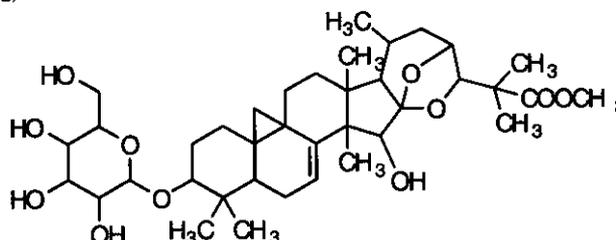
[正確な分子量] 690.397915

[基原] *Cimicifuga simplex*

[性状] 針状結晶

[融点] Mp 213-214 °C

[比旋光度]:  $[\alpha]_D +18.7$  (c, 0.6 in MeOH)



-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR, 結晶構造)

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511, (分離, H-NMR, C13-NMR)

§ 16,23:16,24-Diepoxyart-7-ene-3,15,25-triol; (3  $\beta$ , 15  $\alpha$ , 23R, 24S)-form, O<sup>25</sup>-Me,

3-O- $\beta$ -D-galactopyranoside

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

[構造式]

[分子式]  $C_{37}H_{58}O_{10}$

[分子量] 662.859

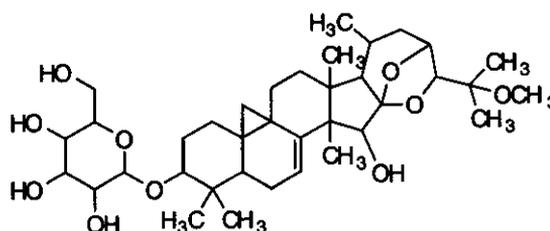
[正確な分子量] 662.403

[基原] *Cimicifuga simplex*

[性状] 針状結晶

[融点] Mp 209-210 °C

[比旋光度]:  $[\alpha]_D +20.4$  (c, 0.5 in MeOH)



-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR, 結晶構造)

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511, (分離, H-NMR, C13-NMR)

§ 16,23:22,25-Diepoxyart-7-ene-3,23,24-triol; (3  $\beta$ , 16  $\beta$ , 20S, 22R, 23R, 24R)-form,

7,8  $\beta$ -Dihydro, 3-O- $\beta$ -D-xylopyranoside

[化学名・別名] Cimiaceroside B

[CAS No.] 210643-84-8

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

[構造式]

[分子式]  $C_{35}H_{56}O_9$

[分子量] 620.822

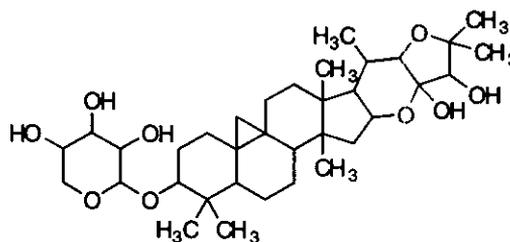
[正確な分子量] 620.392435

[基原] *Cimicifuga acerina*, *Cimicifuga simplex*

[性状] 針状結晶 (MeOH)

[融点] Mp 278-280 °C

[比旋光度]:  $[\alpha]_D^{25} -2.4$  (c, 0.4 in MeOH)



-----文献-----

Kusano, A. et al., *Heterocycles*, 1998, 48, 1003, (分離, H-NMR, C13-NMR)

Kusano, A. et al., *Chem. Pharm. Bull.*, 1999, 47, 1175, (2'-O-Malonylcimiaceroside B)

§ 16,23:22,25-Diepoxycholeart-7-ene-3,23,24-triol; (3  $\beta$ ,16  $\beta$ ,20S,22R,23R,24R)-form, 7,8  $\beta$ -Dihydro, 3-O-(2-O-malonyl- $\beta$ -D-xylopyranoside)

[化学名・別名] 2'-O-Malonylcimiaceroside B

[CAS No.] 245494-51-3

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

[構造式]

[分子式]  $C_{38}H_{58}O_{12}$

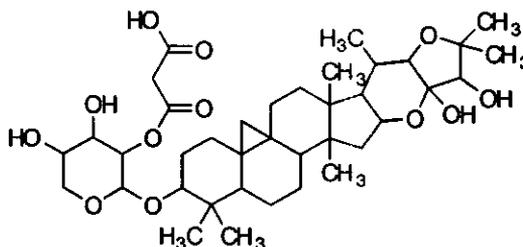
[分子量] 706.869

[正確な分子量] 706.39283

[基原] *Cimicifuga simplex*

[性状] 粉末

[比旋光度]:  $[\alpha]_D^{25} -0.72$  (c, 0.33 in MeOH)



-----文献-----

Kusano, A. et al., *Chem. Pharm. Bull.*, 1999, 47, 1175, (2'-O-Malonylcimiaceroside B)

§ 16,23-Epoxycholeartane-1,3,15,16,24,25-hexol; (1  $\alpha$ ,3  $\beta$ ,15  $\alpha$ ,16  $\xi$ ,23R,24S)-form, 25-Me ether, 3-O- $\beta$ -D-xylopyranoside, 24-Ac

[CAS No.] 173180-29-5

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

[構造式]

[分子式]  $C_{38}H_{60}O_{12}$

[分子量] 710.901

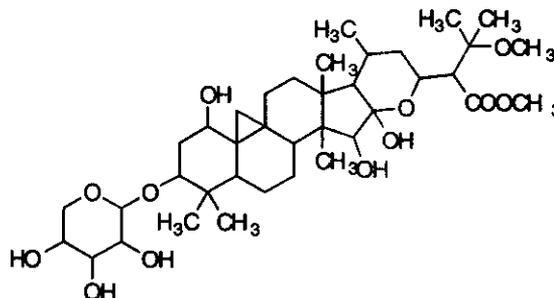
[正確な分子量] 710.42413

[基原] *Cimicifuga simplex*

[性状] 粉末

[融点] Mp 149-150 °C

[比旋光度]:  $[\alpha]_D^{25} +5$  (c, 1.15 in MeOH)



-----文献-----

Kusano, A. et al., *Chem. Pharm. Bull.*, 1996, 44, 167, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxycholeartane-3,7,15,16,24,25-hexol; (3  $\beta$ ,7  $\beta$ ,15  $\alpha$ ,16  $\xi$ ,23R,24R)-form, 3-O- $\beta$ -D-Xylopyranoside, 24-Ac

[CAS No.] 173180-26-2

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

[構造式]

[分子式]  $C_{37}H_{60}O_{12}$

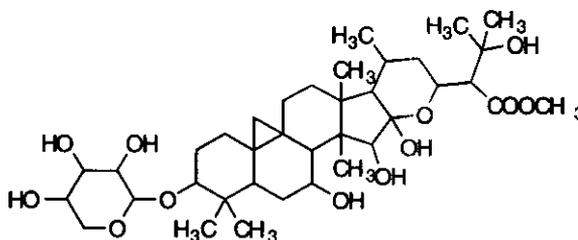
[分子量] 696.874

[正確な分子量] 696.40848

[基原] *Cimicifuga simplex*

[性状] 針状結晶

[融点] Mp 276-277 °C



[比旋光度]:  $[\alpha]_D +10.3$  (c, 0.6 in MeOH)

-----文献-----

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 167, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-cycloartane-3,7,15,16,24,25-hexol; (3  $\beta$ , 7  $\beta$ , 15  $\alpha$ , 16  $\xi$ , 23R,24S)-form, 25-Me ether, 3-O- $\beta$ -D-xylopyranoside, 24-Ac

[CAS No.] 173180-28-4

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

[構造式]

[分子式]  $C_{38}H_{62}O_{12}$

[分子量] 710.901

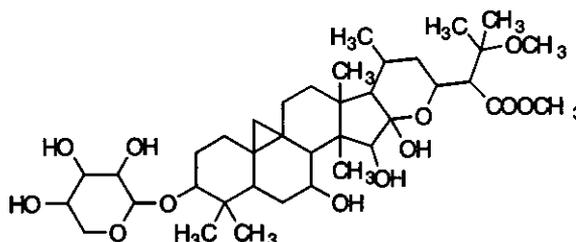
[正確な分子量] 710.42413

[基原] *Cimicifuga simplex*

[性状] 針状結晶

[融点] Mp 199-200 °C

[比旋光度]:  $[\alpha]_D +4.6$  (c, 0.52 in MeOH)



-----文献-----

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 167, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-cycloartane-3,15,16,24,25-pentol; (3  $\beta$ , 15  $\alpha$ , 16  $\alpha$  OH, 23R,24R)-form, 3-O- $\beta$ -D-Galactopyranoside, 24-Ac

[CAS No.] 184419-89-4

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

[

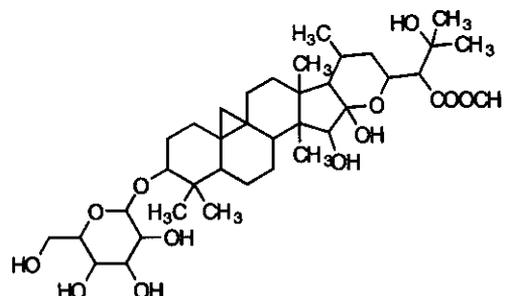
構造式]

[分子式]  $C_{38}H_{62}O_{12}$

[分子量] 710.901

[正確な分子量] 710.42413

[基原] *Cimicifuga simplex*



-----文献-----

Sakurai, N. et al., Chem. Pharm. Bull., 1994, 42, 48, (*Cimicifuga dahurica* const.)

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 167; 2078, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-cycloartane-3,15,16,24,25-pentol; (3  $\beta$ , 15  $\alpha$ , 16  $\xi$ , 23R,24S)-form, 25-Me ether, 3-O- $\beta$ -D-xylopyranoside, 24-Ac

[CAS No.] 173180-27-3

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

[構造式]

[分子式]  $C_{38}H_{62}O_{11}$

[分子量] 694.901

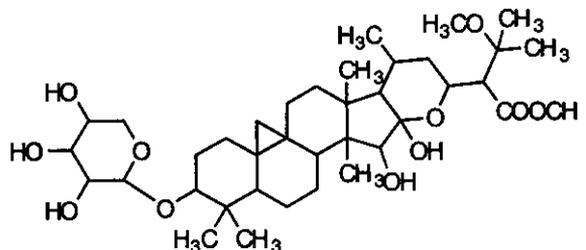
[正確な分子量] 694.429215

[基原] *Cimicifuga simplex*

[性状] 針状結晶

[融点] Mp 205-206 °C

[比旋光度]:  $[\alpha]_D -1.5$  (c, 0.55 in MeOH)



-----文献-----

Sakurai, N. et al., Chem. Pharm. Bull., 1994, 42, 48, (*Cimicifuga dahurica* const.)

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 167; 2078, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-cycloart-7-ene-3,15,16,24,25-pentol; (3  $\beta$ , 15  $\alpha$ , 16  $\alpha$  OH, 23R,24R)-form, 24-Ac, 3-O- $\alpha$ -L-arabinopyranoside

[CAS No.] 228251-26-1

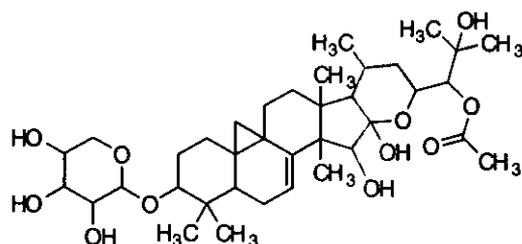
[化合物分類]テルペノイド (Cycloartane triterpenoid)

[構造式]

[分子式]  $C_{37}H_{58}O_{11}$

[分子量] 678.859  
[正確な分子量] 678.397915

[基原] *Cimicifuga simplex*  
[性状] 針状結晶 (MeOH)  
[融点] Mp 221-222 °C  
[比旋光度]:  $[\alpha]_D^{25} -9.2$  (c, 0.5 in MeOH)



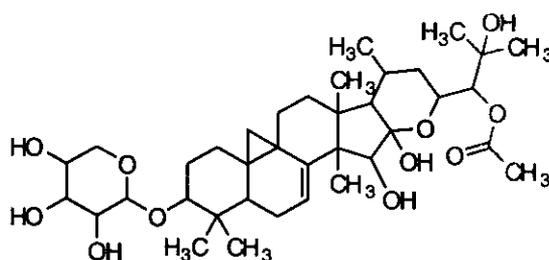
-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-3,15,16,24,25-pentol; (3 β,15 α,16 α OH,23R,24R)-form,  
24-Ac, 3-O-β-D-xylopyranoside

[CAS No.] 228251-25-0  
[化合物分類] テルペノイド (Cycloartane triterpenoid)  
[構造式]

[分子式] C<sub>37</sub>H<sub>58</sub>O<sub>11</sub>  
[分子量] 678.859  
[正確な分子量] 678.397915  
[基原] *Cimicifuga simplex*  
[性状] 針状結晶 (MeOH)  
[融点] Mp 224-225 °C  
[比旋光度]:  $[\alpha]_D^{25} -25.5$  (c, 1 in MeOH)



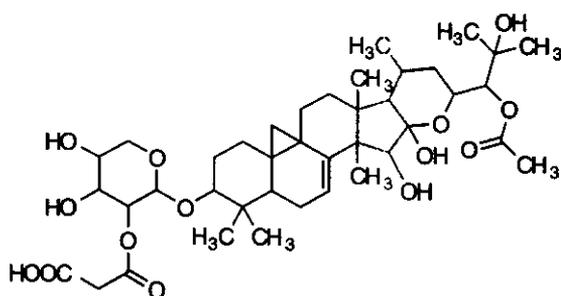
-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-3,15,16,24,25-pentol; (3 β,15 α,16 α OH,23R,24R)-form,  
24-Ac, 3-O-(2-O-malonyl-β-D-xylopyranoside)

[CAS No.] 245494-50-2  
[化合物分類] テルペノイド (Cycloartane triterpenoid)  
[構造式]

[分子式] C<sub>40</sub>H<sub>60</sub>O<sub>14</sub>  
[分子量] 764.906  
[正確な分子量] 764.39831  
[基原] *Cimicifuga simplex*  
[性状] 粉末  
[比旋光度]:  $[\alpha]_D^{25} -8$  (c, 0.52 in MeOH)



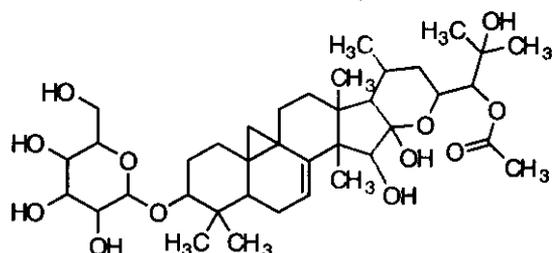
-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-3,15,16,24,25-pentol; (3 β,15 α,16 α OH,23R,24R)-form,  
24-Ac, 3-O-β-D-galactopyranoside

[化合物分類] テルペノイド (Cycloartane triterpenoid)  
[構造式]

[分子式] C<sub>38</sub>H<sub>60</sub>O<sub>12</sub>  
[分子量] 708.885  
[正確な分子量] 708.40848  
[基原] *Cimicifuga simplex*  
[性状] 針状結晶 (MeOH)



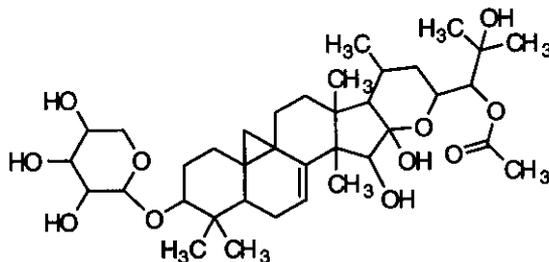
[融点] Mp 243-244 °C  
[比旋光度]:  $[\alpha]_D -11.4$  (c, 1.1 in MeOH)

-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-cycloart-7-ene-3,15,16,24,25-pentol; (3  $\beta$ , 15  $\alpha$ , 16  $\alpha$  OH, 23R, 24S)-form,  
24-Ac, 3-O- $\alpha$ -L-arabinopyranoside

[CAS No.] 228251-27-2  
[化合物分類] テルペノイド (Cycloartane triterpenoid)  
[構造式]  
[分子量] 678.859  
[正確な分子量] 678.397915  
[基原] *Cimicifuga simplex*  
[性状] 粉末 (MeOH)  
[融点] Mp 172-173 °C  
[比旋光度]:  $[\alpha]_D -14.1$  (c, 0.51 in MeOH)

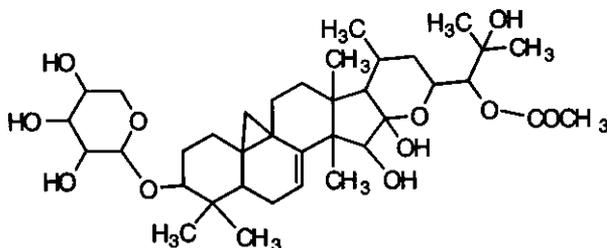


-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-cycloart-7-ene-3,15,16,24,25-pentol; (3  $\beta$ , 15  $\alpha$ , 16  $\alpha$  H, 23R, 24S)-form,  
24-Ac, 3-O- $\beta$ -D-xylopyranoside

[CAS No.] 150972-78-4  
[化合物分類] テルペノイド (Cycloartane triterpenoid)  
[構造式]  
[分子式]  $C_{37}H_{58}O_{11}$   
[分子量] 678.859  
[正確な分子量] 678.397915  
[基原] *Cimicifuga heracleifolia*, *Cimicifuga simplex*  
[性状] 針状結晶 (MeOH)  
[融点] Mp 227-228 °C  
[比旋光度]:  $[\alpha]_D -27.4$  (c, 0.62 in  $CHCl_3/MeOH$ ).  $[\alpha]_D -29.7$  (c, 0.77 in MeOH)

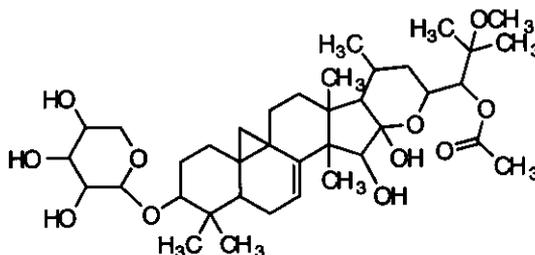


-----文献-----

Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)

§ 16,23-Epoxy-cycloart-7-ene-3,15,16,24,25-pentol; (3  $\beta$ , 15  $\alpha$ , 16  $\alpha$  OH, 23R, 24S)-form, 25-Me ether,  
24-Ac, 3-O- $\beta$ -D-xylopyranoside

[CAS No.] 245494-54-6  
[化合物分類] テルペノイド (Cycloartane triterpenoid)  
[構造式]  
[分子式]  $C_{38}H_{60}O_{11}$   
[分子量] 692.885  
[正確な分子量] 692.413565  
[基原] *Cimicifuga simplex*  
[性状] 針状結晶 (MeOH)  
[融点] Mp 216-217 °C  
[比旋光度]:  $[\alpha]_D -14.7$  (c, 0.51 in MeOH)



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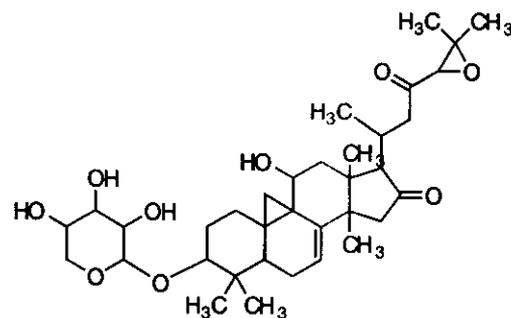
Li, J.X. et al., Chem. Pharm. Bull., 1993, 41, 832, (分離, H-NMR, C13-NMR)  
Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)

§ 24,25-Epoxy-3,11-dihydroxycycloart-7-ene-16,23-dione; (3  $\beta$ , 11  $\beta$ , 24R)-form,

3-O-β-D-Xylopyranoside

[化学名・別名] Cimicifugoside H1. Cimicifugoside H  
[化合物分類] テルペノイド (Cycloartane triterpenoid)  
[構造式]

[分子式] C<sub>35</sub>H<sub>52</sub>O<sub>9</sub>  
[分子量] 616.79  
[正確な分子量] 616.361135  
[基原] *Cimicifuga simplex*  
[性状] 結晶 (MeOH)  
[融点] Mp 262 °C  
[比旋光度]: [α]<sub>D</sub> -43.5 (c, 0.5 in MeOH)



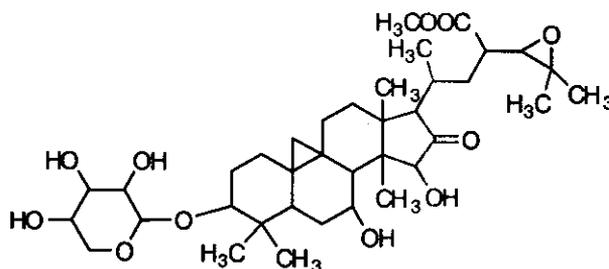
-----文献-----

Koeda, M. et al., Chem. Pharm. Bull., 1994, 42, 2205; 1995, 43, 771, (分離, H-NMR, C13-NMR)  
Kadota, S. et al., Tetrahedron, 1995, 51, 1143, (分離, H-NMR, C13-NMR)

§ 24,25-Epoxy-3,7,15,23-tetrahydrocycloartan-16-one; (3β,7β,16α,23S,24R)-form, 3-O-β-D-Xylopyranoside, 23-Ac

[CAS No.] 156759-68-1  
[化合物分類] テルペノイド (Cycloartane triterpenoid)

[構造式]  
[分子式] C<sub>37</sub>H<sub>58</sub>O<sub>11</sub>  
[分子量] 678.859  
[正確な分子量] 678.397915  
[基原] *Cimicifuga simplex*  
[性状] 針状結晶 (EtOH/diisopropyl ether)  
[融点] Mp 252-253 °C  
[比旋光度]: [α]<sub>D</sub> -51.4 (c, 0.14 in MeOH)



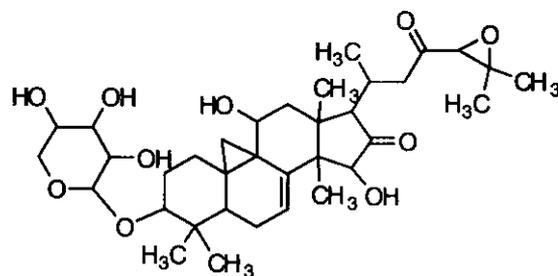
-----文献-----

Kusano, G. et al., Chem. Pharm. Bull., 1994, 42, 1106, (分離, H-NMR, C13-NMR)

§ 24,25-Epoxy-3,11,15-trihydroxycycloart-7-ene-16,23-dione; (3β,11β,15ε,24R)-form, 3-O-β-D-Xylopyranoside

[化学名・別名] Cimicifugoside H5  
[CAS No.] 168075-12-5  
[化合物分類] テルペノイド (Cycloartane triterpenoid)  
[構造式]

[分子式] C<sub>35</sub>H<sub>52</sub>O<sub>10</sub>  
[分子量] 632.79  
[正確な分子量] 632.35605  
[基原] *Cimicifuga simplex*  
[性状] 結晶 (MeOH 溶液)  
[融点] Mp 262-264 °C  
[比旋光度]: [α]<sub>D</sub> -22.9 (c, 1.9 in MeOH)



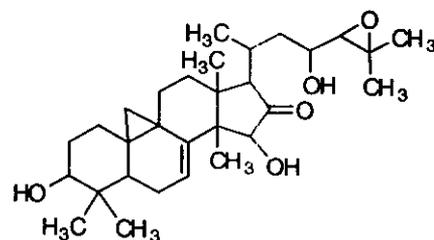
-----文献-----

Koeda, M. et al., Chem. Pharm. Bull., 1995, 43, 771, (分離, H-NMR, C13-NMR)

§ 24,25-Epoxy-3,15,23-trihydroxy-7-cycloarten-16-one; (3β,15α,23R,24S)-form

[化学名・別名] 7,8-Didehydroshengmanol  
[化合物分類] テルペノイド (Cycloartane triterpenoid)  
[構造式]

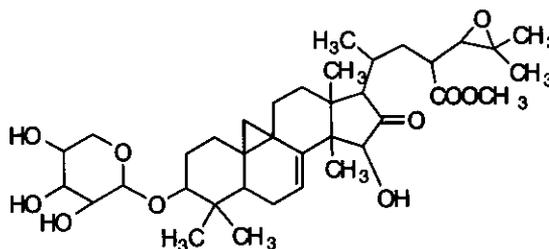
[基原] Sapogenin from *Cimicifuga simplex*



-----文献-----

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)  
**§ 24,25-Epoxy-3,15,23-trihydroxy-7-cycloarten-16-one; (3  $\beta$ ,15  $\alpha$ ,23R,24S)-form, 23-Ac,**  
 3-O- $\alpha$ -L-arabinopyranoside

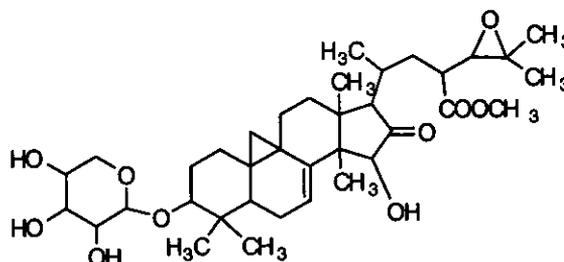
[CAS No.]184419-86-1  
 [化合物分類]テルペノイド (Cycloartane triterpenoid)  
 [構造式]  
 [分子式] C<sub>37</sub>H<sub>56</sub>O<sub>10</sub>  
 [分子量] 660.843  
 [正確な分子量] 660.38735  
 [基原] *Cimicifuga simplex*  
 [性状] 針状結晶 (MeOH)  
 [融点] Mp 239-240 °C  
 [比旋光度]: [ $\alpha$ ]<sub>D</sub> -55.5



-----文献-----

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)  
**§ 24,25-Epoxy-3,15,23-trihydroxy-7-cycloarten-16-one; (3  $\beta$ ,15  $\alpha$ ,23R,24S)-form, 23-Ac,**  
 3-O- $\beta$ -D-xylopyranoside

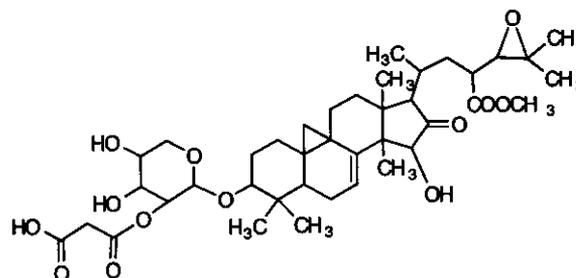
[CAS No.]245494-52-4  
 [化合物分類]テルペノイド (Cycloartane triterpenoid)  
 [構造式]  
 [分子式] C<sub>37</sub>H<sub>56</sub>O<sub>10</sub>  
 [分子量] 660.843  
 [正確な分子量] 660.38735  
 [基原] *Cimicifuga simplex*  
 [性状] 粉末 (MeOH/EtOAc/diisopropyl ether)  
 [融点] Mp 268-269 °C  
 [比旋光度]: [ $\alpha$ ]<sub>D</sub><sup>25</sup> -49.6 (c, 1.27 in MeOH)



-----文献-----

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)  
**§ 24,25-Epoxy-3,15,23-trihydroxy-7-cycloarten-16-one; (3  $\beta$ ,15  $\alpha$ ,23R,24S)-form, 23-Ac, 3-O-**  
**(2-O-malonyl- $\beta$ -D-xylopyranoside)**

[CAS No.]245494-48-8  
 [化合物分類]テルペノイド (Cycloartane triterpenoid)  
 [構造式]  
 [分子式] C<sub>40</sub>H<sub>58</sub>O<sub>13</sub>  
 [分子量] 746.89  
 [正確な分子量] 746.387745  
 [基原] *Cimicifuga simplex*  
 [性状] 粉末  
 [比旋光度]: [ $\alpha$ ]<sub>D</sub> -16.7 (c, 0.39 in MeOH)

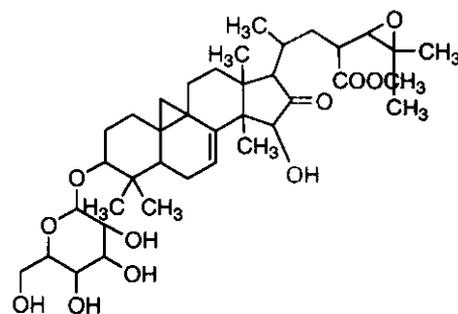


-----文献-----

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)  
**§ 24,25-Epoxy-3,15,23-trihydroxy-7-cycloarten-16-one; (3  $\beta$ ,15  $\alpha$ ,23R,24S)-form, 23-Ac, 3-O- $\beta$**

**-D-galactopyranoside**

[CAS No.] 228251-33-0  
[化合物分類]テルペノイド (Cycloartane triterpenoid)  
[構造式]  
[分子式]  $C_{38}H_{58}O_{11}$   
[分子量] 690.87  
[正確な分子量] 690.397915  
[基原] *Cimicifuga simplex*  
[性状] 粉末 (MeOH/MeCN)  
[融点] Mp 170-171 °C  
[比旋光度]:  $[\alpha]_D -44.1$  (c, 0.47 in MeOH)

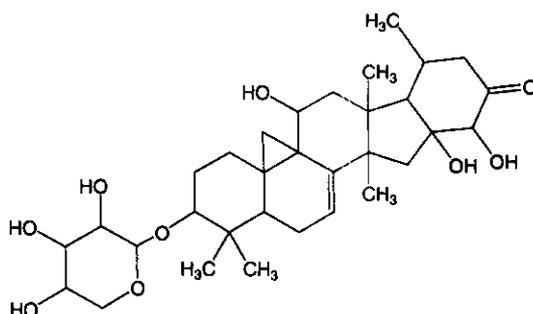


-----文献-----

Kusano, A. et al., Chem. Pharm. Bull., 1996, 44, 2078; 1999, 47, 511; 1175, (分離, H-NMR, C13-NMR)

**§ Foetidinol; 3-O-β-D-Xylopyranoside**

[化学名・別名] Cimicifugoside H4. Neocimicide  
[CAS No.] 161097-79-6  
[化合物分類]テルペノイド (Cycloartane triterpenoid)  
[構造式]  
[分子式]  $C_{32}H_{48}O_9$   
[分子量] 576.726  
[正確な分子量] 576.329835  
[基原] *Cimicifuga foetida*, *Cimicifuga simplex*  
[性状] 黄色の無定型粉末もしくは結晶 (MeOH)  
[融点] Mp 265-267 °C  
[比旋光度]:  $[\alpha]_D -43.46$  (c, 0.27 in  $CHCl_3/MeOH$ ).  $[\alpha]_D -75$  (c, 1 in  $CHCl_3/MeOH$ )

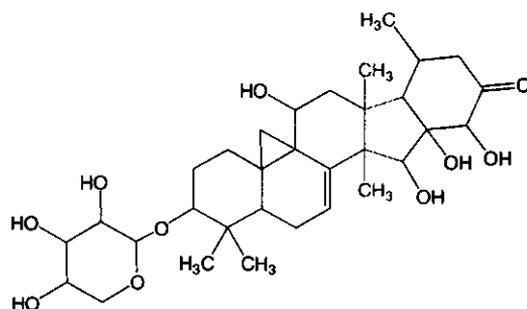


-----文献-----

Li, J.X. et al., Tet. Lett., 1994, 35, 4575, (分離, H-NMR, C13-NMR)  
Sakurai, N. et al., Chem. Pharm. Bull., 1995, 43, 1475, (Cimicifugoside)  
Kadota, S. et al., Tetrahedron, 1995, 51, 1143, (分離, H-NMR, C13-NMR)

**§ Foetidinol; 15 α-Hydroxy, 3-O-β-D-xylopyranoside**

[化学名・別名] Cimicifugoside H6  
[CAS No.] 161097-80-9  
[化合物分類]テルペノイド (Cycloartane triterpenoid)  
[構造式]  
[分子式]  $C_{32}H_{48}O_{10}$   
[分子量] 592.725  
[正確な分子量] 592.32475  
[基原] *Cimicifuga foetida*, *Cimicifuga simplex*  
[性状] 粉末もしくは結晶 (MeOH)  
[融点] Mp 275-276 °C  
[比旋光度]:  $[\alpha]_D -73.64$  (c, 0.36 in  $CHCl_3/MeOH$ ) ((-64.3))



-----文献-----

Li, J.X. et al., Tet. Lett., 1994, 35, 4575, (分離, H-NMR, C13-NMR)  
Sakurai, N. et al., Chem. Pharm. Bull., 1995, 43, 1475, (Cimicifugoside)  
Kadota, S. et al., Tetrahedron, 1995, 51, 1143, (分離, H-NMR, C13-NMR)

**§ Fukiic acid; (2S,3R)-form, 2-O-(3-Hydroxy-4-methoxycinnamoyl) (E-), 1-Me ester**

[化合物分類]炭水化物(Aldaric acid)

[構造式]

[分子式]  $C_{22}H_{22}O_{11}$

[分子量] 462.409

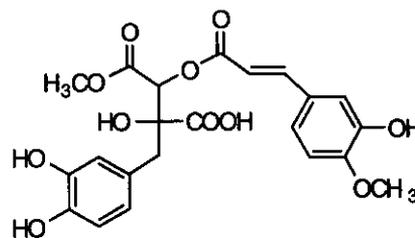
[正確な分子量] 462.116215

[基原] *Cimicifuga simplex*

[性状] 青白い黄色の粉末

[比旋光度]:  $[\alpha]_D +36.4$  (c, 0.37 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  235 (sh) (log  $\epsilon$  4.3); 290 (log  $\epsilon$  4.19); 325 (log  $\epsilon$  4.22) (MeOH)



-----文献-----

Sakamura, S. et al., Agric. Biol. Chem., 1969, 33, 1795; 1973, 37, 1915, (分離, 構造決定, 誘導体)

Yoshihara, T. et al., Tet. Lett., 1971, 3809, (stereochem)

Heller, W. et al., Helv. Chim. Acta, 1975, 58, 974, (分離)

Kusano, G. et al., Biol. Pharm. Bull., 1998, 21, 997, (活性, Fukinolic acid)

Takahira, M. et al., Chem. Pharm. Bull., 1998, 46, 362, (分離, UV, H-NMR, C13-NMR, Mas)

Takahira, M. et al., Phytochemistry, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)

### § Fukiic acid; (2S,3R)-form, 2-O-(4-Hydroxy-3-methoxycinnamoyl) (E-), 1-Me ester

[化合物分類]炭水化物(Aldaric acid)

[構造式]

[分子式]  $C_{22}H_{22}O_{11}$

[分子量] 462.409

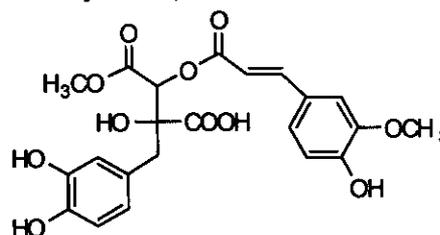
[正確な分子量] 462.116215

[基原] *Cimicifuga simplex*

[性状] 青白い黄色の粉末

[比旋光度]:  $[\alpha]_D +41.3$  (c, 0.42 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  235 (sh) (log  $\epsilon$  4.36); 291 (log  $\epsilon$  4.25); 327 (log  $\epsilon$  4.36) (MeOH)



-----文献-----

Sakamura, S. et al., Agric. Biol. Chem., 1969, 33, 1795; 1973, 37, 1915, (分離, 構造決定, 誘導体)

Yoshihara, T. et al., Tet. Lett., 1971, 3809, (stereochem)

Heller, W. et al., Helv. Chim. Acta, 1975, 58, 974, (分離)

Kusano, G. et al., Biol. Pharm. Bull., 1998, 21, 997, (活性, Fukinolic acid)

Takahira, M. et al., Chem. Pharm. Bull., 1998, 46, 362, (分離, UV, H-NMR, C13-NMR, Mas)

Takahira, M. et al., Phytochemistry, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)

### § Fukiic acid; (2S,3R)-form, 2-O-(4-Hydroxycinnamoyl)

[化学名・別名] Cimicifugic acid C

[化合物分類]炭水化物(Aldaric acid)

[構造式]

[分子式]  $C_{20}H_{18}O_{10}$

[分子量] 418.356

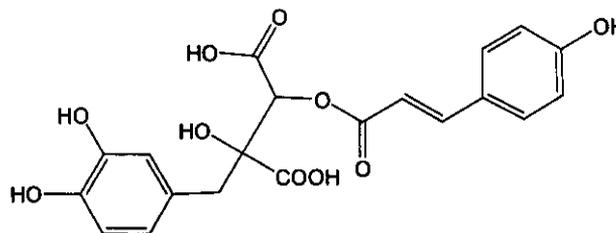
[正確な分子量] 418.09

[基原] *Cimicifuga simplex*

[性状] 青白い黄色の粉末 (CHCl<sub>3</sub>/MeOH)

[比旋光度]:  $[\alpha]_D^{25} +38.7$  (c, 0.3 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  224 (log  $\epsilon$  4.23); 286 (sh) (log  $\epsilon$  4.16); 313 (log  $\epsilon$  4.27) (MeOH)



-----文献-----

Sakamura, S. et al., Agric. Biol. Chem., 1969, 33, 1795; 1973, 37, 1915, (分離, 構造決定, 誘導体)

Yoshihara, T. et al., Tet. Lett., 1971, 3809, (stereochem)

Heller, W. et al., Helv. Chim. Acta, 1975, 58, 974, (分離)

Kusano, G. et al., Biol. Pharm. Bull., 1998, 21, 997, (活性, Fukinolic acid)

Takahira, M. et al., Chem. Pharm. Bull., 1998, 46, 362, (分離, UV, H-NMR, C13-NMR, Mas)

Takahira, M. et al., Phytochemistry, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)

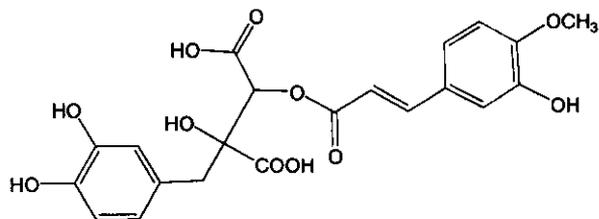
### § Fukiic acid; (2S,3R)-form, 2-O-(3-Hydroxy-4-methoxycinnamoyl)

[化学名・別名] Cimicifugic acid B  
[化合物分類] 炭水化物 (Aldaric acid)  
[構造式]

[分子式]  $C_{21}H_{20}O_{11}$   
[分子量] 448.382  
[正確な分子量] 448.100565

[基原] *Cimicifuga simplex*  
[性状] 青白い黄色の粉末 (CHCl<sub>3</sub>/MeOH)  
[比旋光度]:  $[\alpha]_D^{25} +42.5$  (c, 0.5 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  224 (log  $\epsilon$  4.23); 286 (sh) (log  $\epsilon$  4.16); 313 (log  $\epsilon$  4.27) (MeOH)



-----文献-----

Sakamura, S. et al., Agric. Biol. Chem., 1969, 33, 1795; 1973, 37, 1915, (分離, 構造決定, 誘導体)  
Yoshihara, T. et al., Tet. Lett., 1971, 3809, (stereochem)  
Heller, W. et al., Helv. Chim. Acta, 1975, 58, 974, (分離)  
Kusano, G. et al., Biol. Pharm. Bull., 1998, 21, 997, (活性, Fukinolic acid)  
Takahira, M. et al., Chem. Pharm. Bull., 1998, 46, 362, (分離, UV, H-NMR, C13-NMR, Mas)  
Takahira, M. et al., Phytochemistry, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)

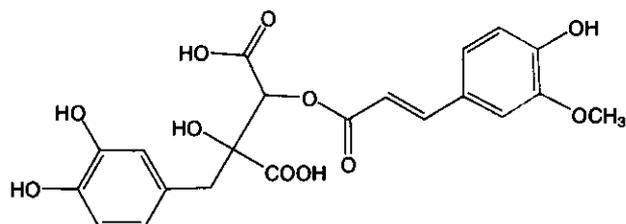
### § Fukiic acid; (2*S*,3*R*)-form, 2-*O*-(4-Hydroxy-3-methoxycinnamoyl)

[化学名・別名] Cimicifugia acid A  
[化合物分類] 炭水化物 (Aldaric acid)  
[構造式]

[分子式]  $C_{21}H_{20}O_{11}$   
[分子量] 448.382  
[正確な分子量] 448.100565

[基原] *Cimicifuga simplex*  
[性状] 青白い黄色の粉末 (CHCl<sub>3</sub>/MeOH)  
[比旋光度]:  $[\alpha]_D^{25} +47.8$  (c, 0.9 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  234 (log  $\epsilon$  4.16); 287 (sh) (log  $\epsilon$  4.08); 328 (log  $\epsilon$  4.28) (MeOH)



-----文献-----

Sakamura, S. et al., Agric. Biol. Chem., 1969, 33, 1795; 1973, 37, 1915, (分離, 構造決定, 誘導体)  
Yoshihara, T. et al., Tet. Lett., 1971, 3809, (stereochem)  
Heller, W. et al., Helv. Chim. Acta, 1975, 58, 974, (分離)  
Kusano, G. et al., Biol. Pharm. Bull., 1998, 21, 997, (活性, Fukinolic acid)  
Takahira, M. et al., Chem. Pharm. Bull., 1998, 46, 362, (分離, UV, H-NMR, C13-NMR, Mas)  
Takahira, M. et al., Phytochemistry, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)

### § 2-Hydroxy-7-methyl-9*H*-carbazole

[化学名・別名] 7-Methyl-9*H*-carbazol-2-ol (CAS 名)

[CAS No.] 151985-61-4

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

[構造式]

[分子式]  $C_{13}H_{11}NO$

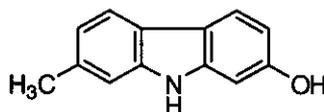
[分子量] 197.236

[正確な分子量] 197.084064

[基原] 次の植物の地上部から得られるアルカロイド: *Cimicifuga simplex* (キンポウゲ科)

[性状] 青白い黄色の無定型粉末 (CHCl<sub>3</sub>/MeOH)

[融点] Mp 269-271 °C

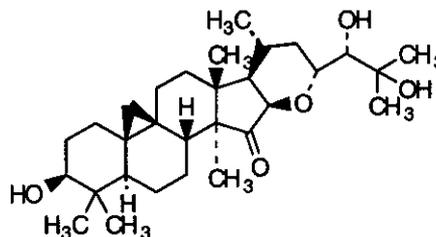


-----文献-----

Kusano, G. et al., Heterocycles, 1993, 36, 2367, (分離, UV, IR, H-NMR, C13-NMR, Mass, 構造決定)

### § Isodahurinol

[CAS No.] 59331-33-8  
 [化合物分類] テルペノイド (Cycloartane triterpenoid)  
 [構造式]  
 [分子式]  $C_{30}H_{48}O_5$   
 [分子量] 488.706  
 [正確な分子量] 488.350175  
 [基原] *Cimicifuga acerina*, *Cimicifuga simplex*  
 [性状] 結晶  
 [融点] Mp 216-222 °C

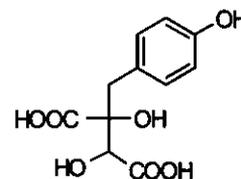


-----文献-----

Kusano, G. et al., *Yakugaku Zasshi*, 1976, 96, 82

§ **Piscidic acid; (2R,3S)-form**

[CAS No.] 35388-57-9  
 [化合物分類] AF8100, 炭水化物 (Aldaric acid)  
 [構造式]  
 [基原] 次の植物から分離: *Piscidia erythrina* の樹皮, *Narcissus poeticus*, *Cimicifuga simplex*, *Agave americana*, *Opuntia ficus-indica*  
 [性状] 細長いプリズム結晶 (EtOAc/CHCl<sub>3</sub>)  
 [融点] Mp 186-187 °C  
 [比旋光度]:  $[\alpha]_D +42.8$  (c, 0.8 in MeOH)  
 [UV]: [neutral]  $\lambda_{max}$  255 (log  $\epsilon$  3.88); 277 (log  $\epsilon$  3.17) (MeOH)

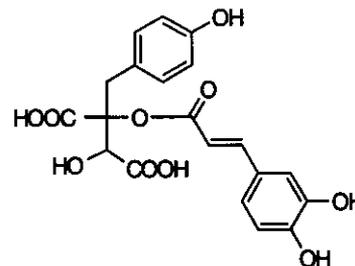


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Nordal, A. et al., *Acta Chem. Scand.*, 1964, 18, 1979; 1966, 20, 1431, (分離)  
 Yoshihara, T. et al., *Tet. Lett.*, 1971, 3809, (stereochem)  
 Takahira, M. et al., *Phytochemistry*, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)  
 Kruse, S.O. et al., *Planta Med.*, 1999, 65, 763, (分離)

§ **Piscidic acid; (2R,3S)-form, 3-O-(3,4-Dihydroxycinnamoyl) (E-)**

[化学名・別名] 3-O-Caffeoylpiscidic acid. 2-O-Caffeoylpiscidic acid  
 [CAS No.] 219986-51-3  
 [構造式]  
 [分子式]  $C_{20}H_{18}O_{10}$   
 [分子量] 418.356  
 [正確な分子量] 418.09  
 [基原] *Cimicifuga simplex*  
 [性状] 青白い黄色の粉末  
 [比旋光度]:  $[\alpha]_D +67.3$  (c, 0.34 in MeOH)  
 [UV]: [neutral]  $\lambda_{max}$  248 (sh) (log  $\epsilon$  4.02); 291 (log  $\epsilon$  4.07); 332 (log  $\epsilon$  4.25) (MeOH)



-----文献-----

Nordal, A. et al., *Acta Chem. Scand.*, 1964, 18, 1979; 1966, 20, 1431, (分離)  
 Yoshihara, T. et al., *Tet. Lett.*, 1971, 3809, (stereochem)  
 Takahira, M. et al., *Phytochemistry*, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)  
 Toshima, H. et al., *Biosci., Biotechnol., Biochem.*, 1999, 63, 964; 1934, (合成法)  
 Kruse, S.O. et al., *Planta Med.*, 1999, 65, 763, (分離)

§ **Piscidic acid; (2R,3S)-form, 3-O-(3-Hydroxy-4-methoxycinnamoyl) (E-)**

[化学名・別名] 3-O-Isoferuloylpiscidic acid. 2-O-Isoferuloylpiscidic acid. Cimicifugic acid F

[CAS No.] 220618-91-7

[構造式]

[分子式]  $C_{21}H_{20}O_{10}$

[分子量] 432.383

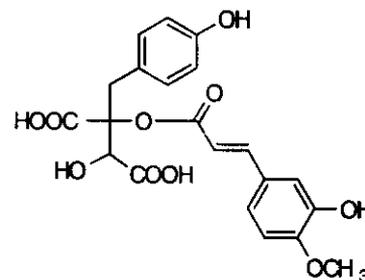
[正確な分子量] 432.10565

[基原] *Cimicifuga simplex*

[性状] 青白い黄色の粉末

[比旋光度]:  $[\alpha]_D +37.6$  (c, 0.5 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  245 (sh) (log  $\epsilon$  4.1); 297 (log  $\epsilon$  4.19); 326 (log  $\epsilon$  4.25) (MeOH)



-----文献-----

Buckle, A.L.J. et al., J.C.S., 1954, 3981, (合成法)

Nordal, A. et al., Acta Chem. Scand., 1964, 18, 1979; 1966, 20, 1431, (分離)

Yoshihara, T. et al., Tet. Lett., 1971, 3809, (stereochem)

Takahira, M. et al., Phytochemistry, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)

Toshima, H. et al., Biosci., Biotechnol., Biochem., 1999, 63, 964; 1934, (合成法)

Kruse, S.O. et al., Planta Med., 1999, 65, 763, (分離)

**§ Piscidic acid; (2R,3S)-form, 3-O-(3-Hydroxy-4-methoxycinnamoyl) (E-), 4-Me ester**

[CAS No.] 220618-93-9

[構造式]

[分子式]  $C_{22}H_{22}O_{10}$

[分子量] 446.41

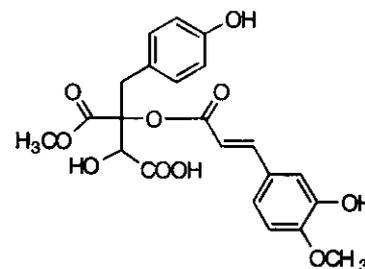
[正確な分子量] 446.1213

[基原] *Cimicifuga simplex*

[性状] 青白い黄色の粉末

[比旋光度]:  $[\alpha]_D +33.6$  (c, 0.2 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  245 (sh) (log  $\epsilon$  3.92); 295 (log  $\epsilon$  3.93); 325 (log  $\epsilon$  3.97) (MeOH)



-----文献-----

Buckle, A.L.J. et al., J.C.S., 1954, 3981, (合成法)

Nordal, A. et al., Acta Chem. Scand., 1964, 18, 1979; 1966, 20, 1431, (分離)

Yoshihara, T. et al., Tet. Lett., 1971, 3809, (stereochem)

Takahira, M. et al., Phytochemistry, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)

Toshima, H. et al., Biosci., Biotechnol., Biochem., 1999, 63, 964; 1934, (合成法)

Kruse, S.O. et al., Planta Med., 1999, 65, 763, (分離)

**§ Piscidic acid; (2R,3S)-form, 3-O-(4-Hydroxy-3-methoxycinnamoyl) (E-)**

[化学名・別名] 3-O-Feruloylpiscidic acid. 2-O-Feruloylpiscidic acid. Cimicifugic acid E

[CAS No.] 219986-67-1

[構造式]

[分子式]  $C_{21}H_{20}O_{10}$

[分子量] 432.383

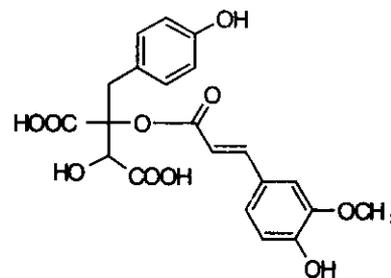
[正確な分子量] 432.10565

[基原] *Cimicifuga simplex*

[性状] 青白い黄色の粉末

[比旋光度]:  $[\alpha]_D +50.3$  (c, 0.2 in MeOH)

[UV]: [neutral]  $\lambda_{max}$  291 (log  $\epsilon$  3.98); 325 (log  $\epsilon$  4.16) (MeOH)



-----文献-----

Nordal, A. et al., Acta Chem. Scand., 1964, 18, 1979; 1966, 20, 1431, (分離)

Yoshihara, T. et al., Tet. Lett., 1971, 3809, (stereochem)

Takahira, M. et al., Phytochemistry, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)

Toshima, H. et al., Biosci., Biotechnol., Biochem., 1999, 63, 964; 1934, (合成法)

Kruse, S.O. et al., Planta Med., 1999, 65, 763, (分離)

§ Piscidic acid; (2*R*,3*S*)-form, 3-*O*-(4-Hydroxy-3-methoxycinnamoyl) (*E*-), 4-Me ester

[CAS No.] 220618-92-8

[構造式]

[分子式] C<sub>22</sub>H<sub>22</sub>O<sub>10</sub>

[分子量] 446.41

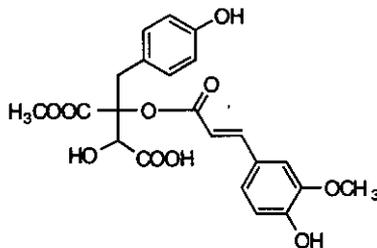
[正確な分子量] 446.1213

[基原] *Cimicifuga simplex*

[性状] 青白い黄色の粉末

[比旋光度]: [α]<sub>D</sub> +32.8 (c, 0.3 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 246 (sh) (log ε 4.03); 292 (sh) (log ε 4.07); 326 (log ε 4.24) (MeOH)



-----文献-----

Buckle, A.L.J. et al., J.C.S., 1954, 3981, (合成法)

Nordal, A. et al., Acta Chem. Scand., 1964, 18, 1979; 1966, 20, 1431, (分離)

Yoshihara, T. et al., Tet. Lett., 1971, 3809, (stereochem)

Takahira, M. et al., Phytochemistry, 1998, 49, 2115, (分離, UV, H-NMR, C13-NMR, Mas)

Kruse, S.O. et al., Planta Med., 1999, 65, 763, (分離)

§ Shengmanol; 23-Ac, 3-*O*-(2-*O*-malonyl-β-D-xylopyranoside)

[CAS No.] 245494-49-9

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

[構造式]

[分子式] C<sub>40</sub>H<sub>60</sub>O<sub>13</sub>

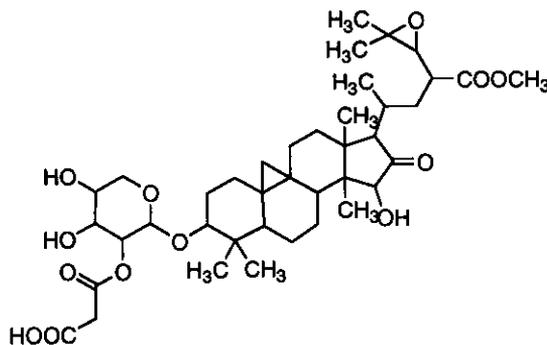
[分子量] 748.906

[正確な分子量] 748.403395

[基原] *Cimicifuga simplex*

[性状] 粉末

[比旋光度]: [α]<sub>D</sub> -19.6 (c, 1.59 in MeOH)



-----文献-----

Sakurai, N. et al., Chem. Pharm. Bull., 1979, 27, 158

Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1999, 47, 1175, (分離, H-NMR, C13-NMR, 誘導体)

§ Shengmanol; 23-Ac, 3-*O*-[β-D-glucopyranosyl-(1 → 3)-β-D-xylopyranoside]

[CAS No.] 163860-88-6

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

[構造式]

[分子式] C<sub>43</sub>H<sub>68</sub>O<sub>15</sub>

[分子量] 825.001

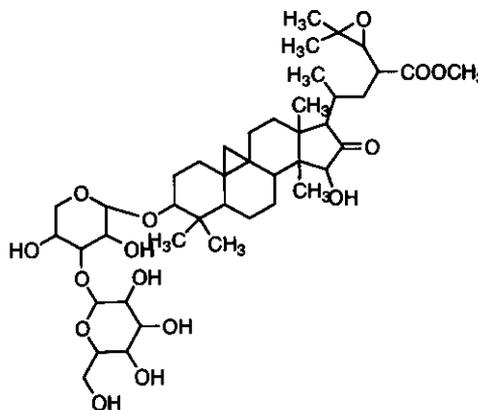
[正確な分子量] 824.455825

[基原] *Cimicifuga simplex*

[性状] 針状結晶

[融点] Mp 245-246 °C

[比旋光度]: [α]<sub>D</sub> -38.2 (c, 1 in MeOH)



-----文献-----

Sakurai, N. et al., Chem. Pharm. Bull., 1979, 27, 158

Kusano, A. et al., Chem. Pharm. Bull., 1994, 42, 1940; 1995, 43, 279; 1999, 47, 1175, (分離, H-NMR, C13-NMR, 誘導体)