

[化合物分類]テルペノイド(Oleanane triterpenoid)

[構造式]

[分子式]  $C_{70}H_{104}O_{32}$

[分子量] 1457.572

[正確な分子量] 1456.65108

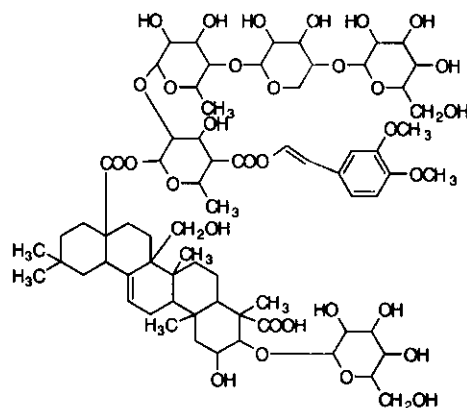
[基原] 次の植物から分離: *Polygala senega*

[性状] 結晶・四水和物

[融点] Mp 247-248 °C

[比旋光度]:  $[\alpha]_D^{20}$  -6.2 (MeOH)

[傷害・毒性] BERDY HAZD : 50 % 致死量(LD<sub>50</sub>) (マウス, 腹腔内投与) 3 mg/kg



-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2  $\beta$ , 3  $\beta$ )-form, 3-O- $\beta$ -D-Glucopyranoside, 28-O-[ $\beta$ -D-galactopyranosyl-(1  $\rightarrow$  4)- $\beta$ -D-xylopyranosyl-(1  $\rightarrow$  4)- $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  2)-[(3,4-dimethoxy-Z-cinnamoyl)-(1  $\rightarrow$  4)- $\beta$ -D-fucopyranosyl]] ester

[化学名・別名] Z-Senegin II

[CAS No.] 162681-52-9

[化合物分類]テルペノイド(Oleanane triterpenoid)

[構造式]

[分子式]  $C_{70}H_{104}O_{32}$

[分子量] 1457.572

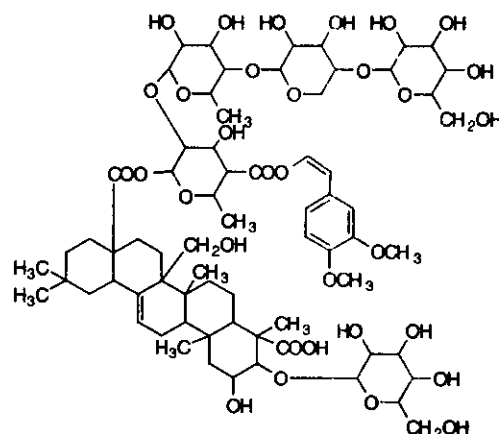
[正確な分子量] 1456.65108

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 238-242 °C

[比旋光度]:  $[\alpha]_D$  -24 (MeOH)



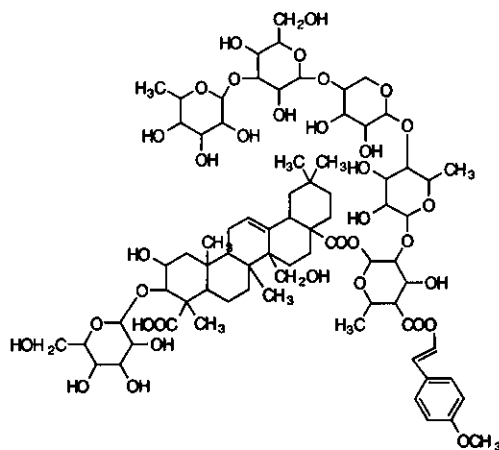
-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2  $\beta$ , 3  $\beta$ )-form, 3-O- $\beta$ -D-Glucopyranoside, 28-O-[ $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  3)- $\beta$ -D-galactopyranosyl-(1  $\rightarrow$  4)- $\beta$ -D-xylopyranosyl-(1  $\rightarrow$  4)- $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  2)-[4-methoxycinnamoyl-(1  $\rightarrow$  4)- $\beta$ -D-fucopyranosyl]] ester

[化学名・別名] Onjisaponin B. Senegin III. Sinegin 3  
 [CAS No.] 35906-36-6  
 [化合物分類] テルペノイド (Oleanane triterpenoid)  
 [構造式]



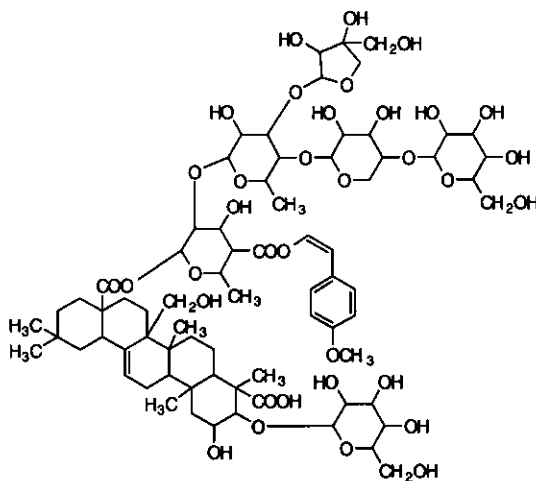
[分子式]  $C_{75}H_{112}O_{35}$   
 [分子量] 1573.689  
 [正確な分子量] 1572.698425  
 [基原] 次の植物から分離: *Polygala senega* and *Polygala tenuifolia*  
 [性状] 粉末 (EtOH 溶液)  
 [融点] Mp 249-251 °C で分解  
 [比旋光度]:  $[\alpha]_D^{17} -10.2$  (c, 1.08 in MeOH)

-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2 $\beta$ ,3 $\beta$ )-form, 3-O- $\beta$ -D-Glucopyranoside, 28-O- $\beta$ -D-galactopyranosyl-(1 $\rightarrow$ 4)- $\beta$ -D-xylopyranosyl-(1 $\rightarrow$ 4)-[ $\beta$ -D-apiofuranosyl-(1 $\rightarrow$ 3)]- $\alpha$ -L-rhamnopyranosyl-(1 $\rightarrow$ 2)-[4-methoxy-E-cinnamoyl-( $\rightarrow$ 4)]- $\beta$ -D-fucopyranosyl] ester

[化学名・別名] E-Senegasaponin A  
 [CAS No.] 162762-97-2  
 [化合物分類] テルペノイド (Oleanane triterpenoid)



[構造式]  
 [分子式]  $C_{74}H_{110}O_{35}$   
 [分子量] 1559.662  
 [正確な分子量] 1558.682775  
 [基原] *Polygala senega* var. *latifolia*  
 [性状] 結晶  
 [融点] Mp 228-231 °C  
 [比旋光度]:  $[\alpha]_D -12.9$  (MeOH)

-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

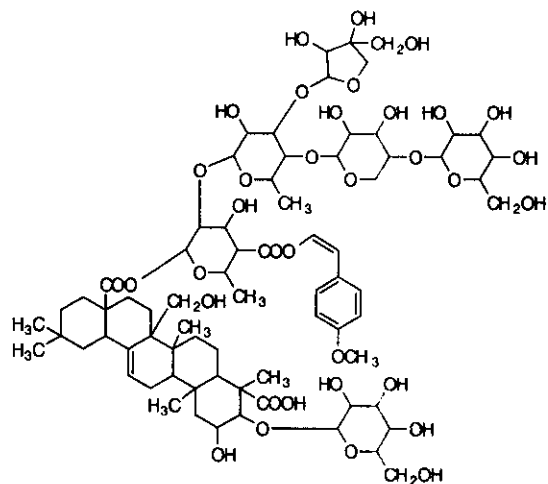
§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2 $\beta$ ,3 $\beta$ )-form, 3-O- $\beta$ -D-Glucopyranoside, 28-O- $\beta$ -D-galactopyranosyl-(1 $\rightarrow$ 4)- $\beta$ -D-xylopyranosyl-(1 $\rightarrow$ 4)-[ $\beta$ -D-apiofuranosyl-(1 $\rightarrow$ 3)]- $\alpha$ -L-rhamnopyranosyl-(1 $\rightarrow$ 2)-[4-methoxy-Z-cinnamoyl-( $\rightarrow$ 4)]- $\beta$ -D-fucopyranosyl] ester

[化学名・別名] Z-Senegasaponin A

[CAS No.] 162613-72-1

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

[構造式]



[分子式]  $C_{74}H_{110}O_{35}$

[分子量] 1559.662

[正確な分子量] 1558.682775

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 237-240 °C

-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)

Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

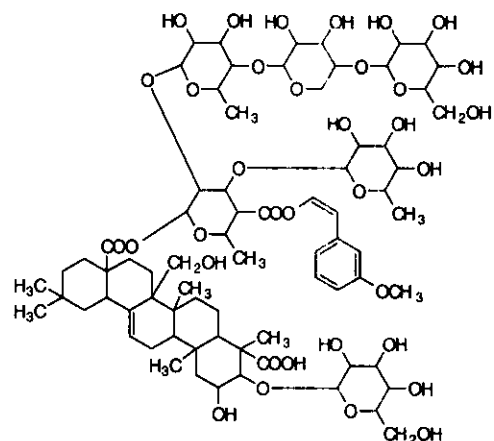
§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2  $\beta$ , 3  $\beta$ )-form, 3-O- $\beta$ -D-Glucopyranoside, 28-O- $[\beta$ -D-galactopyranosyl-(1  $\rightarrow$  4)- $\beta$ -D-xylopyranosyl-(1  $\rightarrow$  4)- $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  2)- $[\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  3)]-[3-methoxy-Z-cinnamoyl-( $\rightarrow$  4)- $\beta$ -D-fucopyranosyl]] ester

[化学名・別名] Z-Senegin III

[CAS No.] 162681-53-0

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

[構造式]



[分子式]  $C_{75}H_{112}O_{35}$

[分子量] 1573.689

[正確な分子量] 1572.698425

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 243-246 °C

[比旋光度]:  $[\alpha]_D -17$  (MeOH)

-----文献-----

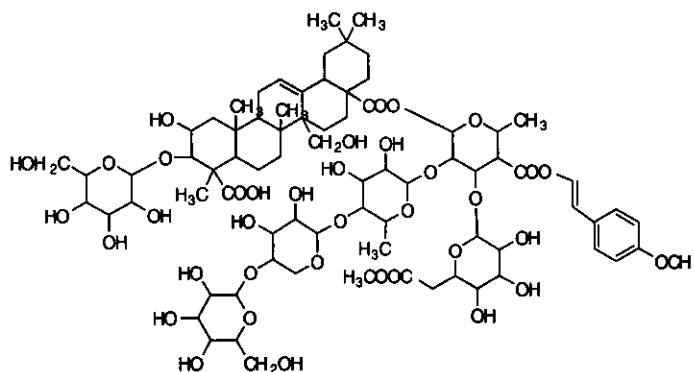
Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)

Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2  $\beta$ , 3  $\beta$ )-form, 3-O- $\beta$ -D-Glucopyranoside, 28-O- $[\beta$ -D-galactopyranosyl-(1  $\rightarrow$  4)- $\beta$ -D-xylopyranosyl-(1  $\rightarrow$  4)- $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  2)-[6-O-acetyl- $\beta$ -D-glucopyranosyl-(1  $\rightarrow$  3)]-[4-methoxy-E-cinnamoyl-( $\rightarrow$  4)]- $\beta$ -D-fucopyranosyl]] ester

[化学名・別名] *E*-Senegasaponin C  
 [CAS No.] 180387-69-3  
 [化合物分類] テルペノイド (Oleanane triterpenoid)  
 [構造式]  
 [分子式]  $C_{77}H_{114}O_{37}$   
 [分子量] 1631.725  
 [正確な分子量] 1630.703905  
 [基原] *Polygala senega* var. *latifolia*  
 [性状] 結晶  
 [融点] Mp 230-232 °C  
 [比旋光度]:  $[\alpha]_D^{29} +11.4$  (c, 0.1 in MeOH)

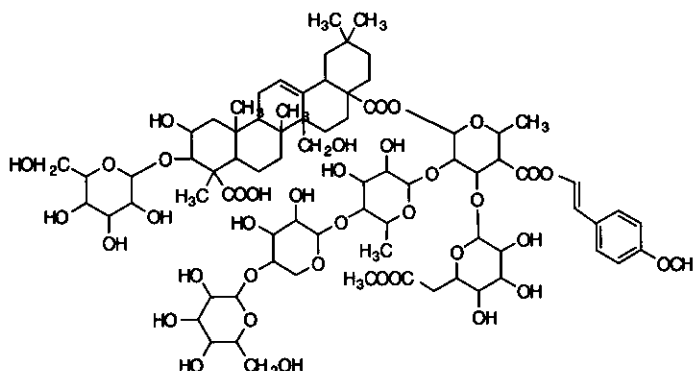


-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2  $\beta$ , 3  $\beta$ )-form, 3-*O*- $\beta$ -D-Glucopyranoside, 28-*O*-[ $\beta$ -D-galactopyranosyl-(1  $\rightarrow$  4)- $\beta$ -D-xylopyranosyl-(1  $\rightarrow$  4)- $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  2)-[6-*O*-acetyl- $\beta$ -D-glucopyranosyl-(1  $\rightarrow$  3)]-[4-methoxy-*Z*-cinnamoyl-( $\rightarrow$  4)]- $\beta$ -D-fucopyranosyl] ester  
 [化学名・別名] *Z*-Senegasaponin C

[CAS No.] 180684-11-1  
 [化合物分類] テルペノイド (Oleanane triterpenoid)  
 [構造式]  
 [分子式]  $C_{77}H_{114}O_{37}$   
 [分子量] 1631.725  
 [正確な分子量] 1630.703905  
 [基原] *Polygala senega* var. *latifolia*  
 [性状] 結晶  
 [融点] Mp 229-232 °C  
 [比旋光度]:  $[\alpha]_D^{29} -4.1$  (c, 0.1 in MeOH)

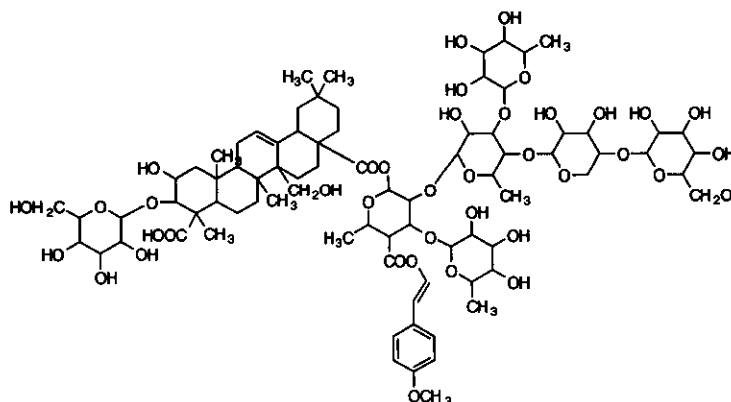


-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2  $\beta$ , 3  $\beta$ )-form, 3-*O*- $\beta$ -D-Glucopyranoside, 28-*O*-[ $\beta$ -D-galactopyranosyl-(1  $\rightarrow$  4)- $\beta$ -D-xylopyranosyl-(1  $\rightarrow$  4)-[ $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  3)]- $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  2)-[ $\alpha$ -L-rhamnopyranosyl-(1  $\rightarrow$  3)]-[4-methoxycinnamoyl-( $\rightarrow$  4)]- $\beta$ -D-fucopyranosyl] ester  
 [化学名・別名] Senegin IV. Sinegin 4

[CAS No.] 51005-46-0  
 [化合物分類] テルペノイド (Oleanane triterpenoid)  
 [構造式]  
 [分子式]  $C_{81}H_{122}O_{39}$   
 [分子量] 1719.831  
 [正確な分子量] 1718.756335  
 [基原] 次の植物から分離: *Polygala senega*  
 [融点] Mp 249-250 °C で分解  
 [比旋光度]:  $[\alpha]_D^{20} -20.2$  (c, 2 in MeOH)



-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ § ヒメハギ科ヒロハセネガ (*Polygala senega* Linne var. *latifolia* Torrey et Gray) の根。

§ Senegose D

[CAS No.] 151466-63-6  
 [化合物分類] 炭水化物 (Oligosaccharide)  
 [構造式]

[分子式] C<sub>57</sub>H<sub>72</sub>O<sub>33</sub>

[分子量] 1285.176

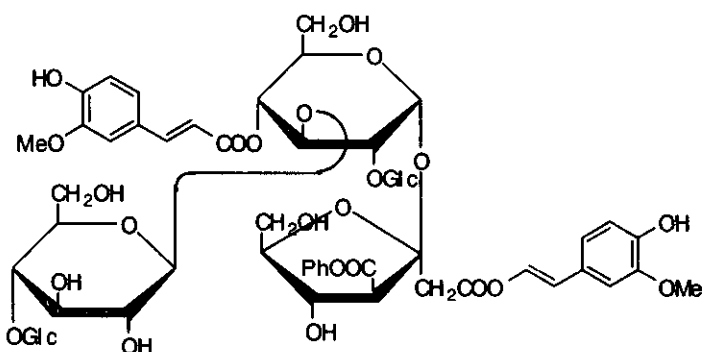
[正確な分子量] 1284.395595

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科) の根

[性状] 無定型の粉末・二水和物

[比旋光度]: [α]<sub>D</sub><sup>23</sup> -6.9 (c, 1 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 220 (ε 28180); 233 (ε 29510); 284 (sh) (ε 17780); 299 (sh) (ε 24550); 325 (ε 33880) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6<sup>a</sup>-Ac

[化学名・別名] Senegose C

[CAS No.] 151466-62-5

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C<sub>59</sub>H<sub>74</sub>O<sub>34</sub>

[分子量] 1327.213

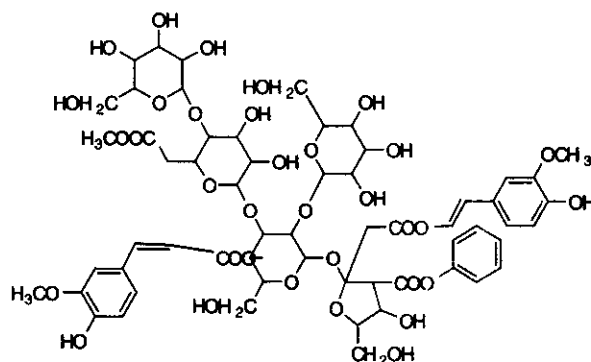
[正確な分子量] 1326.40616

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末・二水和物

[比旋光度]: [α]<sub>D</sub><sup>23</sup> -16 (c, 1.3 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 219 (ε 33110); 233 (ε 33880); 284 (sh) (ε 20420); 297 (sh) (ε 26910); 327 (ε 40740) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6<sup>c</sup>-Ac

[化学名・別名] Senegose B

[CAS No.] 151466-61-4

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C<sub>59</sub>H<sub>74</sub>O<sub>34</sub>

[分子量] 1327.213

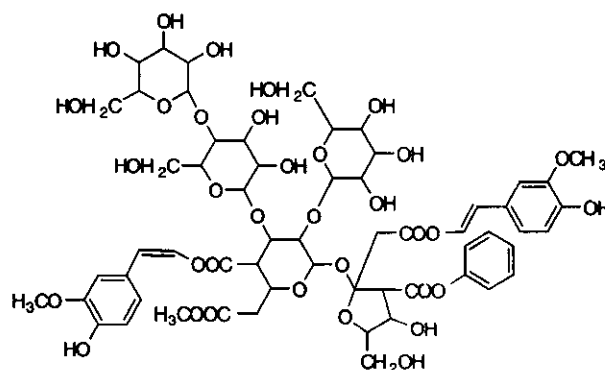
[正確な分子量] 1326.40616

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末・一水和物

[比旋光度]: [α]<sub>D</sub><sup>23</sup> -10.2 (c, 1.2 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 220 (ε 38020); 233 (ε 38020); 284 (sh) (ε 24550); 299 (sh) (ε 30200); 327 (ε 43650) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6<sup>β</sup>,6<sup>α</sup>-Di-Ac

[化学名・別名] Senegose A

[CAS No.] 151466-60-3

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C<sub>61</sub>H<sub>76</sub>O<sub>35</sub>

[分子量] 1369.25

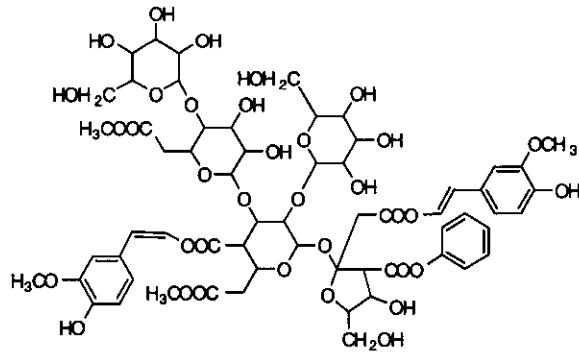
[正確な分子量] 1368.416725

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末 + 4·1/2H<sub>2</sub>O

[比旋光度]: [α]<sub>D</sub><sup>23</sup> -9.9 (c, 1.2 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 220 (ε 33110); 233 (ε 33110); 284 (sh) (ε 20420); 299 (sh) (ε 26300); 328 (ε 38900) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 6<sup>β</sup>,6<sup>α</sup>-Di-Ac, 2'-Z-isomer

[化学名・別名] Senegose E

[CAS No.] 151530-27-7

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C<sub>61</sub>H<sub>76</sub>O<sub>35</sub>

[分子量] 1369.25

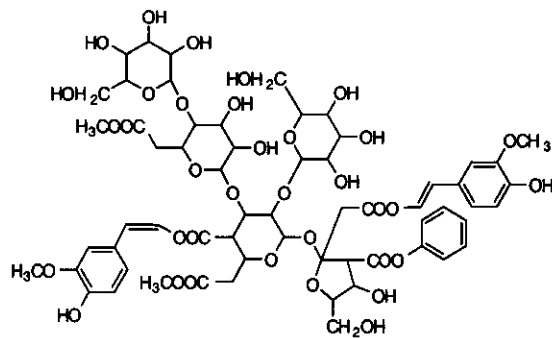
[正確な分子量] 1368.416725

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末・三水和物

[比旋光度]: [α]<sub>D</sub><sup>23</sup> +64.5 (c, 0.6 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 220 (ε 35480); 232 (ε 35480); 284 (sh) (ε 19500); 301 (sh) (ε 25700); 327 (ε 36310) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 4<sup>β</sup>-Deglucosyl, 6<sup>β</sup>-Ac

[化学名・別名] Senegose G

[CAS No.] 156031-87-7

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C<sub>55</sub>H<sub>64</sub>O<sub>29</sub>

[分子量] 1165.071

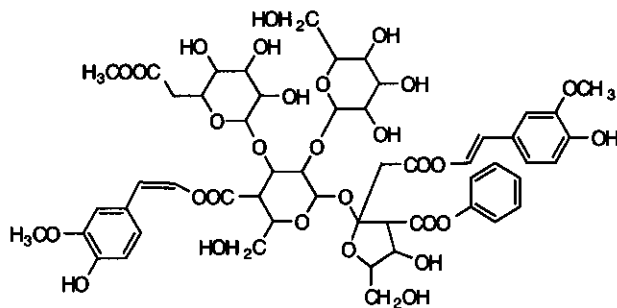
[正確な分子量] 1164.353335

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末・三水和物

[比旋光度]: [α]<sub>D</sub> +1.2 (c, 1.2 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 220 (ε 29510); 233 (ε 30200); 285 (sh) (ε 17380); 299 (sh) (ε 22910); 327 (ε 34670) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 4<sup>p</sup>-Deglucosyl, 6<sup>c</sup>-Ac

[化学名・別名] Senegose H

[CAS No.] 156031-88-8

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C<sub>53</sub>H<sub>64</sub>O<sub>29</sub>

[分子量] 1165.071

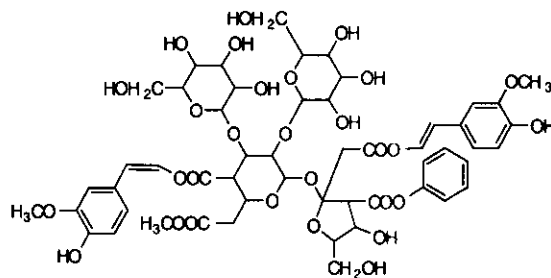
[正確な分子量] 1164.353335

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末 + 2・1/2H<sub>2</sub>O

[比旋光度]: [α]<sub>D</sub><sup>20</sup> -3 (c, 0.66 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 219 (ε 38020); 233 (ε 38020); 286 (sh) (ε 22390); 301 (sh) (ε 29510); 328 (ε 43650) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 4<sup>p</sup>-Deglucosyl, 6<sup>p</sup>,6<sup>c</sup>-di-Ac

[化学名・別名] Senegose F

[CAS No.] 156031-89-9

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C<sub>55</sub>H<sub>66</sub>O<sub>30</sub>

[分子量] 1207.108

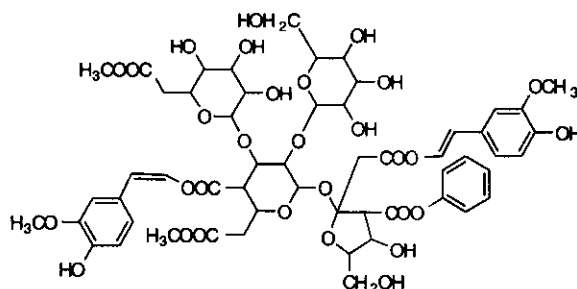
[正確な分子量] 1206.3639

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末・三水和物

[比旋光度]: [α]<sub>D</sub><sup>22</sup> -11.5 (c, 1.2 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 219 (ε 38020); 233 (ε 38020); 285 (sh) (ε 22910); 299 (sh) (ε 28840); 327 (ε 43650) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ Senegose D; 2<sup>c</sup>-Deglucosyl, 6<sup>p</sup>,6<sup>c</sup>-Di-Ac

[化学名・別名] Senegose I

[CAS No.] 156031-86-6

[化合物分類] 炭水化物 (Oligosaccharide)

[構造式]

[分子式] C<sub>55</sub>H<sub>66</sub>O<sub>30</sub>

[分子量] 1207.108

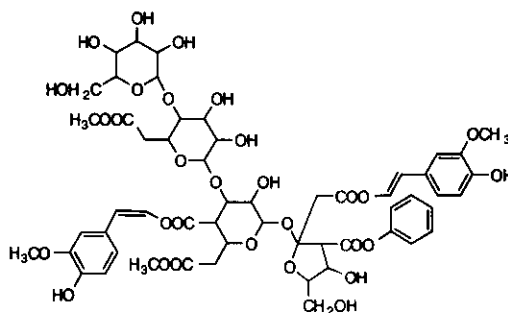
[正確な分子量] 1206.3639

[基原] *Polygala senega* var. *latifolia* (ヒメハギ科)

[性状] 無定型の粉末 + 2・1/2H<sub>2</sub>O

[比旋光度]: [α]<sub>D</sub><sup>22</sup> -29.1 (c, 0.8 in MeOH)

[UV]: [neutral] λ<sub>max</sub> 220 (ε 35480); 234 (ε 35480); 287 (sh) (ε 21880); 300 (sh) (ε 26910); 328 (ε 40740) (MeOH)



-----文献-----

Saitoh, H. et al., Chem. Pharm. Bull., 1993, 41, 1127; 2125; 1994, 42, 641, (分離, UV, H-NMR, C13-NMR)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2 β, 3 β)-form, 3-O-β-D-Glucopyranoside, 28-O-β-D-galactopyranosyl-(1 → 4)-β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-

[4-methoxy-*E*-cinnamoyl-(→4)-β-D-fucopyranosyl]] ester

[化学名・別名] *E*-Senegásaponin B

[CAS No.] 162870-58-8

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

[構造式]

[分子式] C<sub>69</sub>H<sub>102</sub>O<sub>31</sub>

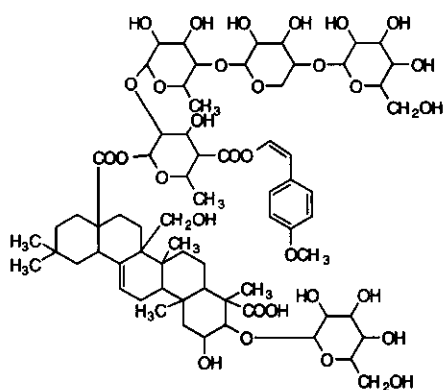
[分子量] 1427.546

[正確な分子量] 1426.640515

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 251-254 °C



-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)

Brieskorn, C.H. et al., Arch. Pharm. (Weinheim, Ger.), 1975, 308, 824, (誘導體)

Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-form, 3-O-β-D-Glucopyranoside, 28-O-β-D-galactopyranosyl-(1→4)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[4-methoxy-Z-cinnamoyl-(→4)-β-D-fucopyranosyl]] ester

[化学名・別名] *Z*-Senegasaponin B

[CAS No.] 162613-71-0

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

[構造式]

[分子式] C<sub>69</sub>H<sub>102</sub>O<sub>31</sub>

[分子量] 1427.546

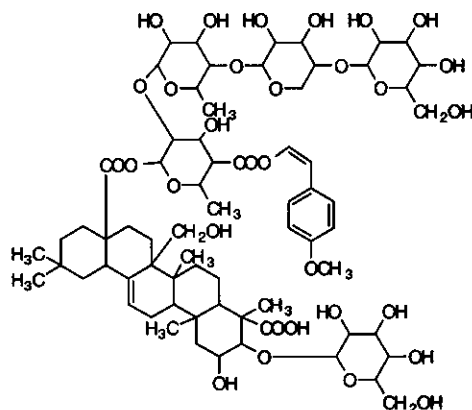
[正確な分子量] 1426.640515

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 252-255 °C

[比旋光度]: [α]<sub>D</sub> -13.2 (MeOH)



-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)

Brieskorn, C.H. et al., Arch. Pharm. (Weinheim, Ger.), 1975, 308, 824, (誘導體)

Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-form, 3-O-β-D-Glucopyranoside, 28-O-β-D-galactopyranosyl-(1→4)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[(3,4-dimethoxy-Z-cinnamoyl)-(→4)-β-D-fucopyranosyl]] ester

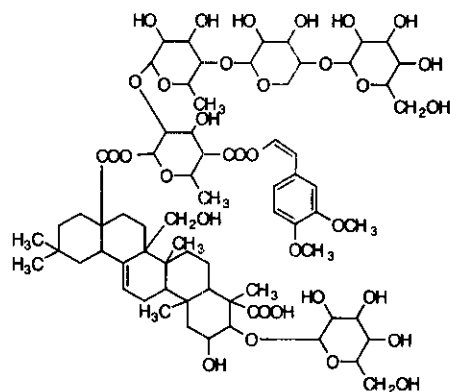
[化学名・別名] *Z*-Senegin II

[CAS No.] 162681-52-9

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



[構造式]  
 [分子式]  $C_{70}H_{104}O_{32}$   
 [分子量] 1457.572  
 [正確な分子量] 1456.65108  
 [基原] *Polygala senega* var. *latifolia*  
 [性状] 結晶  
 [融点] Mp 238-242 °C  
 [比旋光度]:  $[\alpha]_D -24$  (MeOH)

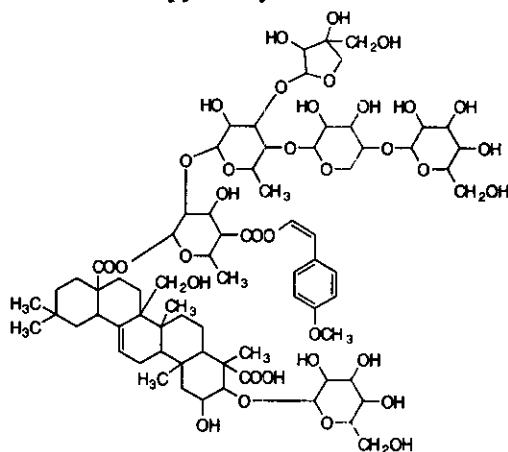


-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2 $\beta$ ,3 $\beta$ )-form, 3-O- $\beta$ -D-Glucopyranoside, 28-O-  
 [ $\beta$ -D-galactopyranosyl-(1 $\rightarrow$ 4)- $\beta$ -D-xylopyranosyl-(1 $\rightarrow$ 4)-[ $\beta$ -D-apiofuranosyl-(1 $\rightarrow$ 3)]- $\alpha$ -  
 L-rhamnopyranosyl-(1 $\rightarrow$ 2)-[4-methoxy-E-cinnamoyl-( $\rightarrow$ 4)]- $\beta$ -D-fucopyranosyl] ester  
 [化学名・別名] E-Senegasaponin A  
 [CAS No.] 162762-97-2  
 [化合物分類] テルペノイド (Oleanane triterpenoid)  
 [構造式]

[分子式]  $C_{74}H_{110}O_{35}$   
 [分子量] 1559.662  
 [正確な分子量] 1558.682775  
 [基原] *Polygala senega* var. *latifolia*  
 [性状] 結晶  
 [融点] Mp 228-231 °C  
 [比旋光度]:  $[\alpha]_D -12.9$  (MeOH)

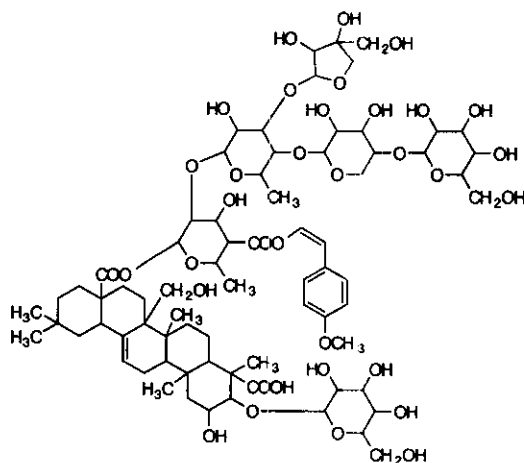


-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2 $\beta$ ,3 $\beta$ )-form, 3-O- $\beta$ -D-Glucopyranoside, 28-O-  
 [ $\beta$ -D-galactopyranosyl-(1 $\rightarrow$ 4)- $\beta$ -D-xylopyranosyl-(1 $\rightarrow$ 4)-[ $\beta$ -D-apiofuranosyl-(1 $\rightarrow$ 3)]- $\alpha$ -  
 L-rhamnopyranosyl-(1 $\rightarrow$ 2)-[4-methoxy-Z-cinnamoyl-( $\rightarrow$ 4)]- $\beta$ -D-fucopyranosyl] ester  
 [化学名・別名] Z-Senegasaponin A  
 [CAS No.] 162613-72-1  
 [化合物分類] テルペノイド (Oleanane triterpenoid)  
 [構造式]

[分子式]  $C_{74}H_{110}O_{35}$   
 [分子量] 1559.662  
 [正確な分子量] 1558.682775  
 [基原] *Polygala senega* var. *latifolia*  
 [性状] 結晶  
 [融点] Mp 237-240 °C



-----文献-----

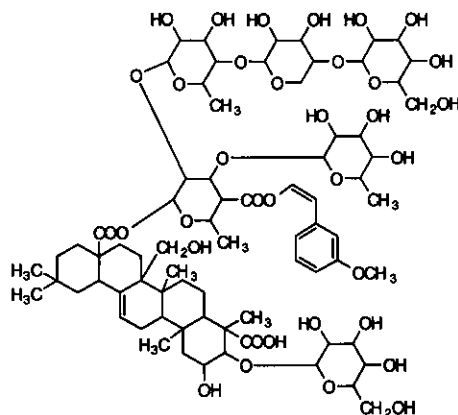
Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-form, 3-O-β-D-Glucopyranoside, 28-O-β-D-galactopyranosyl-(1→4)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-[3-methoxy-Z-cinnamoyl-(→4)-β-D-fucopyranosyl]] ester

[化学名・別名] Z-Senegin III

[CAS No.] 162681-53-0

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



[構造式]

[分子式] C<sub>75</sub>H<sub>112</sub>O<sub>35</sub>

[分子量] 1573.689

[正確な分子量] 1572.698425

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 243-246 °C

[比旋光度]: [α]<sub>D</sub> -17 (MeOH)

-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-form, 3-O-β-D-Glucopyranoside, 28-O-β-D-galactopyranosyl-(1→4)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[6-O-acetyl-β-D-glucopyranosyl-(1→3)]-[4-methoxy-E-cinnamoyl-(→4)]-β-D-fucopyranosyl] ester

[化学名・別名] E-Senegasaponin C

[CAS No.] 180387-69-3

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

[構造式]

[分子式] C<sub>77</sub>H<sub>114</sub>O<sub>37</sub>

[分子量] 1631.725

[正確な分子量] 1630.703905

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 230-232 °C

[比旋光度]: [α]<sub>D</sub><sup>20</sup> +11.4 (c, 0.1 in MeOH)

-----文献-----

Shimizu, Y. et al., J.A.C.S., 1966, 88, 1544, (構造決定)  
 Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)  
 Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)  
 Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

§ 2,3,27-Trihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-form, 3-O-β-D-Glucopyranoside, 28-O-β-D-galactopyranosyl-(1→4)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[6-O-acetyl-β-D-glucopyranosyl-(1→3)]-[4-methoxy-Z-cinnamoyl-(→4)]-β-D-fucopyranosyl] ester

[化学名・別名] Z-Senegasaponin C

[CAS No.] 180684-11-1

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

-----文献-----

[構造式]

[分子式]  $C_{77}H_{114}O_{37}$

[分子量] 1631.725

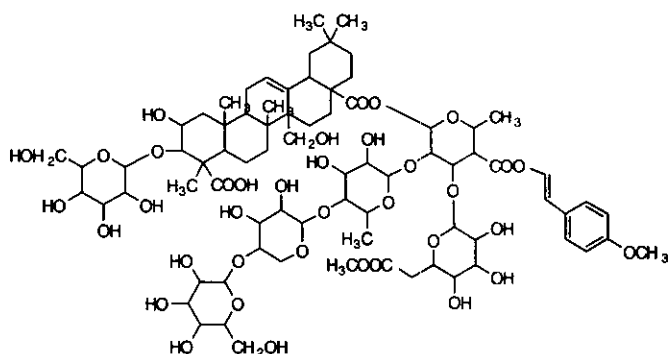
[正確な分子量] 1630.703905

[基原] *Polygala senega* var. *latifolia*

[性状] 結晶

[融点] Mp 229-232 °C

[比旋光度]:  $[\alpha]_D^{29} -4.1$  (c, 0.1 in MeOH)



-----文献-----

Tsukitani, Y. et al., Chem. Pharm. Bull., 1973, 21, 791; 1564, (Senegin)

Sakuma, S. et al., Chem. Pharm. Bull., 1981, 29, 2431; 1982, 30, 810, (C13-NMR, Onjisaponin)

Yoshikawa, M. et al., Chem. Pharm. Bull., 1995, 43, 350; 2115; 1996, 44, 1305, (Senegasaponins, Senegin)

\*\*\*\*\*ゼラニウム (Geranium) \*\*\*\*\*

§ § フウロソウ科ニオイテンジクアオイ (*Pelargonium graveolens* Aiton) の葉, 枝, 茎, 花。

§ 3,7-Dimethyl-2,6-octadien-1-ol; (E)-form, O-β-D-Glucopyranoside

[CAS No.] 22850-13-1

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

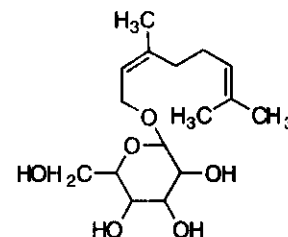
[構造式]

[分子式]  $C_{16}H_{28}O_6$

[分子量] 316.394

[正確な分子量] 316.18859

[基原] 次の植物から分離: *Rosa* spp., *Pelargonium graveolens*, ブドウ (*Vitis vinifera*)



-----文献-----

Francis, M.J.O. et al., Phytochemistry, 1969, 8, 1339, (分離, 配糖体)

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhauser Verlag, Basel, 1972, nos. 118; 119, (生育)

Opdyke, D.L.J., Food Cosmet. Toxicol., 1974, 12, 881, (レビュー, 毒性, Geraniol)

Opdyke, D.L.J., Food Cosmet. Toxicol., Suppl., 1976, 14, 783; 785, (レビュー, エステル)

Ackermann, I.E. et al., Annalen, 1989, 79, (合成法, 配糖体)

Lewis, R.J., Food Additives Handbook, Van Nostrand Reinhold International, New York, 1989, DTD000; DTD200; DTD800

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, DTD000; GCY000; DTD200; DTD800

§ 3,7-Dimethyl-2,6-octadien-1-ol; (Z)-form, O-β-D-Glucopyranoside

[CAS No.] 22850-14-2

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

[構造式]

[分子式]  $C_{16}H_{28}O_6$

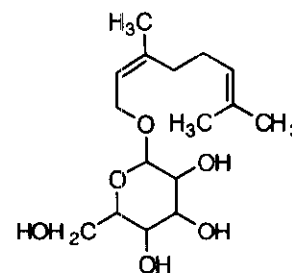
[分子量] 316.394

[正確な分子量] 318.18859

[基原] 次の植物から分離: *Rosa* spp., *Pelargonium graveolens*, ブドウ

[性状] 板状結晶 (EtOH 溶液) (as tetra-Ac)

[融点] Mp 68-70 °C (tetra-Ac)



-----文献-----

Francis, M.J.O. et al., Phytochemistry, 1969, 8, 1339, (分離, 配糖体)

Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhauser Verlag, Basel, 1972, nos. 118; 119, (生育)

Opdyke, D.L.J., Food Cosmet. Toxicol., 1974, 12, 881, (レビュー, 毒性, Geraniol)  
 Opdyke, D.L.J., Food Cosmet. Toxicol., Suppl., 1976, 14, 783; 785, (レビュー, エステル)  
 Ackermann, I.E. et al., Annalen, 1989, 79, (合成法, 配糖体)  
 Lewis, R.J., Food Additives Handbook, Van Nostrand Reinhold International, New York, 1989, DTD000;  
 DTD200; DTD800  
 Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992,  
 DTD000; GCY000; DTD200; DTD800

\*\*\*\*\*セロリー (Celery) \*\*\*\*\*

§ § セリ科セロリー (*Apium graveolens* L.) の種子, 茎葉または根。

§ Apiumetin; (R)-form

[化合物分類] ベンゾピラノイド (7,8-Dioxygenated coumarin), ベンゾピラノイド (Dihydrofuranocoumarin)

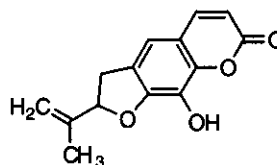
[構造式]

[基原] *Apium graveolens* と *Apium leptophyllum* の種子

[性状] 針状結晶

[融点] Mp 198 °C

[比旋光度]:  $[\alpha]_D^{19}$  -68.29 (c, 0.41 in CHCl<sub>3</sub>)



-----文献-----

Garg, S.K. et al., Phytochemistry, 1978, 17, 2135, (分離, 構造決定)  
 Sharma, B.R. et al., Indian J. Chem., Sect. B, 1979, 17, 647, (Leptophyllidin)  
 Ahluwalia, V.K. et al., Phytochemistry, 1988, 27, 1181, (誘導體)  
 Elgamal, M.H.A. et al., Phytochemistry, 1993, 34, 819, (分離, H-NMR)

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

[CAS No.] 115356-05-3

[化合物分類] ベンゾピラノイド (Dihydrofuranocoumarin), ベンゾピラノイド (7,8-Dioxygenated coumarin)

[構造式]

[分子式] C<sub>20</sub>H<sub>22</sub>O<sub>9</sub>

[分子量] 406.388

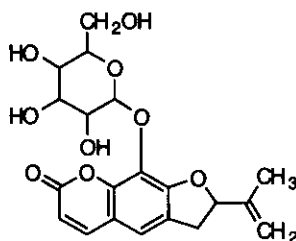
[正確な分子量] 406.126385

[基原] *Apium graveolens*

[性状] 針状結晶 (EtOH)

[融点] Mp 165 °C

[比旋光度]:  $[\alpha]_D^{20}$  -60 (c, 0.16 in CHCl<sub>3</sub>)



-----文献-----

Garg, S.K. et al., Phytochemistry, 1978, 17, 2135, (分離, 構造決定)  
 Sharma, B.R. et al., Indian J. Chem., Sect. B, 1979, 17, 647, (Leptophyllidin)  
 Ahluwalia, V.K. et al., Phytochemistry, 1988, 27, 1181, (誘導體)  
 Elgamal, M.H.A. et al., Phytochemistry, 1993, 34, 819, (分離, H-NMR)

§ Brassinolide; 2-Deoxy

[化学名・別名] 3,22,23-Trihydroxy-24-methyl-B-homo-7-oxacholestan-6-one. 2-Deoxybrassinolide

[CAS No.] 144071-55-6

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

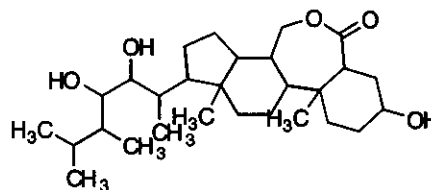
[構造式]

[分子式] C<sub>28</sub>H<sub>48</sub>O<sub>5</sub>

[分子量] 464.684

[正確な分子量] 464.350175

[基原] *Apium graveolens* と *Pisium sativum* の種子



-----文献-----

Sakakibara, M. et al., *Agric. Biol. Chem.*, 1983, 47, 663, (合成法, 成書)

Singh, H. et al., *Indian J. Chem., Sect. B*, 1986, 25, 989, (レビュー)

Yokota, T. et al., *Phytochemistry*, 1996, 42, 509, (2-Deoxybrassinolide)

### § Celereoin

[化学名・別名] 5-Hydroxymarmesin

[CAS No.] 74560-02-4

[化合物分類] ベンゾピラノイド (5,7-Dioxygenated coumarin), ベンゾピラノイド (Dihydrofuranocoumarin)

[構造式]

[分子式]  $C_{14}H_{14}O_5$

[分子量] 262.262

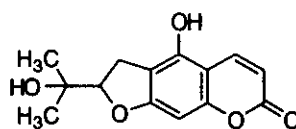
[正確な分子量] 262.084125

[基原] *Apium graveolens*

[性状] 結晶

[融点] Mp 201 °C

[比旋光度]:  $[\alpha]_D^{21} -38$  (MeOH)



-----文献-----

Garg, S.K. et al., *Planta Med.*, 1980, 38, 186, (Celereoside)

### § Celereoin; 3'-O-β-D-Glucopyranoside

[化学名・別名] Celereoside

[CAS No.] 74608-59-6

[化合物分類] ベンゾピラノイド

(Dihydrofuranocoumarin), ベンゾピラノイド (5,7-Dioxygenated coumarin)

[構造式]

[分子式]  $C_{20}H_{24}O_{10}$

[分子量] 424.404

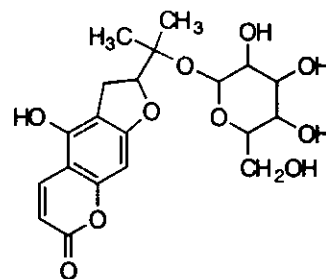
[正確な分子量] 424.13695

[基原] *Apium graveolens*

[性状] 結晶

[融点] Mp 200-201 °C

[比旋光度]:  $[\alpha]_D^{24} -37.27$  (MeOH)



-----文献-----

Garg, S.K. et al., *Planta Med.*, 1980, 38, 186, (Celereoside)

### § Celerin

[化学名・別名] 4-(1,1-Dimethyl-2-propenyl)-8-hydroxy-7-methoxy-2H-1-benzopyran-2-one

[CAS No.] 73815-20-0

[化合物分類] ベンゾピラノイド (7,8-Dioxygenated coumarin)

[構造式]

[分子式]  $C_{15}H_{16}O_4$

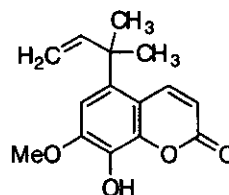
[分子量] 260.289

[正確な分子量] 260.10486

[基原] *Apium graveolens* の種子

[性状] 板状結晶 (EtOAc/petrol)

[融点] Mp 158-159.5 °C



-----文献-----

Garg, S.K. et al., *Planta Med.*, 1980, 38, 186, (分離)

Murray, R.D.H. et al., *Tetrahedron*, 1984, 40, 5229, (構造決定, 合成法)

### § 3a,4-Dihydro-3-(3-methylbutylidene)-1(3H)-isobenzofuranone

[化学名・別名] 3-Isovalidene-3a,4-dihydrophthalide

[化合物分類] ベンゾフラノイド (Isobenzofuran)

[構造式]

[分子式]  $C_{13}H_{16}O_2$

[分子量] 204.268

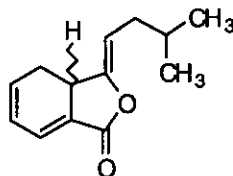
[正確な分子量] 204.11503

[基原] セロリの茎と葉 (*Apium graveolens*) のにおい成分

[性状] 淡黄色のオイル

[沸点]  $Bp_{10}$  175 °C

[その他のデータ]  $\lambda_{max}$  282 (log  $\epsilon$  4.12), 273 (4.14), 227 (4.60) and 197 nm (5.08).  $n_D^{27.5}$  1.5172



-----文献-----

Gold, H.J. et al., J.O.C., 1963, 28, 985, (分離. IR, UV)

### § 7,8-Dihydroxy-2H-1-benzopyran-2-one; Methylene ether

[化学名・別名] 8H-1,3-Dioxolo[4,5-h][1]benzopyran-8-one (CAS 名). 7,8-Methylenedioxy coumarin

[CAS No.] 4361-93-7

[化合物分類] ベンゾピラノイド (7,8-Dioxygenated coumarin)

[構造式]

[分子式]  $C_{10}H_6O_4$

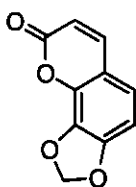
[分子量] 190.155

[正確な分子量] 190.02661

[基原] *Apium graveolens*

[性状] 結晶

[融点]  $Mp$  187-189 °C



-----文献-----

Billek, G. et al., Monatsh. Chem., 1962, 93, 85, (8-Me ether)

Abyshev, A.Z., Khim. Prir. Soedin., 1974, 10, 568; Chem. Nat. Compd. (Engl. Transl.), 1974, 10, 581, (分離)

Rybalko, K.S. et al., Khim. Prir. Soedin., 1976, 12, 294; Chem. Nat. Compd. (Engl. Transl.), 1976, 12, 262, (分離)

Atta-ur-Rahman et al., Phytochemistry, 1997, 44, 683, (7-Me-8-methyloxobutyl)

Tsai, I.-L. et al., J. Chin. Chem. Soc. (Taipei), 1998, 45, 99, (Peroxyschinallylol, Peroxyschinilenol)

### § 4,9-Dihydroxy-7H-furo[3,2-g][1]benzopyran-7-one; 4-Me ether, 9-O-β-D-glucopyranoside

[CAS No.] 115356-06-4

[化合物分類] ベンゾピラノイド (Furanocoumarin), ベンゾピラノイド (5,7,8-Trioxxygenated coumarin)

[構造式]

[分子式]  $C_{18}H_{18}O_{10}$

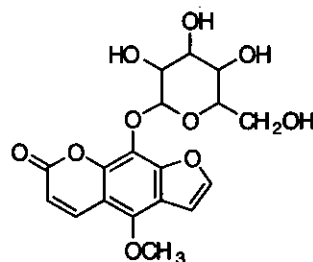
[分子量] 394.334

[正確な分子量] 394.09

[基原] *Apium graveolens*

[性状] 針状結晶 ( $CHCl_3/MeOH$ )

[融点]  $Mp$  230 °C



-----文献-----

Briggs, L.H. et al., Tetrahedron, 1958, 2, 256, (分離, 誘導体)

Komissarenko, N.F. et al., Khim. Prir. Soedin., 1966, 2, 375; Chem. Nat. Compd. (Engl. Transl.), 1966, 2, 307, (Cnidilin)

Abu-Mustafa, G.A. et al., J. Het. Chem., 1973, 10, 443, (成書)

Sokolova, A.I. et al., Khim. Prir. Soedin., 1976, 12, 166; Chem. Nat. Compd. (Engl. Transl.), 1976, 12, 150, (4-Methoxy-9-gernanyloxypsoralen)

Kwon, Y.-S. et al., Phytochemistry, 1997, 44, 887, (bis-dihydroxymethylbutyl)

### § 2-(1,2-Dihydroxy-1-methylethyl)-2,3-dihydro-7H-furo[3,2-g][1]benzopyran-7-one; (1'S,2)-form

[化学名・別名] Dorsteniol

[CAS No.] 80794-85-0

[化合物分類] ベンゾピラノイド (7-Oxygenated coumarins, 6-substituted), ベンゾピラノイド

(Dihydrofuranocoumarin)

[構造式]

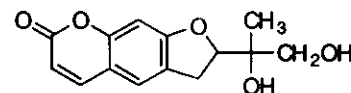
[基原] *Apium graveolens*, *Dorstenia contrajerva*, *Dorstenia excentrica* の根

[性状] プリズム結晶

[融点] Mp 172-173 °C (natural). Mp 185-187 °C (synthetic). Mp 178-180 °C (as 2'-Ac)

[比旋光度]:  $[\alpha]_D +45$  (c, 1 in CHCl<sub>3</sub>) (2'-Ac)

[UV]: [neutral]  $\lambda_{max}$  231 (log  $\epsilon$  3.6); 248 (log  $\epsilon$  3.53); 259 (log  $\epsilon$  3.48); 300 (log  $\epsilon$  3.61); 360 (log  $\epsilon$  4.02) (溶媒の報告はない) (2'-Ac)



-----文献-----

Abyshev, A.Z. et al., *Khim. Prir. Soedin.*, 1974, 10, 574; 1983, 19, 704; *Chem. Nat. Compd.* (Engl. Transl.), 1974, 10, 586; 1983, 19, 668, (Tortuosinol)

Tovar-Miranda, R. et al., *J. Nat. Prod.*, 1998, 61, 1216, (分離, 合成法, H-NMR, C13-NMR, 絶対構造)

Rojas-Lima, S. et al., *Phytochemistry*, 1999, 50, 863, (分離, UV, CD, IR, H-NMR, C13-NMR, Mass, 絶対構造)

Jimenez, B. et al., *Phytochemistry*, 2000, 53, 1025, (Senecioidorsteniol)

§ 7,8-Dihydroxy-6-prenylcoumarin; 8-Me ether

[化学名・別名] 7-Hydroxy-8-methoxy-6-(3-methyl-2-butenyl)-2H-1-benzopyran-2-one.

7-Hydroxy-8-methoxy-6-prenylcoumarin. Apigravin

[CAS No.] 72963-64-5

[化合物分類] ベンゾピラノイド (7,8-Dioxygenated coumarin)

[構造式]

[分子式] C<sub>15</sub>H<sub>16</sub>O<sub>4</sub>

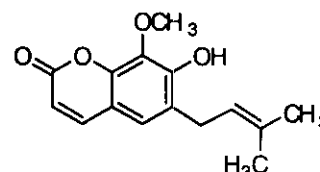
[分子量] 260.289

[正確な分子量] 260.10486

[基原] 次の植物から分離: *Apium graveolens*

[性状] 顆粒

[融点] Mp 167-169 °C



-----文献-----

Garg, S.K. et al., *Phytochemistry*, 1979, 18, 1580, (Apigravin)

§ 3-Hydroxy-4,5-methylenedioxybenzoic acid; Me ether

[化学名・別名] 3-Methoxy-4,5-methylenedioxybenzoic acid. 5-Methoxypiperonylic acid. Myristicin acid.

Myristicin acid

[CAS No.] 526-34-1

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

[構造式]

[分子式] C<sub>9</sub>H<sub>8</sub>O<sub>5</sub>

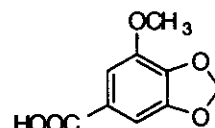
[分子量] 196.159

[正確な分子量] 196.037175

[基原] 次の植物から分離: *Apium graveolens* の種子, Chinese Gaoben

[性状] 針状結晶 (MeOH)

[融点] Mp 212 °C



-----文献-----

Garg, G.P. et al., *Indian J. Chem., Sect. B*, 1978, 16, 658; 1979, 18, 352, (分離)

Baba, K. et al., *CA*, 1984, 101, 97724, (分離)

Barrero, A.F. et al., *Phytochemistry*, 1994, 37, 1351, (分離, 誘導體)

§ 3-(3-Methylbutylidene)-1(3H)-isobenzofuranone (CAS 名)

[化学名・別名] 3-Isovalidenephthalide

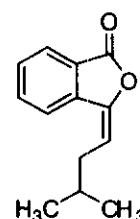
[関連 CAS No.] 56014-70-1, 56014-71-2

[化合物分類] ベンゾフラノイド (Isobenzofuran)

[構造式]

[分子式] C<sub>13</sub>H<sub>14</sub>O<sub>2</sub>

[分子量] 202.252



(E)-form

[正確な分子量] 202.09938

[基原] セロリ (*Apium graveolens*) のにおい副成分

[性状] 青白い黄色のオイル

[沸点] Bp<sub>7</sub> 170-172 °C

-----文献-----

Gold, H.J. et al., J.O.C., 1963, 28, 985, (分離, IR, UV)

Knight, D.W. et al., J.C.S. Perkin 1, 1975, 635, (合成法, IR, H-NMR)

### § Osthenol

[化学名・別名] 7-Hydroxy-8-(3-methyl-2-butenyl)-2H-1-benzopyran-2-one (CAS 名).

7-Hydroxy-8-prenylcoumarin

[CAS No.] 484-14-0

[化合物分類] ベンゾピラノイド (7-Oxygenated coumarins, 8-substituted)

[構造式]

[分子式] C<sub>14</sub>H<sub>14</sub>O<sub>3</sub>

[分子量] 230.263

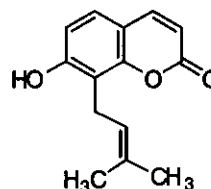
[正確な分子量] 230.094295

[基原] 次の植物から分離: *Seseli sibiricum*, *Haplophyllum ramosissimum*, *Apium graveolens* の種子

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

[融点] Mp 124-125 °C

[沸点] Bp<sub>0.1</sub> 160-169 °C



-----文献-----

Hollis, A.F. et al., Aust. J. Chem., 1961, 14, 101, (Osthol hydrochloride)

Kapoor, S.K. et al., Phytochemistry, 1968, 7, 147, (Osthol)

Danchul, T.Y. et al., Khim. Prir. Soedin., 1977, 13, 575; Chem. Nat. Compd. (Engl. Transl.), 1977, 13, 479, (Osthol)

Kumar, R. et al., Phytochemistry, 1978, 17, 2111, (Osthol)

Sasaki, H. et al., Chem. Pharm. Bull., 1980, 28, 1847, ( $\beta$ -Gentiobiosylsthenol)

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

Meyer, B.N. et al., J. Nat. Prod., 1985, 48, 952, (O-Geranylsthenol)

Fujioka, T. et al., Chem. Pharm. Bull., 1999, 47, 96, (Osthol, H-NMR, C13-NMR)

Cai, J.-N. et al., J. Nat. Prod., 2000, 63, 485, (Osthol hydrate)

### § Rutaretin; (R)-form, 1'-O-[4-Hydroxy-3,5-dimethoxycinnamoyl-( $\rightarrow$ 6)- $\beta$ -D-glucopyranoside]

[化合物分類] ベンゾピラノイド (Dihydrofuranocoumarin), ベンゾピラノイド (7,8-Dioxygenated coumarin)

[構造式]

[分子式] C<sub>31</sub>H<sub>34</sub>O<sub>14</sub>

[分子量] 630.601

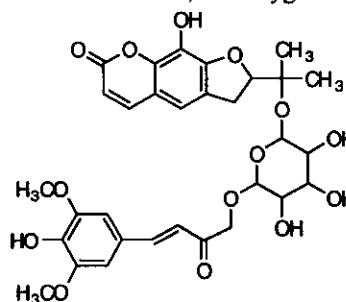
[正確な分子量] 630.19486

[基原] *Apium graveolens*, *Skimmia japonica*

[性状] 板状結晶 (EtOH)

[融点] Mp 166-168 °C

[比旋光度]:  $[\alpha]_D^{25} +75$  (c, 0.38 in MeOH)



-----文献-----

Schneider, G. et al., Arch. Pharm. (Weinheim, Ger.), 1967, 300, 73; 913, (分離, IR, UV, H-NMR, Mas)

Shagova, L.I. et al., Khim. Prir. Soedin., 1973, 9, 665; Chem. Nat. Compd., 1973, 9, 631, (分離)

Varga, E. et al., Acta Pharm. Hung., Suppl. No. 36, 1974, 44; CA, 82, 13996, (分離)

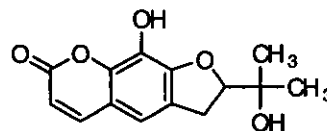
Ahluwalia, V.K. et al., Phytochemistry, 1988, 27, 1181, (配糖体)

### § Rutaretin; (S)-form

[化合物分類] ベンゾピラノイド (7,8-Dioxygenated coumarin), ベンゾピラノイド (Dihydrofuranocoumarin)

[構造式]

[基原] 次の植物から分離: *Herba rutae*, *Apium graveolens* と *Ruta graveolens* の種子





[性状] 青白い黄色の針状結晶  
[融点] Mp 198 °C  
[比旋光度]:  $[\alpha]_D^{25} -30.4$  (c, 0.79 in CHCl<sub>3</sub>)

-----文献-----

Schneider, G. et al., Arch. Pharm. (Weinheim, Ger.), 1967, 300, 73; 913, (分離. IR, UV, H-NMR, Mas)  
Shagova, L.I. et al., Khim. Prir. Soedin., 1973, 9, 665; Chem. Nat. Compd. (Engl. Transl.), 1973, 9, 631, (分離)

Varga, E. et al., Acta Pharm. Hung., Suppl. No. 36, 1974, 44 ; CA, 82, 13996, (分離)

Garg, S.K. et al., Phytochemistry, 1978, 17, 2135; 1979, 18, 1769, (分離. IR, UV, Apiumoside)

Srivastava, S.K. et al., Fitoterapia, 1994, 65, 301, (rutinoside)

### § Rutaretin; (-)-form, 1'-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranoside]

[化学名・別名] Apiumoside

[CAS No.] 73485-93-5

[化合物分類] ベンゾピラノイド (Dihydrofuranocoumarin), ベンゾピラノイド (7,8-Dioxygenated coumarin)

[構造式]

[分子式] C<sub>29</sub>H<sub>30</sub>O<sub>12</sub>

[分子量] 570.549

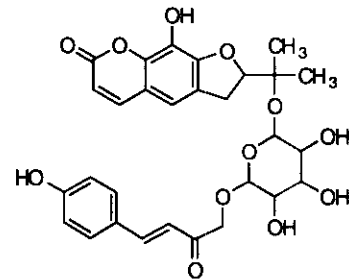
[正確な分子量] 570.17373

[基原] *Apium graveolens*

[性状] 結晶

[比旋光度]:  $[\alpha]_D^{25} -37.37$  (MeOH)

[その他のデータ] Mp > 300 °C



-----文献-----

Garg, S.K. et al., Phytochemistry, 1978, 17, 2135; 1979, 18, 1769, (分離. IR, UV, Apiumoside)

### § Sedanonic acid

[化学名・別名] 6-(1-Oxopentyl)-1-cyclohexene-1-carboxylic acid (CAS 名)

[CAS No.] 6697-07-0

[関連 CAS No.] 62006-38-6

[化合物分類] 脂肪族化合物 (Monocarbocyclic carboxylic acid and lactone)

[構造式]

[分子式] C<sub>12</sub>H<sub>18</sub>O<sub>3</sub>

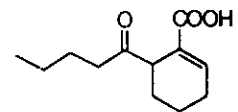
[分子量] 210.272

[正確な分子量] 210.125595

[基原] 次の植物から分離: 加水分解後のセロリオイル (*Apium graveolens*), *Cnidium officinale* の根

[性状] 結晶 (C<sub>6</sub>H<sub>6</sub>)

[融点] Mp 113 °C



-----文献-----

Ciamician, G. et al., Ber., 1897, 30, 492; 501; 1419, (分離, 構造決定)

Barton, D.H.R. et al., J.C.S., 1963, 1916, (分離)

### § 3',4',5,7-Tetrahydroxyflavone; 7-O-[D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]

[化学名・別名] Graveobioside A

[CAS No.] 63808-23-1

[化合物分類] フラボノイド (Flavone; 4 × O-置換基)

[構造式]

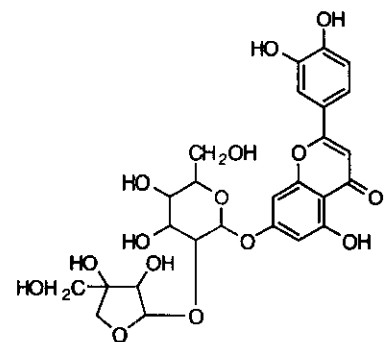
[分子式] C<sub>26</sub>H<sub>28</sub>O<sub>15</sub>

[分子量] 580.498

[正確な分子量] 580.142825

[基原] 次の植物から分離: *Apium graveolens*, *Petroselinum crispum*

[融点] Mp 251-252 °C



-----文献-----

Perkin, A.G., J.C.S., 1900, 77, 1315, (分離)  
 Diller, E., Ber., 1901, 34, 1452, (分離)  
 Karrer, W. et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhaumluser Verlag, Basel, 1972, nos. 1470; 1473, (生育)  
 Markham, K.R. et al., Phytochemistry, 1974, 13, 1553; 1975, 14, 1093; 1978, 17, 1601; 1984, 23, 2049; 1985, 24, 2607, (xylosides, rhamnosides, 3'-xyloside, 7-glucoside, galacturonides,  
 Schulz, M. et al., Phytochemistry, 1985, 24, 343, (glucuronoside)  
 Aritomi, M. et al., Phytochemistry, 1985, 24, 2438, (7-O-glucuronosylglucuronide)  
 Cody, V. et al., Plant Flavonoids in Biology and Medicine II, (eds., Cody, V. et al), A.R. Liss, N.Y., 1988, (生化学的性質)  
 The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988

§ 4',5,7-Trihydroxy-3'-methoxyflavone; 7-O-[ D-Apiofuranosyl-(1 → 2)-β-D-glucopyranoside]

[化学名・別名] Graveobioside B

[CAS No.] 33579-63-4

[化合物分類] フラボノイド (Flavone; 4 × O-置換基)

[構造式]

[分子式] C<sub>27</sub>H<sub>30</sub>O<sub>15</sub>

[分子量] 594.525

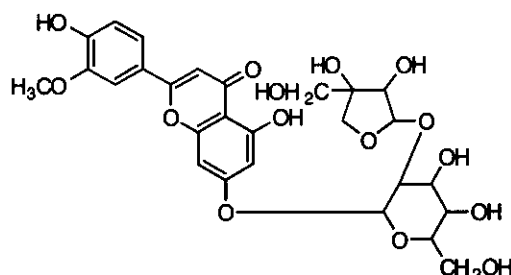
[正確な分子量] 594.158475

[基原] 次の植物から分離: *Apium graveolens*, *Dalbergia volubilis*, その他

[性状] 青白い黄色の針状結晶 (MeOH)

[融点] Mp 214-216 °C

[比旋光度]: [α]<sub>D</sub> -104.4 (Py)



-----文献-----

Schmid, R.D., Tetrahedron, 1972, 28, 3259, (Graveobioside B)

Biswas, K.M. et al., Indian J. Chem., Sect. B, 1977, 15, 396, (Graveobioside B)

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

\*\*\*\*\*センキュウ (Senkyu) \*\*\*\*\*

§ § セリ科センキュウ (*Cnidium officinale* Makino) の根。

§ 3-Butylidene-1(3H)-isobenzofuranone; (Z)-form, 5-Hydroxy

[化学名・別名] 5-Hydroxybutylideneephthalide. Senkyunolide C

[CAS No.] 91652-78-7

[化合物分類] ベンゾフラノイド (Isobenzofuran)

[構造式]

[分子式] C<sub>12</sub>H<sub>12</sub>O<sub>3</sub>

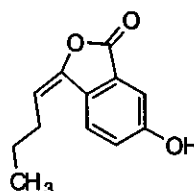
[分子量] 204.225

[正確な分子量] 204.078645

[基原] *Cnidium officinale*

[性状] 結晶

[融点] Mp 95-100 °C



-----文献-----

Mitsuhashi, H. et al., Chem. Pharm. Bull., 1960, 8, 243, (分離)

Banerjee, S.K. et al., Annalen, 1982, 699, (分離)

Opdyke, D.L.J. et al., Food Chem. Toxicol., 1983, 21, 659, (レビュー, 毒性)

Naito, T. et al., Phytochemistry, 1992, 31, 639, (Senkyunolide E)

Li, S. et al., Synth. Commun., 1997, 27, 1783, (Z-form, 合成法, H-NMR, IR)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, BRQ100

§ 3-Butylidene-1(3*H*)-isobenzofuranone; (Z)-form, 7-Hydroxy

[化学名・別名] 7-Hydroxybutylideneisobenzofuranone. Senkyunolide B

[CAS No.] 93236-67-0

[化合物分類] ベンゾフラノイド (Isobenzofuran)

[構造式]

[分子式] C<sub>12</sub>H<sub>12</sub>O<sub>3</sub>

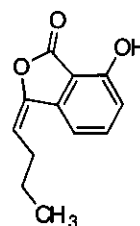
[分子量] 204.225

[正確な分子量] 204.078645

[基原] *Cnidium officinale* の乾燥根茎, the crude drug senkyu

[性状] 結晶

[融点] Mp 150-153 °C



-----文献-----

Mitsuhashi, H. et al., Chem. Pharm. Bull., 1960, 8, 243, (分離)

Banerjee, S.K. et al., Annalen, 1982, 699, (分離)

Opdyke, D.L.J. et al., Food Chem. Toxicol., 1983, 21, 659, (レビュー, 毒性)

Naito, T. et al., Phytochemistry, 1992, 31, 639, (Senkyunolide E)

Ogawa, Y. et al., Synth. Commun., 1992, 22, 315, (合成法)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, BRQ100

§ 3-Butylidene-1(3*H*)-isobenzofuranone; (Z)-form, 9-Hydroxy

[化学名・別名] Senkyunolide E

[CAS No.] 94530-83-3

[化合物分類] ベンゾフラノイド (Isobenzofuran)

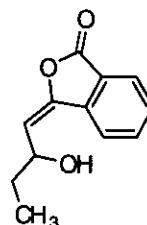
[構造式]

[分子式] C<sub>12</sub>H<sub>12</sub>O<sub>3</sub>

[分子量] 204.225

[正確な分子量] 204.078645

[基原] *Cnidium officinale*



-----文献-----

Naito, T. et al., Phytochemistry, 1992, 31, 639, (Senkyunolide E)

§ Cnidilide

[化学名・別名] 3-Butyl-3a,4,5,7a-tetrahydro-1(3*H*)-isobenzofuranone (CAS 名)

[CAS No.] 3674-03-1

[化合物分類] ベンゾフラノイド (Isobenzofuran)

[構造式]

[分子式] C<sub>12</sub>H<sub>16</sub>O<sub>2</sub>

[分子量] 194.273

[正確な分子量] 194.13068

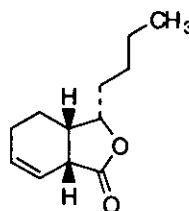
[基原] *Cnidium officinale* の根

[沸点] Bp<sub>2.5</sub> 145-146 °C

[比旋光度]: [α]<sub>D</sub><sup>25</sup> -122.5 (c, 3.5 in CHCl<sub>3</sub>)

[溶解性] BERDY SOL: Sol. メタノール, ベンゼンに可溶; ヘキサンに易溶; 水に難溶

[UV]: [neutral] λ<sub>max</sub> 227 (E1%/1cm 1000); 274 (E1%/1cm 200); 282 (E1%/1cm 186) (MeOH)



-----文献-----

Mitsuhashi, H. et al., Tetrahedron, 1964, 20, 1971; 1965, 21, 1433, (分離, 構造決定)

Cocker, W. et al., J.C.S. (C), 1966, 1152, (合成法)

§ 3-(3,4-Dihydroxyphenyl)-2-propen-1-ol; (E)-form, 3'-Me ether, 1-O-(4-hydroxy-3-methoxycinnamoyl) (E-)

[化学名・別名] Coniferyl ferulate

[化合物分類] 単環芳香族 (Simple phenylpropanoid)

[構造式]

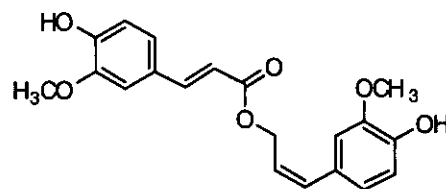
[分子式]  $C_{20}H_{20}O_6$

[分子量] 356.374

[正確な分子量] 356.12599

[基原] *Coreopsis longula*, *Cnidium officinale*, *Ligusticum wallichii*

[性状] オイル



-----文献-----

Metwally, M.A. et al., *Phytochemistry*, 1985, 24, 182, (Coniferyl ferulate)

Ishimaru, K. et al., *Phytochemistry*, 1987, 26, 1147, (*cis*-Coniferyl alcohol galloylglucoside)

Niwa, M. et al., *Chem. Pharm. Bull.*, 1988, 36, 1158, (Coniferinoside)

Jen, C.-M. et al., *J. Nat. Prod.*, 1993, 56, 2019, (Conifegrol)

Francesch, C. et al., *Synthesis*, 1994, 369, (合成法, Coniferyl alcohol)

Greca, M.D. et al., *Phytochemistry*, 1998, 49, 1299, (Coniferyl alcohol, Citrusin D)

### § Ligustilide

[化学名・別名] 3-Butylidene-4,5-dihydro-1(3*H*)-isobenzofuranone (CAS名).

3-Butylidene-4,5-dihydrophthalide (旧CAS名)

[CAS No.] 4431-01-0

[化合物分類] ベンゾフラノイド (Isobenzofuran)

[構造式]

[分子式]  $C_{12}H_{14}O_2$

[分子量] 190.241

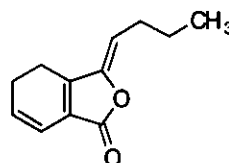
[正確な分子量] 190.09938

[基原] *Ligusticum* and *Angelica* spp., その他のセリ科 (highest content found in *Cnidium officinale*)

[性状] オイル

[沸点]  $Bp_6$  168-169 °C

[UV]: [neutral]  $\lambda_{max}$  320 ( $\epsilon$  2400) (MeOH)



-----文献-----

Stahl, E. et al., *Naturwissenschaften*, 1967, 54, 118, (分離)

Mitsubishi, H., *CA*, 1969, 71, 88456, (分離)

Nikonov, G.K. et al., *Khim. Prir. Soedin.*, 1971, 7, 387; *Chem. Nat. Compd. (Engl. Transl.)*, 373, (分離)

Yamagishi, T. et al., *CA*, 1975, 83, 84751; 1976, 84, 132662, (分離)

Yamagishi, T. et al., *Yakugaku Zasshi*, 1977, 97, 237, (分離)

Pushan, W. et al., *Phytochemistry*, 1984, 23, 2033, (誘導體)

Kobayashi, M. et al., *Chem. Pharm. Bull.*, 1985, 32, 3770; 1987, 35, 4789, (分離, Senkyunolide L)

Naito, T. et al., *Phytochemistry*, 1992, 31, 639, (分離, 絶対構造)

Li, S. et al., *Synth. Commun.*, 1993, 23, 2061; 2909, (合成法, 誘導體)

Grech, J.N. et al., *J. Nat. Prod.*, 1994, 57, 1682, (E-Dihydroxyligustilide)

### § Ligustilide; 9-Hydroxy

[化学名・別名] Senkyunolide F

[CAS No.] 94530-84-4

[化合物分類] ベンゾフラノイド (Isobenzofuran)

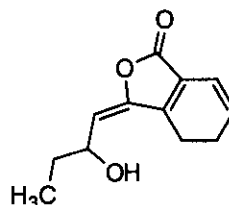
[構造式]

[分子式]  $C_{12}H_{14}O_3$

[分子量] 206.241

[正確な分子量] 206.094295

[基原] *Cnidium officinale*



-----文献-----

Stahl, E. et al., *Naturwissenschaften*, 1967, 54, 118, (分離)

Mitsubishi, H., *CA*, 1969, 71, 88456, (分離)

Nikonov, G.K. et al., *Khim. Prir. Soedin.*, 1971, 7, 387; *Chem. Nat. Compd. (Engl. Transl.)*, 373, (分離)

Yamagishi, T. et al., *CA*, 1975, 83, 84751; 1976, 84, 132662, (分離)

Yamagishi, T. et al., *Yakugaku Zasshi*, 1977, 97, 237, (分離)