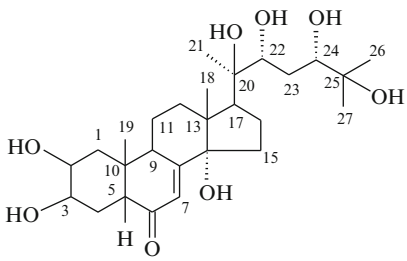
Physicochemical and Biological Properties of Phytoecdysteroids

S.S. Azimova, (ed.), *Natural Compounds – Phytoecdysteroids*,
DOI 10.1007/978-1-4614-0543-6,

Phytoecdysteroids and Their Conjugates

Abutasterone

CAS Registry Number: 88669-02-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Abuta velutina* [1], *Briza maxima* [2], *Lamium album* [3], *Polypodium vulgare* [4], *Vitex strickeri* [5]

$C_{27}H_{44}O_8$: 496.3036

Mp: 257–259°C [1], 270–272°C [5]

$[\alpha]_D^{20}$ + 32° (c 2.0; MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3380, 1660, 1640 [5]

UV λ_{max}^{EtOH} nm (log ε): 242 (4.14) [5]

EI-MS m/z: 460 $[M\text{-}2H_2O]^+$ (1), 442 (1), 424 (2), 363 (3), 345 (10), 327 (6), 319 (1), 301 (4), 283 (4), 177 (4), 159 (15), 141 (15), 133 (8), 123 (12), 115 (34), 103 (3), 97 (28), 89 (4), 85 (17), 71 (100), 67 (13), 59 (80), 53 (10), 41 (15) [1]

^{1}H NMR (J/Hz, C_5D_5N): 1.83–1.58 (Ha-1), 2.07–2.19 (He-1), 4.24 (Ha-2), 4.22 (He-3), 1.70–1.81 (Ha-4), 1.98–2.05 (He-4), 2.97–3.03 (H-5), 6.23 (d, J = 3.0, H-7), 3.58 (m, Ha-9), 1.70–1.81 (Ha-11), 1.83–1.95 (He-11), 2.56 (ddd, J = 13.0, 13.0, 5.0, Ha-12), 1.83–1.95 (He-12), 1.83–1.95 (Ha-15), 2.07–2.19 (Hb-15), 2.41–2.50 (Ha-16), 1.98–2.05 (Hb-16), 2.97–3.03 (H-17), 1.20 (s, CH_3-18), 1.08 (s, CH_3-19), 1.58 (s, CH_3-21), 4.07 (dd, J = 9.0, 1.0, Hb-22), 2.07–2.19 (Ha-23), 2.41–2.50 (Hb-23), 4.19 (dd, J = 12.0, 2.0, Ha-24), 1.45 (s, CH_3-26), 1.50 (s, CH_3-27) [5]

^{13}C NMR (C_5D_5N) [5]:

Table 1

C-1	38.04	C-10	38.66	C-19	24.49
2	68.08	11	21.13	20	76.78
3	68.17	12	31.75	21	21.53
4	32.48	13	48.10	22	78.26
5	51.42	14	84.15	23	32.99
6	203.42	15	31.99	24	80.31
7	121.66	16	21.79	25	72.25
8	166.07	17	50.06	26	26.85
9	34.48	18	17.90	27	25.34

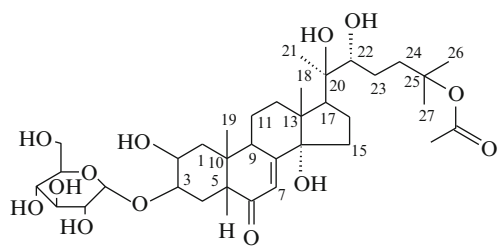
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.4 \times 10^{-7}$M [6].

References

1. M.L.B. Pinheiro, W.W. Filho, A.I.D. Rocha, B. Porter, E. Wenkert, Phytochemistry **22**, 2320 (1983)
2. T. Savchenko, P. Whiting, V. Sik, E. Underwood, S.D. Sarker, L. Dinan, Biochem. Syst. Ecol. **26**, 781 (1998)
3. T. Savchenko, M. Blackford, S.D. Sarker, L. Dinan, Biochem. Syst. Ecol. **29**, 891 (2001)
4. J. Coll, N. Reixach, F. Sanches-Baeza, J. Casas, F. Camps, Tetrahedron **50**, 7247 (1994)
5. M. Zhang, M.J. Stout, I. Kubo, Phytochemistry **31**, 247 (1992)
6. C.Y. Clement, D.A. Bradbrook, R. Lafont, L. Dinan, Insect Biochem. Mol. Biol. **23**, 187 (1993)

25-Acetoxy-20-Hydroxyecdysone-3-Glucoside

CAS Registry Number: 960198-73-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Sida rhombifolia* [1]
$C_{35}H_{56}O_{13}$: 684.3721
Mp: amorphous [1]
$[\alpha]_D^{20}$ + 18.1° (c 2.87; MeOH) [1]
IR (NaCl) ν_{max} cm^{-1}: 3386, 1649, 1373, 1272, 1075 [1]
UV λ_{max}^{MeOH} nm (ε): 244 (1579) [1]
HR-ESI-MS m/z: for $C_{35}H_{56}NaO_{13}$ $[M + Na]^+$ calcd. 707.3619, found 707.3683 [1]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.78 (br s, Ha-1), 2.00–2.06 (He-1), 4.08–4.11 (Ha-2), 4.31 (br s, He-3), 1.67–1.75 (Ha-4), 2.21–2.25 (He-4), 2.91–2.96 (H-5), 6.21 (s, H-7), 3.54 (br s, Ha-9), 1.75–2.04 (Ha-11), 1.83–1.90 (He-11), 2.00–2.04 (Ha-12), 2.54–2.59 (He-12), 2.00–2.06 (Ha-15), 2.54–2.59 (Hb-15), 2.00–2.04 (Ha-16), 2.39–2.45 (Hb-16), 2.96–2.99 (H-17), 1.20 (s, CH_3-18), 0.90 (s, CH_3-19), 1.61 (s, CH_3-21), 3.84 (br d, J = 10.4, Hb-22), 1.67–1.71 (Ha-23), 1.87–1.90 (Hb-23), 2.21–2.25 (Ha-24), 2.39–2.45 (Hb-24), 1.44 (s, CH_3-26), 1.50 (s, CH_3-27), Other: 1.96 (s, $COOCH_3$), β-D-Glcp′: 4.93 (d, J = 7.6, H-1), 4.03 (t, J = 7.2, H-2), 3.93 (br s, H-3), 4.21 (m, H-4), 4.20 (m, H-5), 4.32 (m, Ha-6), 4.52 (d, J = 11.6, Hb-6) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	39.4	C-13	48.4	C-25	82.8
2	67.9	14	84.5	26	26.6
3	78.0	15	32.1	27	26.7
4	31.0	16	21.9	Glc′-1	104.5
5	51.8	17	50.6	2	75.1
6	203.5	18	18.3	3	79.0
7	122.0	19	24.5	4	72.0
8	166.8	20	77.2	5	78.9
9	34.7	21	22.0	6	63.0
10	39.1	22	77.9	$\underline{COO}CH_3$	170.7
11	21.5	23	27.3	$COO\underline{CH_3}$	22.7
12	32.4	24	39.7		

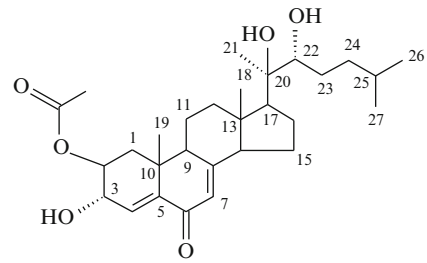
Pharm./Biol.: Antimicrobial tests: inactive > 20 μg/ml; antimalarial test: inactive >4.76 μg/ml; antiprotozoal test: in active >40 μg/ml [1].

References

1. A.N. Jadhav, R.S. Pawar, B. Avula, I.A. Khan, Chem. Biodivers. **4**, 2225 (2007)

Acetylpinnasterol

CAS Registry Number: 80981-66-4



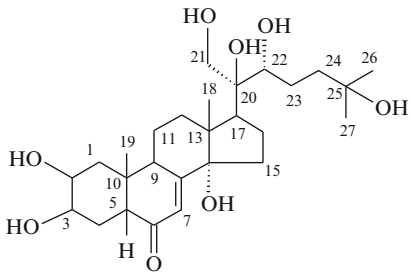
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Laurencia pinnata* [1, 2]
$C_{29}H_{44}O_6$: 488.3137
Mp: 105–107°C [1]
$[\alpha]_D$ + 64° (MeOH) [1]
EI-MS m/z: 488 $[M]^+$ [1]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 5.34 (ddd, J = 10.5, 7.0, 3.5, Ha-2), 4.71 (dd, J = 7.0, 2.0, Ha-3), 6.82 (d, J = 2.0, H-4), 6.03 (t, J = 2.0, H-7), 2.54 (ddd, J = 12.0, 7.0, 2.0, Ha-9), 2.21 (dt, J = 12.0, 2.0, H-14), 1.14 (s, CH_3-18), 1.05 (s, CH_3-19), 1.51 (s, CH_3-21), 3.74 (d, J = 9.0, Ha-22), 0.97 (d, J = 7.0, CH_3-26), 0.98 (d, J = 7.0, CH_3-27), Other: 2.05 (s, $COOCH_3$), 5.00 (s, OH) [1]
Pharm./Biol.: *Sarcophaga* test: ED_{50} = 0.54 μg [2].

References

1. A. Fukuzawa, Y. Kumagai, T. Masamune, A. Furusaki, C. Katayama, T. Masamune, Tetrah. Lett. **22**, 4085 (1981)
2. A. Fukuzawa, M. Miyamoto, Y. Kumagai, T. Masamune, Phytochemistry **25**, 1305 (1986)

Achyranthesterone A

CAS Registry Number: 864753-99-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Achyranthes bidentata* [1], *Froelichia floridana* [2]

$C_{27}H_{44}O_8$: 496.3036

Mp: 300°C [1]

$[\alpha]_D^{30}$ + 13.0° (0.001; MeOH) [1]

UV λ_{max}^{MeOH} nm: 240.8 [1]

ESI-MS m/z: 497.1 $[M + H]^+$, 479.0 $[M + H–H_2O]^+$, 461.0 $[M + H–2H_2O]^+$, 443.1 $[M + H–3H_2O]^+$, 425.1 $[M + H–4H_2O]^+$ [1]

^{1}H NMR (J/Hz, C_5D_5N): 1.90 (m, Ha-1), 2.10 (m, He-1), 4.18 (m, Ha-2), 4.22 (m, He-3), 1.88 (m, Ha-4), 1.98 (m, He-4), 3.00 (dd, J = 3.0, 12.0, H-5), 6.25 (d, J = 3.0, H-7), 3.60 (m, Ha-9), 1.68 (m, Ha-11), 1.80 (m, He-11), 2.16 (m, Ha-12), 1.96 (m, He-12), 2.56 (m, Ha-15), 1.96 (m, He-15), 2.51 (m, Ha-16), 2.08 (m, Hb-16), 3.11 (m, H-17), 1.20 (s, CH_3-18), 1.02 (s, CH_3-19), 4.42 and 4.39 (d, J = 19.2, CH_2OH-21), 4.08 (m, H-22), 2.34 (m, Ha-23), 2.18 (m, Hb-23), 2.32 (m, Ha-24), 1.84 (m, Hb-24), 1.35 (s, CH_3-26), 1.35 (s, CH_3-27) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

C-1	38.0	C-10	38.7	C-19	24.5
2	68.2	11	21.1	20	78.6
3	68.1	12	31.6	21	66.8
4	32.4	13	47.8	22	78.8
5	51.4	14	84.3	23	27.9
6	203.5	15	31.4	24	42.8
7	121.8	16	21.6	25	69.8
8	165.9	17	47.9	26	30.0
9	34.5	18	17.9	27	30.1

Pharm./Biol.: Human DNA Topoisomerase I test: not active [2].

References

1. D.L. Meng, X. Li, J.H. Wang, W. Li, J. Asian Nat. Prod. Res. **7**, 181 (2005)
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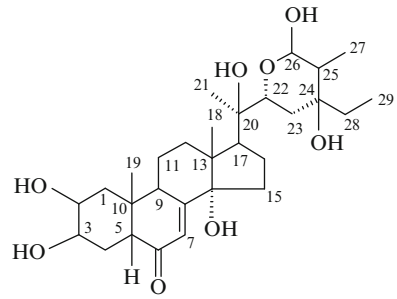
Ajugacetalsterone A

CAS Registry Number: 948300-17-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga nipponensis* [1]

$C_{29}H_{46}O_8$: 522.3192

Mp: amorphous [1]

IR (KBr) ν_{max} cm^{-1}: 3414, 2946, 2964, 2879, 1651, 1547, 1462, 1059, 872 [1]

ES-MS m/z: 545.3 $[M + 23]^+$, 505.3 $[M + H–H_2O]^+$, 487.2 $[M + H–2H_2O]^+$, 451.2 $[M + H–3H_2O]^+$, 557.3 $[M + 35]^+$ [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.96 (Ha-1), 1.72 (He-1), 4.00 (m, Ha-2), 4.08 (m, He-3), 1.89 (Ha-4), 1.64 (He-4), 2.78 (dd, J = 3.7, 13.0, H-5), 6.06 (d, J = 2.4, H-7), 3.38 (H-9), 1.77 (Ha-11), 1.66 (He-11), 2.42 (Ha-12), 1.87 (He-12), 2.05 (dd, J = 7.3, 13.0, Ha-15), 1.78 (Hb-15), 2.26 (q, J = 10.2, Ha-16), 1.95 (Hb-16), 2.81 (t, J = 9.3, H-17), 1.07 (s, CH_3-18), 1.04 (s, CH_3-19), 1.48 (s, CH_3-21), 3.54 (dd, J = 1.0, 12.2, H-22), 2.31 (d, J = 12.9, Ha-23), 1.55 (dd, J = 12.2, 12.9, Hb-23), 2.01 (H-25), 4.88 (d, J = 8.8, H-26), 1.33 (d, J = 7.1, CH_3-27), 1.73 (Ha-28), 1.61 (Hb-28), 1.06 (t, J = 7.8, CH_3-29) [1]:

^{13}C NMR (100.62 MHz, C_5D_5N) [1]:

Table 1

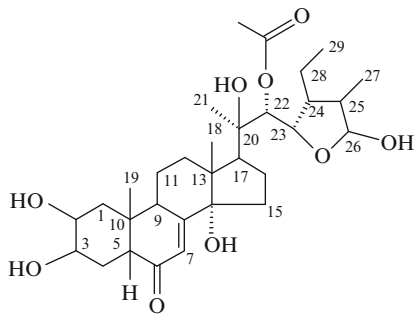
C-1	37.68	C-11	20.93	C-21	22.12
2	67.93	12	31.77	22	76.75
3	67.78	13	47.74	23	36.85
4	32.28	14	83.96	24	72.64
5	51.07	15	31.44	25	50.64
6	203.69	16	21.48	26	98.89
7	121.39	17	49.86	27	9.54
8	166.17	18	17.80	28	23.78
9	34.26	19	24.41	29	7.49
10	38.51	20	75.86		

References

1. J. Coll, Y.A. Tandron, X. Zeng, Steroids **72**, 270 (2007)

Ajugacetalsterone B

CAS Registry Number: 948300-18-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga nipponensis* [1]

$C_{31}H_{48}O_9$: 564.3298

Mp: amorphous [1]

IR (KBr) ν_{max} cm^{-1}: 3457, 2922, 2879, 1729, 1650, 1462, 1383, 1022, 872 [1]

ES-MS m/z: 599.3 $[M + 35]^+$, 563.3 $[M-H]^-$ [1]

^{1}H NMR (400 MHz, J/Hz, $CDCl_3$): 1.89 (Ha-1), 1.39 (He-1), 3.89 (m, Ha-2), 4.04 (m, He-3), 1.84 (Ha-4), 1.62 (He-4), 2.43 (H-5), 5.86 (H-7), 2.99 (br t, J = 7.8, H-9), 1.77 (Ha-11), 1.65 (He-11), 2.07 (Ha-12), 1.89 (He-12), 2.04 (Ha-15), 1.57 (Hb-15), 2.03 (Ha-16), 1.96 (Hb-16), 2.88 (H-17), 0.85 (CH_3-18), 0.98 (CH_3-19), 1.31 (CH_3-21), 4.90 (d, J = 8.5, H-22), 3.81 (dd, J = 6.7, 8.6, H-23), 2.10 (H-24), 2.24 (H-25), 5.10 (d, J = 1.5, H-26), 0.91 (d, J = 7.8, CH_3-27), 1.42 (Ha-28), 1.39 (Hb-28), 0.90 (t, J = 7.3, CH_3-29), 2.11 ($COOCH_3$-22) [1]:

^{13}C NMR (100.62 MHz, C_5D_5N) [1]:

Table 1

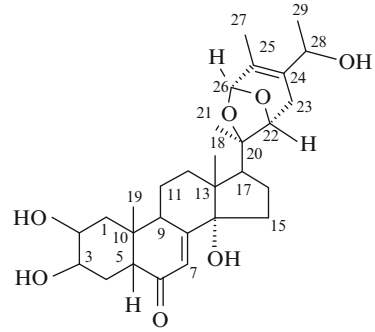
C-1	36.76	C-11	20.41	C-21	22.36
2	67.74	12	31.03	22	80.33
3	67.36	13	47.50	23	81.20
4	31.44	14	85.16	24	46.63
5	50.00	15	31.51	25	41.48
6	201.50	16	20.73	26	104.50
7	121.82	17	48.81	27	11.32
8	165.80	18	17.67	28	20.79
9	33.76	19	23.88	29	12.71
10	38.19	20	76.60	$COOCH_3$	21.05
				$COOCH_3$	171.18

References

1. J. Coll, Y.A. Tandron, X. Zeng, Steroids **72**, 270 (2007)

Ajugacetalsterone C

CAS Registry Number: 1033773-05-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga macrosperma* var. *breviflora* [1]

$C_{29}H_{42}O_7$: 502.2930

Mp: amorphous solid [1]

$[\alpha]_D^{22}$ + 253.9° (c 0.04; MeOH) [1]

HR-ESI-MS m/z: for $C_{29}H_{43}O_7$ $[M + H]^+$ calcd. 503.3009, found 503.3004 [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.91 (t, J = 12.6, Ha-1), 2.10 (He-1), 4.17 (d, J = 10.3, Ha-2), 4.25 (He-3), 1.83 (Ha-4), 2.05 (dt, J = 3.7, 13.7, He-4), 3.01 (dd, J = 3.1, 12.9, H-5), 6.25 (d, J = 1.8, H-7), 3.57 (Ha-9), 1.63 (Ha-11), 1.77 (He-11), 2.50 (td, J = 4.3, 13.0, Ha-12), 1.90 (He-12), 1.81 (Ha-15), 1.86 (Hb-15), 2.13 (Ha-16), 2.22 (m, Hb-16), 2.87 (t, J = 8.8, H-17), 1.02 (s, CH_3-18), 1.03 (s, CH_3-19), 1.66 (s, CH_3-21), 4.56 (d, J = 4.5, Hb-22), 2.67 (d, J = 17.6, Ha-23), 2.75 (d, J = 17.6, Hb-23), 5.46 (s, CH_3-26), 1.72 (s, CH_3-27), 4.95 (Ha-28), 1.36 (d, J = 6.6, CH_3-29), 6.35 (br, OH) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

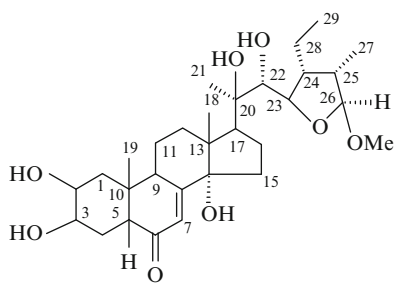
C-1	37.5	C-11	22.0	C-21	23.2
2	67.9	12	31.3	22	80.0
3	67.8	13	47.4	23	26.0
4	32.2	14	83.7	24	132.4
5	51.1	15	31.1	25	129.8
6	203.6	16	22.0	26	101.2
7	121.4	17	54.6	27	14.7
8	165.9	18	16.4	28	64.1
9	34.1	19	24.1	29	21.0
10	38.4	20	85.3		

References

1. A. Castro, J. Coll, Y.A. Tandron, A.K. Pant, C.S. Mathela, J. Nat. Prod. **71**, 1294 (2008)

Ajugacetalsterone D

CAS Registry Number: 1033773-10-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga macrosperma* var. *breviflora* [1]

$C_{30}H_{48}O_8$: 536.3349

Mp: amorphous solid [1]

$[\alpha]_D^{22}$ + 71.6° (c 0.1; MeOH) [1]

HR-ESI-MS m/z: for $C_{30}H_{49}O_8$ $[M + H]^+$ calcd. 537.3427, found 537.3428 [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.82 (dd, J = 12.2, 12.4, Ha-1), 2.03 (He-1), 4.08 (dt, J = 3.8, 11.3, Ha-2), 4.15 (He-3), 1.75 (Ha-4), 2.01 (dt, J = 3.7, 13.7, He-4), 2.93 (dd, J = 3.7, 13.1, H-5), 6.16 (d, J = 2.2, H-7), 3.50 (Ha-9), 1.64 (Ha-11), 2.56 (td, J = 5.1, 13.9, Ha-12), 1.97 (He-12), 1.77 (Ha-15), 2.05 (Hb-15), 2.23 (Ha-16), 2.38 (td, J = 8.8, 10.5, Hb-16), 3.48 (dd, J = 8.8, 9.3, H-17), 1.13 (s, CH_3-18), 0.97 (s, CH_3-19), 1.59 (s, CH_3-21), 3.77 (d, J = 8.0, Hb-22), 3.96 (t, J = 8.0, Ha-23), 2.50 (m, H-24), 2.24 (dq, J = 6.8, H-25), 4.57 (s, CH_3-26), 0.76 (d, J = 7.1, CH_3-27), 1.33 (Ha-28), 2.07 (Hb-28), 0.78 (t, J = 7.3, CH_3-29), 3.40 (s, OCH_3) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-11	21.1	C-21	22.8
2	68.0	12	31.8	22	79.4
3	68.0	13	47.7	23	83.4
4	32.5	14	84.2	24	47.7
5	51.4	15	31.8	25	41.0
6		16	21.7	26	111.6
7	121.4	17	50.1	27	11.6
8		18	18.2	28	21.3
9	34.4	19	24.4	29	13.0
10	38.6	20	76.4	OCH_3	55.4

References

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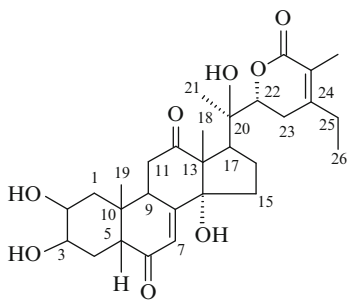
Ajugalactone

CAS Registry Number: 42975-12-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga decumbens* [1], *A. reptans* [2, 3], *A. reptans* var. *atropurpurea* [4], *A. turkestanica* [5], *Eriophyton wallchii* [6]

$C_{29}H_{40}O_8$: 516.2723

Mp: 225–235°C (dec.) [1], 255–260°C (dec, MeOH) [2]

$[\alpha]_D$ + 86.5° (c 5.71, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3440, 1718, 1696, 1654 [1]

UV λ_{max}^{EtOH} nm (ε): 233 (15700) [1]

EI-MS m/z: 516 $[M]^+$ (5), 377 [M-C_{22}-C_{29}] (75), 359 (100), 341 (15), 183 [C_{20}-C_{29}] (71), 139 [C_{22}-C_{29}] (60), 111 (24) [1], 516 $[M]^+$ [2]

HR-MS m/z: for $C_{28}H_{47}O_7$ $[M]^+$ calcd. 516.2719, found 516.2751 [1]

CD (c, dioxane): Δε = +11.56 (244 nm), Δε = −2.84 (204 nm), Δε = +0.86 (340 nm) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 1.96 (Ha-1), 1.96 (He-1), 4.00 (Ha-2), 4.20 (He-3), 2.02, 1.62 (Ha-4), 2.02, 1.62 (He-4), 3.09 (H-5), 6.40 (H-7), 4.00 (H-9), 2.86 (Ha-11), 2.86 (He-11), 2.46, 2.04 (Ha-15), 2.46, 2.04 (Hb-15), 2.62, 2.08 (Ha-16), 2.62, 2.08 (Hb-16), 3.50 (H-17), 1.54 (CH_3-18), 1.16 (CH_3-19), 1.70 (CH_3-21), 4.46 (H-22), 2.42, 2.23 (Ha-23), 2.42, 2.23 (Hb-23), 1.87 (CH_3-27), 0.68 (CH_3-28), 1.87 (H-28) [3, 4]

^{13}C NMR (75 MHz, C_5D_5N) [3, 4]:

Table 1

C-1	37.8	C-11	36.8	C-21	22.1
2	67.9	12	210.2	22	83.1
3	67.6	13	61.5	23	30.1
4	32.1	14	89.1	24	154.2
5	50.8	15	31.9	25	121.2
6	202.7	16	21.0	26	162.2
7	123.3	17	43.8	27	12.2
8	166.8	18	17.4	28	27.0
9	36.8	19	23.7	29	11.5
10	39.8	20	74.9		

Pharm./Biol.: *Chilo suppressalis* biotest: moulting hormone inhibitor [1], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.6 \times 10^{-7}$M [7, 8].

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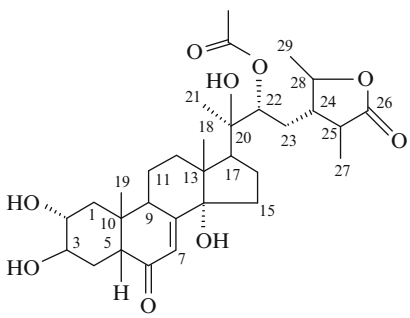
Ajugalide E

CAS Registry Number: 866016-98-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Ajuga taiwanensis* [1]
$C_{31}H_{46}O_9$: 562.3142
Mp: 210–212°C [1]
$[\alpha]_D^{25}$ + 133.6° (c 0.007, $CHCl_3$) [1]
IR (KBr) ν_{max} cm^{-1}: 3375, 1730, 1654, 1248, 1197, 1063, 1038 [1]
UV λ_{max}^{MeOH} nm (log ε): 240 (4.10) [1]
FAB-MS m/z: 563 $[M + H]^+$ (1), 562 (1), 544 (1), 526 (1), 516 (1), 508 (3), 498 (2), 484 (1), 466 (1), 456 (1), 451 (1), 448 (2), 433 (2), 377 (2), 371 (13), 363 (3), 360 (2), 353 (3), 345 (2), 327 (3), 301 (4), 300 (3), 299 (3), 250 (3), 249 (5), 183 (8), 149 (100), 139 (20) [1]
HR-FAB-MS m/z: for $C_{31}H_{47}O_9$ $[M + H]^+$ calcd. 563.3220, found 563.3221 [1]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 2.20–2.00 (m, Ha-1), 2.00–1.60 (m, He-1), 3.81 (ddd, J = 4.0, 7.6, 7.6, Ha-2), 4.18 (ddd, J = 4.0, 7.6, 7.6, He-3), 2.43–2.38 (m, Ha-4), 1.45–1.38 (m, He-4), 2.43–2.38 (m, H-5), 6.21 (br s, H-7), 3.67 (t, J = 9.0, H-9), 2.00–1.60 (m, H-11), 2.59–2.53 (m, Ha-12), 2.00–1.60 (m, He-12), 2.20–2.00 (m, Ha-15), 2.00–1.60 (m, Hb-15), 2.59–2.53 (m, Ha-16), 2.20–2.00 (m, Hb-16), 2.79 (t, J = 8.8, H-17), 1.14 (s, CH_3-18), 1.01 (s, CH_3-19), 1.53 (s, CH_3-21), 5.43 (d, J = 10.0, H-22), 2.00–1.60 (m, H-23), 2.00–1.60 (m, H-24), 2.25 (qd, J = 6.8, 6.8, H-25), 1.41 (d, J = 6.8, CH_3-27), 3.95 (qd, J = 6.8, 6.8, H-28), 1.29 (d, J = 6.8, CH_3-29), Other: 2.01 (s, $COOCH_3$-22), 5.53 (s, OH-2), 6.53 (s, OH-3) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	33.7	C-11	21.0	C-21	21.7
2	75.2	12	31.9	22	76.9
3	71.8	13	48.1	23	33.1
4	43.1	14	84.0	24	48.2
5	57.1	15	31.8	25	42.7
6	201.6	16	21.5	26	178.6
7	121.7	17	50.2	27	15.6
8	165.6	18	17.8	28	79.2
9	35.2	19	23.9	29	19.0
10	39.0	20	76.2	$COOCH_3$	21.2,
				$COOCH_3$	170.9

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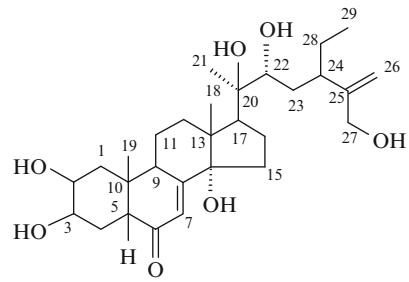
Ajugasterone B

CAS Registry Number: 21490-21-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Ajuga incisa* [1], *Ajuga iva* [2], *A. reptans* [3], *A. turkestanica* [4]
$C_{29}H_{46}O_7$: 506.3243
Mp: 240°C [1]
$[\alpha]_D$ + 54.7° (c, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3400, 1650 [1]
UV λ_{max}^{MeOH} nm (ε): 244 (10675) [1]
EI-MS m/z: 506 $[M]^+$, 363, 345, 327, 143 $[M\text{-}C_{22}\text{-}C_{27}]^+$, 125, 107 [1]
^{1}H NMR (J/Hz, C_5D_5N): 4.05 (Ha-2), 4.14 (He-3), 6.18 (H-7), 1.16 (CH_3-18), 1.05 (CH_3-19), 1.54 (CH_3-21), 3.85 (dd, H-22), 0.86 (t, J = 7.0, CH_3-29), 4.36 (CH_2–OH), 5.03, 5.33 (CH_2=) [1]
Pharm./Biol.: *Chilo* test: highly active [1].

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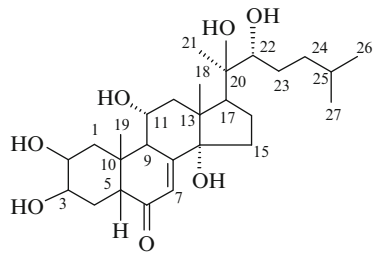
Ajugasterone C

CAS Registry Number: 23044-80-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga decumbens, A. japonica* [1], *A. nipponensis* [2], *A. remota* [3], *Centaurea moschata* [4], *Cyanotus longifolia* [5], *Dacrudium pierrei* [6], *Dioscorea dumetorum* [7], *Leuzea carthamoides* [8–10], *Rhaponticum uniflorum* [11], *Schizea dichotoma* [12], *Serratula coronata* [13], *S. strangulate* [14], *Vitex fisherii* [15], *V. madiensis* [16], *V. polygama* [17], *V. scabra* [18], *V. strickeri* [19]

$C_{27}H_{44}O_7$: 480.3087

Mp: 216–216.5°C [11], amorphous [9, 19]

$[\alpha]_D^{18}$ + 48.5° (c 1.1, MeOH) [13]

IR (KBr) ν_{max} cm^{-1}: 3400, 1655 [1]

UV λ_{max}^{MeOH} nm (ε): 243 (10320) [1]

EI-MS m/z: 462 $[M\text{-}H_2O]^+$, 379 (5), 361 (16), 343 (64), 335 (1), 325 (39), 317 (2), 299 (6), 281 (4), 145 (23), 127 (6), 109 (21), 101 (2), 83 (25), 43 (100) [1]

FAB-MS m/z: 481 $[M + H]^+$ [19]

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.39 (Ha-1), 2.59 (dd, J = 4.2, 13.0, He-1), 4.01 (Ha-2), 3.96 (He-3), 1.72 (Ha-4), 1.89 (He-4), 2.35 (H-5), 5.80 (d, J = 2.5, H-7), 3.15 (dd, J = 2.8, 8.8, Ha-9), 4.07 (m, Ha-11), 2.22 (Ha-12), 2.16 (He-12), 1.95 (Ha-15), 1.58 (Hb-15), 1.98 (Ha-16), 1.74 (Hb-16), 2.41 (m, H-17), 0.88 (s, CH_3-18), 1.06 (s, CH_3-19), 1.20 (s, CH_3-21), 3.32 (dd, J = 2.0, 11.0, Hb-22), 1.22 (Ha-23), 1.55 (H-25), 0.92 (d, J = 6.4, CH_3-26), 0.93 (d, J = 6.4, CH_3-27) [8]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 3.44 (Ha-1), 4.60 (Ha-2), 4.21 (He-3), 3.11 (H-5), 6.30 (H-7), 3.87 (Ha-9), 4.60 (Ha-11), 3.03 (Ha-12), 2.70 (He-12), 1.33 (CH_3-18), 1.28 (CH_3-19), 1.58 (CH_3-21), 3.79 (Hb-22), 5.53 (H-24), 0.83 (CH_3-26), 0.82 (CH_3-27) [15]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 2.01 (Ha-1), 3.44 (dd, J = 4.0, 16.0, He-1), 4.59 (Ha-2), 4.21 (m, He-3), 1.80 (ddd, J = 3.0, 14.0, 14.0, Ha-4), 2.03 (ddt, J = 4.0, 14.0, 14.0, He-4), 3.02 (H-5), 6.30 (d, J = 3.0, H-7), 3.87 (dd, J = 3.0, 9.0, Ha-9), 4.59 (Ha-11), 3.40 (dd, J = 12.0, 12.0, Ha-12), 2.70 (dd, J = 6.0, 12.0, He-12), 1.95 (Ha-15), 2.24 (Hb-15), 2.11 (Ha-16), 2.48 (Hb-16), 3.02 (H-17), 1.29 (s, CH_3-18), 1.33 (s, CH_3-19), 1.57 (s, CH_3-21), 3.79 (dd, J = 5.0, 10.0, Hb-22), 1.39 (Ha-23), 1.68 (Hb-23), 1.46 (Ha-24), 1.71 (Hb-24), 1.51 (H-25), 0.82 (d, J = 3.0, CH_3-26), 0.80 (d, J = 3.0, CH_3-27) [19]

^{13}C NMR (75 MHz, CD_3OD) [13]: **^{13}C NMR** (100 MHz, C_5D_5N) [15]:

Table 1

C-1	39.92 (t)	C-15	31.84 (t)	C-1	39.5	C-15	31.9
2	68.92 (d)	16	21.52 (t)	2	68.1	16	21.5
3	68.55 (d)	17	50.26 (d)	3	68.4	17	50.0
4	33.26 (t)	18	18.92 (q)	4	32.9	18	19.0
5	52.75 (d)	19	24.64 (q)	5	52.5	19	24.9
6	206.84 (s)	20	77.85 (s)	6	203.8	20	76.8
7	122.73 (d)	21	20.98 (q)	7	122.3	21	21.5
8	165.82 (s)	22	77.95 (d)	8	164.1	22	76.7
9	42.90 (d)	23	30.45 (t)	9	42.8	23	30.3
10	39.02 (s)	24	37.64 (t)	10	39.9	24	37.1
11	69.52 (d)	25	29.23 (d)	11	68.9	25	28.2
12	43.74 (t)	26	23.49 (q)	12	44.2	26	22.4
13		27	22.80 (q)	13	48.2	27	23.3
14	84.90 (s)			14	84.2		

^{13}C NMR (125 MHz, C_5D_5N) [19]:

Table 2

C-1	39.54	C-10	39.92	C-19	24.89
2	68.14	11	68.89	20	76.80
3	68.42	12	44.21	21	21.53
4	32.90	13	48.22	22	76.74
5	52.50	14	84.25	23	30.31
6	203.90	15	31.96	24	37.15
7	122.33	16	21.53	25	28.16
8	164.20	17	49.96	26	23.31
9	42.83	18	18.91	27	22.37

Pharm./Biol.: *Chilo* test: 0.5–1 μg [1], *Candida* tests: Not active (MIC > 200 μg/ml) [7], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 6.2 \times 10^{-8}$ M [13], $EC_{50} = 3.0 \times 10^{-8}$ M [20–23], $EC_{50} = 8.0 \times 10^{-8}$ M [21–23].

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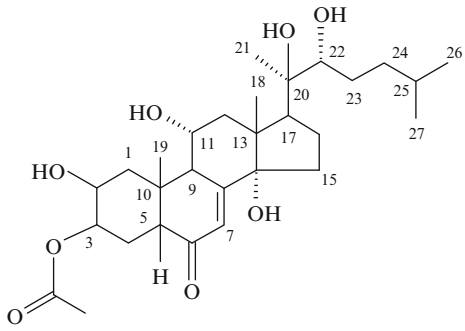
Ajugasterone C 3-Acetate



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotus longifolia* [1]

$C_{29}H_{46}O_8$: 522.3192

CI-MS m/z: 523 $[M + H]^+$, 505 $[M + H–H_2O]^+$, 487 $[M + H–2H_2O]^+$, 469 $[M + H–3H_2O]^+$, 451 $[M + H–4H_2O]^+$,463 $[M + H–CH_3COOH]^+$, 445 $[M + H–H_2O–CH_3COOH]^+$, 427 $[M + H–2H_2O–CH_3COOH]^+$, 409 $[M + H–3H_2O–CH_3COOH]^+$ [1]

^{1}H NMR (J/Hz, D_2O): 1.51 (t, J = 13.3, Ha-1), 2.60 (dd, J = 12.8, 3.8, He-1), 4.23 (m, Ha-2), 5.20 (m, He-3), 1.78 (Ha-4), 1.84 (He-4), 2.34 (H-5), 6.00 (d, J = 2.3, H-7), 3.14 (dd, J = 8.5, 2.5, H-9), 4.25 (Ha-11), 2.06 (Ha-12), 2.29 (He-12), 2.05 (Ha-15), 1.66 (Hb-15), 1.88 (Ha-16), 1.81 (Hb-16), 2.36 (t, J = 9.5, H-17), 0.87 (s, CH_3-18), 1.13 (s, CH_3-19), 1.25 (s, CH_3-21), 3.44 (d, J = 9.3, H-22), 1.28 (Ha-23), 1.61 (Hb-23), 1.28 (Ha-24), 1.38 (Hb-24), 1.58 (H-25), 0.90 (d, J = 6.4, CH_3-26), 0.92 (d, J = 6.4, CH_3-27), 2.19 (s, CH_3COO-3) [1]

^{13}C NMR (D_2O) [1]:

Table 1

C-1	40.4	C-11	70.6	C-21	21.6
2	68.2	12	44.0	22	79.2
3	73.3	13	49.4	23	30.9
4	33.7	14	86.7	24	37.9
5	53.7	15	32.6	25	29.6
6	209.7	16	22.1	26	23.8
7	123.9	17	50.9	27	24.5
8	167.7	18	19.8	$\underline{CH_3}COO$	22.9
9	43.7	19	25.4	$CH_3\underline{COO}$	176.4
10	40.9	20	80.0		

References

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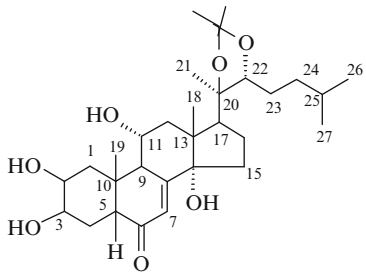
Ajugasterone C-20,22-Acetonide

CAS Registry Number: 142735-64-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum uniflorum* [1], *Serratula coronata* [2], *S. wolffi* [3], *Vitex polygama* [4], *V. strickeri* [5]

$C_{30}H_{48}O_7$: 520.3400

Mp: 248–250°C [1], 287–288°C [3], 246–249°C [5]

IR (KBr) ν_{max} cm^{-1}: 3400–3440, 1675 [3]

IR (Nujol) ν_{max} cm^{-1}: 3200, 1650 [5]

UV λ_{max}^{MeOH} nm: 237 [5]

EI-MS m/z: 520 $[M]^+$ (0.3), 505 $[M\text{-}CH_3]^+$ (0.7), 502 $[M\text{-}H_2O]^+$ (0.3), 487 $[M\text{-}CH_3\text{–}H_2O]^+$ (0.7), 469 $[M\text{-}CH_3\text{–}2H_2O]^+$ (0.4), 462 (5.6), 444 (3.0), 427 (3.9), 379 (3.5), 344 (3.2), 317 (8.0), 266 (10.3), 185 (68.4), 127 (88.7), 109 (44.4), 59 (100) [1], 520 $[M]^+$ (10), 505 (20), 502 (5), 487 (10), 469 (4), 462 (98), 445 (20), 444 (28), 427 (33), 426 (32), 420 (33), 411 10), 409 (20), 402 (13), 379 (20), 361 (17), 299 (12), 281 (7), 266 (33), 185 (100), 142 (58), 127 (83), 114 (33), 109 (33), 84 (60) [2], 379, 361, 325, 317, 299, 185 [5]

CI-MS m/z: 538 $[M + H + NH_3]^+$, 521 $[M + H]^+$, 503 $[M + H\text{–}H_2O]^+$, 490, 480, 464, 447, 429, 413, 394, 391, 380, 364, 279, 230, 212, 178, 136, 124 [2]

FAB-MS m/z: 543 $[M + Na]^+$, 527 $[M + Li]^+$ [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 2.00 (d, J = 12.0, Ha-1), 3.42 (dd, J = 12.0, 5.0, He-1), 4.52 (Ha-2), 4.21 (d, J = 4.0, He-3), 1.78 (ddd, J = 14.0, 14.0, 4.0, Ha-4), 2.03 (dt, J = 14.0, 4.0, 4.0, 4.0, He-4), 3.04 (dd, J = 14.0, 4.0, H-5), 6.29 (d, J = 5.0, H-7), 3.82 (Ha-9), 4.57 (Ha-11), 2.95 (dd, J = 12.0, 12.0, Ha-12), 2.57 (dd, J = 12.0, 7.0, He-12), 1.95 (Ha-15), 2.19 (Hb-15), 2.13 (Ha-16), 2.23 (Hb-16), 2.79 (dd, J = 8.0, 8.0, H-17), 1.31 (s, CH_3-18), 1.32 (s, CH_3-19), 1.08 (s, CH_3-21), 3.86 (H-22), 1.55 (Ha-23), 1.39 (Hb-23), 1.55 (Ha-24), 1.50 (Hb-24), 1.46 (H-25), 0.81 (d, J = 8.0, CH_3-26), 0.81 (d, J = 8.0, CH_3-27), Other: 1.52 and 1.46 (20,22-iPr) [5]

^{13}C NMR (C_5D_5N) [3]:

Table 1

C-1	39.45	C-11	68.83	C-21	22.24
2	68.37	12	43.83	22	81.94
3	68.09	13	47.82	23	27.10
4	32.86	14	84.13	24	36.86
5	52.43	15	31.75	25	28.24
6	203.88	16	22.13	26	22.81
7	122.37	17	49.72	27	22.43
8	163.68	18	18.23	20,22-iPr	29.37
9	42.69	19	24.81		29.37
10	39.81	20	84.81		106.93

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 6.0 \times 10^{-7}$M [2].

References

1. J.K. Cheng, Y.H. Zhang, Z.Y. Zhang, D.L. Cheng, G.L. Zhang, Chem. J. Chinese Univ. **23**, 2084 (2002)
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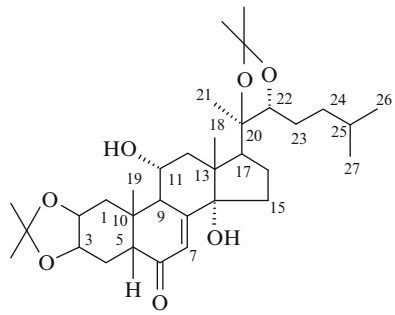
Ajugasterone C-2,3;20,22-Diacetonide

CAS Registry Number: 84028-24-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum uniflorum* [1]

$C_{33}H_{52}O_7$: 560.3713

Mp: 134–136°C [1]

IR (KBr) ν_{max} cm^{-1}: 3431, 2929, 1662, 1459, 1384, 1375, 1217, 1165, 1056 [1]

EI-MS m/z: 560 $[M]^+$, 545 $[M\text{-}CH_3]^+$, 502, 484, 460, 419, 379, 344, 317, 306, 185, 142, 127, 109 [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.44 (d, J = 11.4, Ha-1), 2.56 (dd, J = 4.8, 11.4, He-1), 4.52 (m, Ha-2), 4.29 (m, He-3), 1.74 (Ha-4), 1.87 (He-4), 2.23 (dd, J = 4.1, 12.2, H-5), 5.58 (d, H-7), 2.84 (m, H-9), 4.12 (Ha-11), 2.12 (Ha-12), 2.23 (He-12), 1.74 (Ha-15), 2.10 (Hb-15), 2.04 (Ha-16), 2.13 (Hb-16), 2.21 (H-17), 0.78 (s, CH_3-18), 1.04 (s, CH_3-19), 1.16 (s, CH_3-21), 3.60 (dd, J = 5.5, 7.0, H-22), 1.37 (Ha-23), 1.54 (Hb-23), 1.58 (H-25), 0.89 (d, J = 6.5, CH_3-26), 0.91 (d, J = 6.5, CH_3-27), Other: 1.32 (CH_3-2), 1.33(CH_3-3), 1.41 (CH_3-20), 1.49 (CH_3-22) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	39.98	C-11	68.09	C-21	21.84
2	72.54	12	42.39	22	81.57
3	71.59	13	47.14	23	27.12
4	27.48	14	84.42	24	36.38
5	52.09	15	31.65	25	28.22
6	203.29	16	21.16	26	22.45
7	122.13	17	48.79	27	22.58
8	161.14	18	17.70	CH_3	26.76, 26.83, 29.04, 30.87
9	41.88	19	23.59	OCO	108.09, 106.81
10	38.58	20	83.90		

(*continued*)

References

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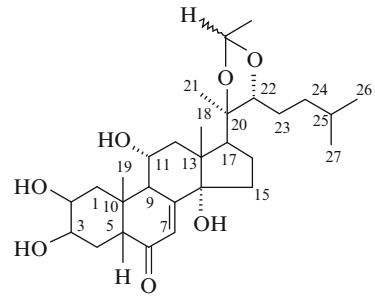
Ajugasterone C-20,22-O-R-Ethylidene

CAS Registry Number: 899428-76-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula coronata* [1]

$C_{29}H_{46}O_7$: 506.3243

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.38 (m, Ha-1), 2.48 (dd, J = 13.5, 4.0, He-1), 4.09 (m, Ha-2), 4.09 (m, He-3), 1.74 (t, Ha-4), 1.74 (t, He-4), 2.32 (m, H-5), 5.98 (d, J = 2.5, H-7), 3.11 (br d, J = 8.5, H-9), 4.20 (m, Ha-11), 2.02 (m, Ha-12), 2.18 (m, He-12), 1.67 (m, Ha-15), 2.05 (m, Hb-15), 1.95 (m, Ha-16), 1.80 (m, Hb-16), 2.31 (m, H-17), 0.84 (s, CH_3-18), 1.09 (s, CH_3-19), 1.24 (s, CH_3-21), 3.83 (m, H-22), 1.56 (m, Ha-23), 1.36 (m, Hb-23), 1.53 (m, Ha-24), 1.30 (m, Hb-24), 1.60 (m, H-25), 0.90 (d, J = 6.9, CH_3-26), 0.91 (d, J = 6.9, CH_3-27), Other: –OC(CH_3)O: 1.38 (d, J = 5.0), OCHO: 5.15 (q, J = 5.0) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

C-1	38.8 (t)	C-11	69.9 (d)	C-21	24.1 (q)
2	68.8 (d)	12		22	
3	68.8 (d)	13	47.9 (s)	23	
4		14	86.4 (s)	24	37.4 (t)
5	52.4 (d)	15		25	29.1 (d)
6		16		26	23.5 (q)
7	123.4 (d)	17	51.7 (d)	27	23.5 (q)
8		18	19.1 (q)	$COCH_3$	21.7 (q)
9	38.8 (d)	19	24.8 (q)	OCO	102.2 (d)
10	42.3 (s)	20	87.3 (s)		

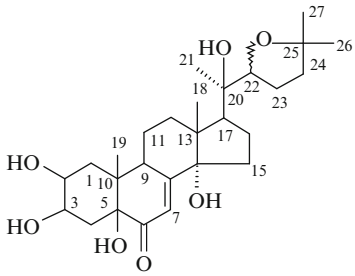
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 6.2 \times 10^{-7}$M [1].

References

1. V.N. Odinokov, S. Kumpun, I.V. Galyautdinov, N. Edvard-Todeschi, N.A. Veskina, L.M. Khalilov, J.P. Girault, L. Dinan, R. Lafont, Coll. Czech. Chem. Comm. **70**, 2038 (2005)

Ajugasterone D

CAS Registry Number: 80651-74-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga nipponensis* [1,2]

$C_{27}H_{42}O_7$: 478.2930

Mp: 234–237°C [1]

IR (KBr) ν_{max} cm^{-1}: 3400, 1690 [1]

UV λ_{max}^{EtOH} nm (log ε): 244–246 (4.07) [1]

EI-MS m/z: 479 $[M + H]^+$, 443, 379, 361, 343, 325, 143, 125, 99, 81 [1]

^{1}H NMR (C_5D_5N): 0.94 (s, CH_3-18), 1.04 (s, CH_3-19), 1.28 (s, CH_3-21), 1.10 (s, CH_3-26), 1.10 (s, CH_3-27) [1]

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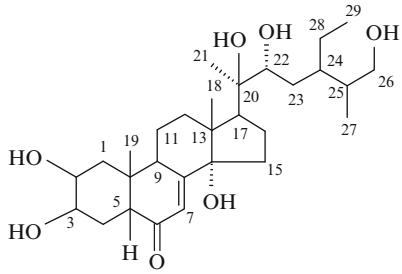
Amarasterone A

CAS Registry Number: 20853-88-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga australis* [1], *Cyathula capitata* [2], *Leuzea carthamoides* [3], *Microsorum scolopendria* [4]

$C_{29}H_{48}O_7$: 508.3400

Mp: 210–211°C [2]

$[\alpha]_D^{20}$ + 75° (dioxan) [2]

IR (KBr) ν_{max} cm^{-1}: 1650 [2], 3465, 3387, 1658, 1061, 1054 [3]

UV λ_{max}^{EtOH} nm: 244 [2]

EI-MS m/z: 508 $[M]^+$, 363 $[M - C_{22}\text{-}C_{29}]^+$, 345, 327, 145 $[C_{22}\text{-}C_{29}]^+$, 127, 109 [2]

ESI-MS m/z: 509 $[M + H]^+$, 491 $[M + H–H_2O]^+$, 473 $[M + H–2H_2O]^+$, 455 $[M + H–3H_2O]^+$, 437 $[M + H–4H_2O]^+$ [3]

CI/D-MS m/z: 526 $[M + NH_4]^+$, 509 $[M + H]^+$, 491 $[M + H–H_2O]^+$, 473 $[M + H–2H_2O]^+$, 455 $[M + H–3H_2O]^+$, 364 $[M + NH_4–H_2O–C_{22}–C_{29}]^+$, 347

[M + H–H_2O–C_{22}–C_{29}]$^+$, 329 [M + H–2H_2O–C_{22}–C_{29}]$^+$, 171, 127, 124 [4]

HR-MS m/z: for $C_{28}H_{47}O_7$ $[M]^+$ calcd. 516.2719, found 516.2751 [1]

HR-ESI-MS m/z: for $C_{29}H_{48}O_7Na$ $[M + Na]^+$ calcd. 531.3277, found 531.3298 [3]

CD (c, dioxane): $\Delta\varepsilon = +11.56$ (244 nm), $\Delta\varepsilon = -2.84$ (204 nm), $\Delta\varepsilon = +0.86$ (340 nm) [1]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 6.23 (H-7), 1.21 (s, CH_3-18), 1.06 (s, CH_3-19), 1.56 (s, CH_3-21), 1.11 (d, CH_3-27), 0.92 (t, CH_3-29) [2]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (dd, J = 4.2, 13.4, Ha-1), 1.43 (dd, J = 12.0, 13.4, He-1), 3.83 (ddd, J = 3.0, 4.2, 12.0, Ha-2), 3.95 (q, J = 3.0, He-3), 1.70–1.75 (Ha-4), 1.70–1.75 (He-4), 2.88 (dd, J = 4.5, 12.6, H-5), 5.81 (d, J = 2.6, H-7), 3.15 (ddd, J = 2.6, 7.0, 11.5, Ha-9), 1.81 (Ha-11), 1.70 (He-11), 2.11 (td, J = 5.0, 13.0, 13.0, Ha-12), 1.88 (He-12), 1.96 (Ha-15), 1.61 (Hb-15), 1.75 (Ha-16), 2.00 (Hb-16), 2.34 (dd, J = 8.4, 9.8, H-17), 0.894 (s, CH_3-18), 0.968 (s, CH_3-19), 1.179 (s, CH_3-21), 3.45 (dd, J = 2.3, 10.4, Hb-22), 1.21 (Ha-23), 1.21 (Hb-23), 1.68 (Ha-24), 1.85 (H-25), 3.50 (dd, J = 7.3, 11.0, Ha-26), 3.40 (dd, J = 6.8, 11.0, Ha-26), 0.786 (d, J = 7.0, CH_3-27), 1.51 (Ha-28), 1.28 (Hb-28), 0.935 (t, J = 6.4, CH_3-29) [3]

^{1}H NMR (J/Hz, D_2O): 1.38 (Ha-1), 1.88 (He-1), 3.99 (Ha-2), 4.07 (He-3), 1.75 (Ha-4), 1.75 (He-4), 2.34 (t, H-5), 5.97 (d, J = 2.0, H-7), 3.11 (Ha-9), 1.73 (Ha-11), 1.86 (He-11), 1.99 (Ha-12), 1.96 (He-12), 1.65 (Ha-15), 2.05 (Hb-15), 1.89 (Ha-16), 1.80 (Hb-16), 2.32 (m, H-17), 0.867 (s, CH_3-18), 1.00 (s, CH_3-19), 1.23 (s, CH_3-21), 3.54 (d, J = 10.0, Hb-22), 1.36 (Ha-23), 1.42 (Hb-23), 1.50 (m, Ha-24), 1.82 (H-25), 3.39 (dd, J = 8.3, 10.8, Ha-26), 3.65 (dd, J = 5.0, 10.8, Ha-26), 0.932 (d, J = 6.8, CH_3-27), 1.40 (Ha-28), 1.40 (Hb-28), 0.913 (t, J = 7.1, CH_3-29) [4]

^{13}C NMR (D_2O) [4]:

Table 1

C-1	38.3	C-11	23.0	C-21	22.4
2	70.2	12	33.9	22	78.8
3	70.1	13	50.3	23	35.4
4	34.1	14	88.1	24	41.4
5	53.3	15	33.4	25	40.0
6	211.4	16	22.4	26	68.0
7	124.1	17	52.1	27	18.8
8		18	19.9	28	25.1
9	36.7	19	25.9	29	14.2
10	41.0	20	81.0		

(*continued*)

Table 1 (continued)

9	36.7	19	25.9	29	14.2
10	41.0	20	81.0		

^{13}C NMR (125.7 MHz, CD_3OD) [3]:

Table 2

C-1	37.36	C-11	21.53	C-21	20.90
2	68.70	12	32.52	22	75.71
3	68.52	13	49.00	23	32.02
4	33.86	14	85.21	24	37.85
5	51.79	15	31.79	25	37.60
6	206.44	16	21.47	26	66.75
7	122.14	17	50.34	27	11.51
8	167.94	18	18.06	28	25.40
9	35.10	19	24.41	29	12.29
10	39.26	20	77.96		

Pharm./Biol.: *Sarcophaga* test: highly active [2].

References

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3. M. Budesinsky, K. Vokas, J. Harmatha, J. Cvacka, Steroids **73**, 502 (2008)
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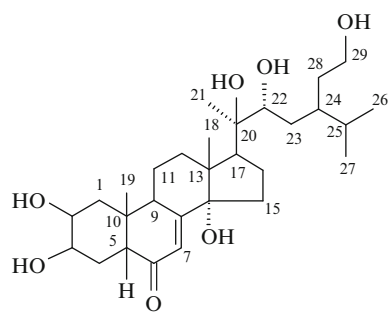
Amarasterone B

CAS Registry Number: 21132-15-0



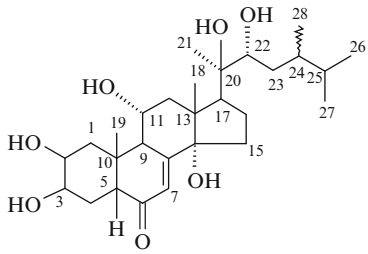
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Cyathula capitata* [1]
$C_{29}H_{48}O_7$: 508.3400
Mp: 284–285°C [1]
$[\alpha]_D^{20}$ + 82° (dioxan) [1]
IR (KBr) ν_{max} cm^{-1}: 1650 [1]
UV λ_{max}^{EtOH} nm: 244 [1]
EI-MS m/z: 508 $[M]^+$, 363 $[M\text{-}C_{22}\text{-}C_{29}]^+$, 345, 327, 145 $[C_{22}\text{-}C_{29}]^+$, 127, 109 [1]
^{1}H NMR (100 MHz, C_5D_5N): 6.22 (H-7), 1.22 (s, CH_3-18), 1.07 (s, CH_3-19), 1.56 (s, CH_3-21), 0.91 (d, CH_3-26), 0.91 (d, CH_3-27) [1]
Pharm./Biol.: *Sarcophaga* biotest: highly active [1].

References

1. T. Takemoto, K. Nomoto, H. Hikino, Tetrah. Lett. **48**, 4953 (1968)

Atrotosterone A

CAS Registry Number: 190519-38-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Paxillis atrotomentosus* [1, 2], *Cyanotus longifolia* [3]
$C_{28}H_{46}O_7$: 494.3243
IR (KBr) ν_{max} cm^{-1}: 3412, 1658, 1050 [2]
EI-MS m/z: 379 (4), 361 (18), 343 (100), 325 (66), 307 (12), 300 (6), 283 (6), 267 (43), 255 (6), 241 (3), 225 (4), 213 (5), 187 (7), 173 (6), 161 (3), 143 (3), 123 (5), 95 (5), 83 (5), 71 (7), 55 (4), 43 (14) [2]
FAB-MS m/z: 517 $[M + Na]^+$ (8), 495 $[M + H]^+$ (12), 477 (14), 459 (8), 441 (5), 423 (3), 399 (5), 345 (5), 329 (5), 317 (5), 299 (9), 281 (6), 249 (6), 225 (7), 149 (24), 129 (15), 113 (17), 95 (38), 83 (41), 71 (74), 55 (100) [2]
HR-MS m/z: for $C_{28}H_{47}O_7$ $[M + H]^+$ calcd. 495.3322, found 495.3334 [2]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.38 (dd, J = 12.8, 12.0, Ha-1), 2.59 (dd, J = 12.8, 4.2, He-1), 4.01 (ddd, J = 12.0, 4.2, 3.3, Ha-2), 3.95 (q, He-3), 1.77 (ddd, J = 14.0, 13.0, 2.5, Ha-4), 1.69 (ddd, J = 14.0, 4.0, 3.2, He-4), 2.33 (dd, J = 13.0, 4.0, H-5), 5.80 (dd, J = 2.7, 1.0, H-7), 3.16 (dd, J = 9.0, 2.7, H-9), 4.10 (ddd, J = 10.6, 9.0, 6.0, Ha-11), 2.21 (dd, J = 12.1, 10.6, Ha-12), 2.15 (dd, J = 12.1, 6.0, He-12), 1.95 (Ha-15), 1.58 (Hb-15), 2.01 (Ha-16), 1.74 (Hb-16), 2.42 (dd, J = 9.5, 8.5, H-17), 0.874 (s, CH_3-18), 1.056 (s, CH_3-19), 1.197 (s, CH_3-21), 3.45 (dd, J = 10.5, 1.7, H-22), 1.53 (Ha-23), 1.09 (ddd, J = 14.1, 10.5, 4.6, Hb-23), 1.67 (H-24), 1.78 (dh, J = 3.4, 6.8 (6x), H-25), 0.935 (d, J = 7.0, CH_3-26), 0.801 (d, J = 6.8, CH_3-27), 0.851 (d, J = 7.0, CH_3-28) [2]
^{1}H NMR (J/Hz, D_2O): 1.41 (t, J = 13.3, Ha-1), 2.50 (dd, J = 13.3, 3.8, He-1), 4.11 (m, Ha-2), 4.10 (m, He-3), 1.78 (Ha-4), 1.78 (He-4), 2.32 (t, H-5), 5.99 (d, J = 2.4, H-7), 3.14 (dd, J = 9.0, 2.5, H-9), 4.23 (ddd, Ha-11), 2.06 (Ha-12), 2.29 (He-12), 2.06 (Ha-15), 1.67 (Hb-15), 1.91 (Ha-16), 1.83 (Hb-16), 2.39 (t, J = 9.5, H-17), 0.87 (s, CH_3-18), 1.11 (s, CH_3-19), 1.25 (s, CH_3-21), 3.57 (d, J = 10.0, H-22), 1.17 (Ha-23), 1.63 (Hb-23), 1.63 (Ha-24), 1.58 (H-25), 0.80 (d, J = 6.9, CH_3-26), 0.93 (d, J = 6.9, CH_3-27), 0.85 (d, J = 6.7, CH_3-28) [3]
^{13}C NMR (125.7 MHz, CD_3OD) [2]:

Table 1

C-1	39.08	C-11	69.54	C-21	20.75
2	68.95	12	43.76	22	75.50
3	68.54	13		23	37.50
4	33.31	14	84.76	24	36.68
5	52.78	15	31.81	25	30.37
6	206.74	16	21.55	26	16.21
7	122.68	17	50.17	27	15.70
8	165.89	18	18.85	28	21.58
9	42.94	19	24.60		
10	39.88	20	77.86		

^{13}C NMR (D_2O) [3]:

Table 2

C-1	39.1	C-11	70.0	C-21	21.0
2	69.3	12	43.7	22	76.5
3	69.1	13	49.1	23	37.8
4	33.4	14	86.4	24	36.8
5	53.2	15	32.1	25	30.6
6	n.d.	16	21.9	26	22.3
7	123.7	17	50.4	27	16.9
8	n.d.	18	19.5	28	16.5
9	43.2	19	25.0		
10	40.3	20	79.8		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 2.5 \times 10^{-8}$M [4].

References

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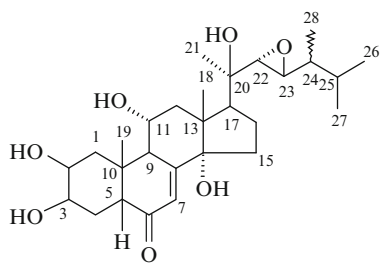
2. K. Vokas, M. Budesinsky, J. Harmatha, J. Pis, Tetrahedron **54**, 1657 (1998)
3. S. Crouzet, A. Maria, L. Dinan, R. Lafont, J.P. Girault, Arch. Insect Biochem. Physiol. **72**, 194 (2009)
4. J. Harmatha, L. Dinan, Arch. Insect Biochem. Physiol. **35**, 219 (1997)

Atrotosterone B

CAS Registry Number: 190519-40-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Paxillis atrotomentosus* [1, 2]

$C_{28}H_{44}O_7$: 492.3087

IR (KBr) ν_{max} cm^{-1}: 3406, 1657, 1061 [2]

EI-MS m/z: 456 $[M\text{-}2H_2O]^+$ (1), 438 (2), 423 (1), 409 (1), 395 (1), 367 (2), 343 (7), 325 (8), 309 (5), 300 (25), 285 (25), 267 (21), 185 (13), 171 (17), 157 (15), 139 (13), 129 (17), 118 (33), 83 (45), 71 (43), 55 (53), 43 (100) [2]

FAB-MS m/z: 515 $[M + Na]^+$ (8), 493 $[M + H]^+$ (10), 475 (35), 457 (7), 439 (3), 316 (10), 299 (8), 283 (8), 281 (8), 250 (58), 231 (11), 213 (13), 133 (55), 115 (35), 105 (33), 91 (60), 83 (87), 71 (55), 55 (100) [2]

HR-MS m/z: for $C_{28}H_{45}O_7$ $[M + H]^+$ calcd. 493.3165, found 493.3261 [2]

^{1}H NMR (500 MHz, J/Hz, CD_3OD):1.38 (dd, J = 12.8, 12.0, Ha-1), 2.59 (dd, J = 12.8, 4.2, He-1), 4.01 (ddd, J = 11.7, 4.0, 3.3, Ha-2), 3.96 (q, J = 2.9, He-3), 1.78 (dt, J = 13.5, 13.5, 2.4, Ha-4), 1.69 (dt, J = 14.0, 3.6, 3.6, He-4), 2.34 (dd, J = 13.0, 4.0, H-5), 5.81 (dd, J = 2.7, 1.0, H-7), 3.16 (dd, J = 9.0, 2.7, H-9), 4.10 (ddd, J = 10.7, 8.7, 6.0, Ha-11), 2.25 (dd, J = 12.0, 11.0, Ha-12), 2.14 (dd, J = 12.2, 5.8, He-12), 1.96 (m, Ha-15), 1.62 (m, Hb-15), 1.96 (m, Ha-16), 1.96 (m, Hb-16), 2.49 (dd, J = 9.5, 8.5, H-17), 0.843 (s, CH_3-18), 1.055 (s, CH_3-19), 1.306 (s, CH_3-21), 2.85 (d, J = 2.4, H-22), 2.72 (dd, J = 7.8, 2.4, H-23), 1.12 (m, H-24), 1.68 (m, H-25), 0.987 (d, J = 6.8, CH_3-26), 0.962 (d, J = 6.8, CH_3-27), 0.987 (d, J = 6.8, CH_3-28) [2]

^{13}C NMR (125.7 MHz, CD_3OD) [2]:

Table 1

C-1	39.09	C-11	69.47	C-21	24.01
2	68.95	12	43.52	22	66.75
3	68.58	13		23	59.93
4	33.30	14	84.69	24	43.11
5	52.78	15	31.84	25	34.42
6	206.71	16	21.88	26	20.85
7	122.71	17	54.26	27	19.90
8	165.70	18	18.75	28	13.94
9	42.96	19	24.60		
10	39.89	20	72.80		

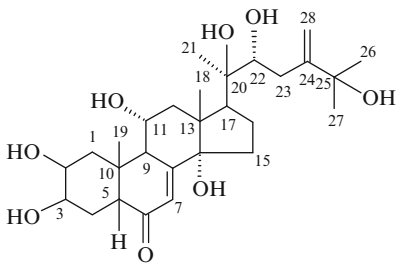
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 6.5 \times 10^{-6}$M [3].

References

1. K. Vokas, M. Budesinsky, J. Harmatha, in *Abstracts of the 16th Conference on Isoprenoids*, Prague, 1995, p. 77
2. K. Vokas, M. Budesinsky, J. Harmatha, J. Pis, Tetrahedron **54**, 1657 (1998)
3. J. Harmatha, L. Dinan, Arch. Insect Biochem. Physiol. **35**, 219 (1997)

Atrotosterone C

CAS Registry Number: 190519-42-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Klaseopsis chinensis* [1], *Paxillis atrotomentosus* [2]

$C_{28}H_{44}O_8$: 508.3036

IR (KBr) ν_{max} cm^{-1}: 3406, 1657, 1073, 1051 [2]

FAB-MS m/z: 531 $[M + Na]^+$ (3), 509 $[M + H]^+$ (1), 491 (2), 473 (3), 455 (4), 437 (2), 345 (5), 317 (7), 299 (12), 239 (18), 121 (49), 105 (51), 91 (87), 81 (63), 69 (70), 55 (100) [2]

HR-MS m/z: for $C_{28}H_{45}O_8$ $[M + H]^+$ calcd. 509.3114, found 509.3035 [2]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.38 (dd, J = 12.8, 12.0, Ha-1), 2.59 (dd, J = 12.8, 4.2, He-1), 4.01 (ddd, J = 11.3, 4.8, 3.0, Ha-2), 3.95 (q, J = 3.0, He-3), 1.78 (dt, J = 13.0, 13.0, 2.5, Ha-4), 1.69 (dt, J = 14.0, 3.7, 3.7, He-4), 2.34 (dd, J = 13.0, 3.8, H-5), 5.81 (bd, J = 2.7, H-7), 3.15 (dd, J = 8.8, 2.8, H-9), 4.11 (ddd, J = 10.5, 9.0, 6.0, Ha-11), 2.23 (dd, J = 12.0, 10.5, Ha-12), 2.17 (dd, J = 12.0, 6.2, He-12), 1.97 (m, Ha-15), 1.59 (m, Hb-15), 2.04 (m, Ha-16), 1.82 (m, Hb-16), 2.46 (dd, J = 9.5, 8.7, H-17), 0.885 (s, CH_3-18), 1.060 (s, CH_3-19), 1.256 (s, CH_3-21), 3.58 (dd, J = 10.6, 1.8, H-22), 2.39 (bd, J = 14.5, Ha-23), 2.14 (bd, J = 14.5, 10.6, Hb-24), 1.376 (s, CH_3-26), 1.323 (s, CH_3-27) [2]

^{13}C NMR (125.7 MHz, CD_3OD) [2]:

Table 1

C-1	39.08	C-11	69.51	C-21	20.98
2	68.96	12	43.77	22	78.02
3	68.59	13		23	34.59
4	33.28	14	84.93	24	155.34
5	52.78	15	31.85	25	73.63
6	206.72	16	21.56	26	30.21
7	122.77	17	50.30	27	29.76
8	165.71	18	18.89	28	110.42
9	42.94	19	24.60		
10	39.90	20	77.72		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 3.0 \times 10^{-6}$M [3–5].

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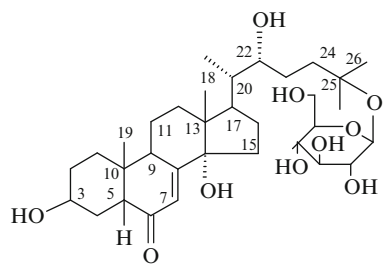
Blechnoside B

CAS Registry Number: 104387-06-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Asparagus dumosus* [1], *Blechnum minus* [2], *Froelichia floridana* [3]

$C_{33}H_{54}O_{10}$: 610.3716

Mp: 218–220°C (EtOAc-MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3440, 1660 [2]

UV λ_{max}^{EtOH} nm (log ε): 243 (4.03) [2]

CD (c, 0.12, EtOH): $\Delta\varepsilon = -1.28$ (253 nm), $\Delta\varepsilon = +1.35$ (330 nm) [2]

DEI m/z: 611 [M + 1] (0.4%); 431 [M + 1-glucose] (10%) [2]

Anal. Calcd. for $C_{33}H_{54}O_{10}$: C, 63.0; H, 9.0. Found: C, 62.9; H, 8.8 [2]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 3.86 (br m, J = 10.0, He-3), 2.89 (H-5), 6.19 (br d, J = 2.0, H-7), 3.48 (m, Ha-9), 0.72 (s, CH_3-18), 0.88 (s, CH_3-19), 1.29 (d, J = 6.5, CH_3-21), 4.10 (Hb-22), 1.40 (s, CH_3-26), 1.40 (s, CH_3-27), β-D-Glcp′: 4.90 (d, J = 7.5, H-1) [2]

^{13}C NMR (62.9 MHz, C_5D_5N) [2]:

Table 1

C-1	29.9	C-12	31.8	C-23	25.8
2	29.5	13	48.2	24	42.5
3	72.5	14	84.1	25	69.8
4	27.6	15	31.8	26	30.0
5	51.5	16	26.8	27	30.3
6	203.0	17	48.4	Glc′-1	103.3
7	121.3	18	15.9	2	75.3
8	165.9	19	24.0	3	78.3
9	34.7	20	43.0	4	71.9
10	36.8	21	13.7	5	78.7
11	21.6	22	74.1	6	63.0

Pharm./Biol.: *Calliphora* bioassay: high active [2], Human DNA Topoisomerase I test: not active [3].

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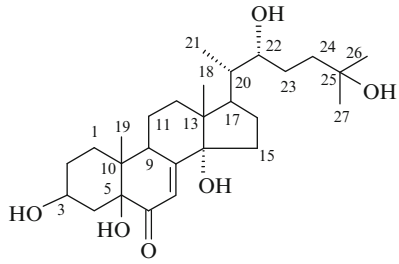
Brahuisterone

CAS Registry Number: 169238-28-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1]

$C_{27}H_{44}O_6$: 464.3137

Mp: 186–188°C ($CHCl_3$–MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3300–3500, 1680 [1]

EI-MS m/z: 464 $[M]^+$ (1), 446 (11), 431 (14), 428 (15), 418 (11), 413 (16), 410 (11), 395 (15), 378 (27), 359 (15), 348 (100), 330 (63), 300 (61), 279 (98), 99 (99), 81 (98) [1]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 3.92 (br m, He-3), 6.06 (br s, H-7), 3.39 (br m, Ha-9), 0.60 (s, CH_3-18), 1.00 (s, CH_3-19), 1.15 (dd, J = 6.0, 4.0, CH_3-21), 3.92 (br m, H-22), 1.26 (s, CH_3-26), 1.26 (s, CH_3-27) [1]

References

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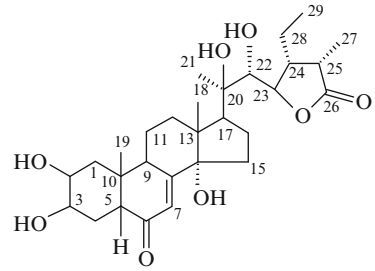
Briviflorasterone

CAS Registry Number: 1033773-08-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga macrosperma* var. *breviflora* [1], *Ajuga reptans* var. *reptans* [2]

$C_{29}H_{44}O_8$: 520.3036

Mp: amorphous solid [1], 268–270°C [2]

$[\alpha]_D^{22}$ −159.3° (c 0.23; MeOH) [1], $[\alpha]_D^{25}$ + 15° (c 0.1, MeOH) [2]

UV λ_{max}^{MeOH} nm (log ε): 242 (3.9459) [2]

HR-ESI-MS m/z: for $C_{29}H_{45}O_8$ $[M + H]^+$ calcd. 521.3114, found 521.3140 [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.93 (dd, J = 12.0, 13.4, Ha-1), 2.14 (He-1), 4.20 (br d, Ha-2), 4.27 (He-3), 1.83 (br t, J = 13.4, Ha-4), 2.07 (dt, J = 3.7, 13.7, He-4), 3.02 (dd, J = 3.5, 13.5, H-5), 6.24 (d, J = 2.2, H-7), 3.60 (m, Ha-9), 1.72 (qd, J = 4.4, 12.0, Ha-11), 1.87 (Hb-12), 2.00 (br d, J = 12.4, Ha-12), 2.60 (td, J = 4.6, 12.4, He-12), 1.89 (Ha-15), 2.15 (Hb-15), 2.15 (Ha-16), 2.44 (m, Hb-16), 3.06 (t, J = 9.0, H-17), 1.19 (s, CH_3-18), 1.07 (s, CH_3-19), 1.65 (s, CH_3-21), 4.19 (br s, Hb-22), 4.62 (br d, J = 2.4, Ha-23), 2.81 (td, J = 4.5, 9.0, H-24), 3.45 (q, J = 7.7, H-25), 1.14 (d, J = 7.6, CH_3-27), 1.22 (m, Ha-28), 1.48 (m, Hb-28), 0.98 (t, J = 7.3, CH_3-29), 6.40 (br, OH), 7.35 (br, OH) [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.43 (Ha-1), 1.81 (He-1), 3.84 (Ha-2), 3.95 (He-3), 1.71 (Ha-4), 1.78 (He-4), 2.38 (H-5), 5.81 (H-7), 3.16 (Ha-9), 1.70 (Ha-11), 1.82 (Hb-12), 1.87 (Ha-12), 2.16 (He-12), 1.63 (Ha-15), 1.98 (Hb-15), 2.00 (Ha-16), 1.81 (Hb-16), 2.57 (H-17), 0.88 (s, CH_3-18), 0.97 (s, CH_3-19), 1.30 (s, CH_3-21), 3.62 (d, J = 4.3, Hb-22), 4.34 (dd, J = 4.3, 2.0, Ha-23), 2.62 (tdd, J = 8.7, 5.1, 2.1, H-24), 3.10 (dq, J = 8.2, 7.6, H-25), 1.13 (d, J = 7.6, CH_3-27), 1.35 (ddd, J = 14.2, 8.9, 7.3, Ha-28), 1.59 (Hb-28), 1.00 (t, J = 7.3, CH_3-29) [2]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-11	21.4	C-21	22.5
2	68.1	12	31.9	22	77.8
3	68.0	13	48.1	23	82.9
4	32.5	14	84.0	24	40.9
5	51.4	15	31.6	25	38.1
6	203.5	16	21.0	26	180.4
7	121.6	17	50.7	27	10.6
8	166.0	18	18.0	28	22.0
9	34.4	19	24.4	29	12.0
10	38.6	20	75.8		

(*continued*)

Table 1 (continued)

7	121.6	17	50.7	27	10.6
8	166.0	18	18.0	28	22.0
9	34.4	19	24.4	29	12.0
10	38.6	20	75.8		

^{13}C NMR (125 MHz, CD_3OD) [2]:

Table 2

C-1	37.5	C-11	21.6	C-21	22.0
2	68.8	12	32.6	22	78.1
3	68.6	13	49.2	23	84.4
4	33.0	14	85.3	24	42.3
5	51.9	15	31.8	25	38.8
6	206.6	16	21.6	26	182.9
7	122.2	17	51.2	27	10.6
8	168.1	18	18.3	28	22.7
9	35.2	19	24.5	29	12.0
10	39.4	20	77.1		

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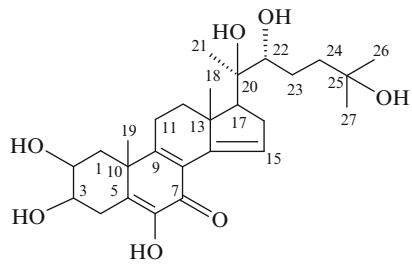
Calonysterone

CAS Registry Number: 51787-31-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Asparagus dumosus* [1], *Asparagus filicinus* [2], *Ipomoea calonyction* [3–5], *Vitex canascens* [6], *V. glabrata* [7], *V. scabra* [8]

$C_{27}H_{40}O_7$: 476.2774

Mp: 234–235°C (MeOH) [3], 253–254°C (Me_2CO) [3–5]

$[\alpha]_D^{20}$ + 76.8° (c 1.0, MeOH) [3–5]

IR (KBr) ν_{max} cm^{-1}: 3380, 3350, 1638, 1620, 845 [3, 4]

UV λ_{max}^{EtOH} nm (ε): 222 (20700), 244 (13500), 294 (7850) [3, 5]

EI-MS m/z: 476 (14.4), 458 (32.4), 443 (18.0), 442 (16.2), 440 (38.8), 425 (22.8), 424 (9.2), 422 (18.2), 407 (12.8), 406 (5.9), 359 (56.5), 343 (48), 342 (100), 341 (59.1), 327 (93.1), 325 (41.0), 323 (39.2), 315 (64.2), 314 (80.5), 298 (75.8), 296 (40.5), 161, 143, 125, 107, 99, 81, 69, 55 [4]

HR-MS m/z: for $C_{27}H_{40}O_7$ $[M]^+$ calcd. 476.2774, found 476.2774 [4]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 7.41 (m, H-15), 1.40 (s, CH_3-18), 1.72 (s, CH_3-19), 1.56 (s, CH_3-21), 1.42 (s, CH_3-26), 1.42 (s, CH_3-27) [4]

^{1}H NMR (DMSO-d_6): 6.78 (s, H-15), 1.00 (s, CH_3-18), 1.41 (s, CH_3-19), 1.16 (s, CH_3-21), 1.05 (s, CH_3-26), 1.07 (s, CH_3-27) [5]

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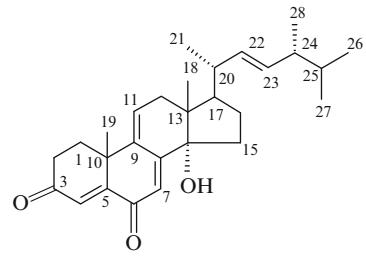
Calvasterol A

CAS Registry Number: 162857-85-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Calvatia cyathiformis* [1]

$C_{28}H_{38}O_3$: 422.2820

Mp: 190–192°C (n-hexane-$CHCl_3$) [1]

$[\alpha]_D^{20}$ + 93° (c 0.39, $CHCl_3$) [1]

IR (KBr) ν_{max} cm^{-1}: 3450, 1660 [1]

UV λ_{max}^{MeOH} nm (log ε): 250 (4.35), 340 (4.06) [1]

EI-MS m/z: 422.2815 $[M]^+$ (2), 404 $[M - H_2O]^+$ (60), 280 (55), 265 (38) [1]

CD (c, MeOH): Δε = -3.46 (275 nm), Δε = +1.57 (234 nm) [1]

^{1}H NMR (600 MHz, J/Hz, $CDCl_3$): 2.28 (ddd, J = 5.5, 13.6, 14.3, Ha-1), 2.42 (ddd, J = 4.5, 5.1, 13.6, Hb-1), 2.65 (ddd, J = 5.1, 14.3, 19.4, Ha-2), 2.59 (ddd, J = 4.5, 5.5, 19.4, Hb-2), 6.45 (s, H-4), 6.17 (s, H-7), 6.22 (dd, J = 1.8, 6.6, H-11), 2.72 (dd, J = 1.8, 18.3, Ha-12), 2.38 (dd, J = 6.6, 18.3, Hb-12), 2.00 (m, Ha-15), 1.77 (m, Hb-15), 2.00 (m, Ha-16), 1.44 (m, Hb-16), 2.11 (m, H-17), 0.76 (s, CH_3-18), 1.46 (s, CH_3-19), 2.09 (m, H-20), 1.04 (d, J = 5.9, CH_3-21), 5.22 (dd, J = 7.7, 15.4, H-22), 5.30 (dd, J = 7.7, 15.4, H-23), 1.89 (m, H-24), 1.50 (m, H-25), 0.84 (d, J = 6.9, CH_3-26), 0.85 (d, J = 6.9, CH_3-27), 0.93 (d, J = 6.9, CH_3-28) [1]

^{13}C NMR (150 MHz, $CDCl_3$) [1]:

Table 1

C-1	34.5	C-11	132.9	C-21	20.9
2	34.3	12	37.4	22	135.4

(*continued*)

Table 1 (continued)

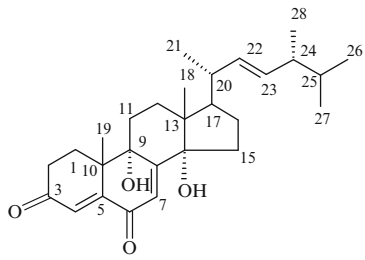
3	199.7	13	46.3	23	133.3
4	127.0	14	84.7	24	42.9
5	156.3	15	31.2	25	33.2
6	188.7	16	27.2	26	20.0
7	121.8	17	50.4	27	19.7
8	156.0	18	16.2	28	17.6
9	138.5	19	29.5		
10	38.8	20	40.1		

References

1. N. Kawahara, S. Sekita, M. Satake, Phytochemistry **38**, 947 (1995)

Calvasterol B

CAS Registry Number: 162857-86-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Calvatia cyathiformis* [1]

$C_{28}H_{40}O_4$: 440.2926

Mp: 173–175°C [1], 176–185°C (hexane) [2]

$[\alpha]_D^{20}$ − 103° (c 0.27, $CHCl_3$) [1]

IR (KBr) ν_{max} cm^{-1}: 3450, 1660 [1]

UV λ_{max}^{MeOH} nm: 266 (log ε 4.09) [1], 267 (ε 11100) [2]

EI-MS m/z: 440.2932 $[M]^+$ (4), 422 $[M - H_2O]^+$ (38), 297 (26), 229 (87) [1]

CD (c, MeOH): Δε = -2.94 (290 nm), Δε = +4.30 (248 nm) [1]

^{1}H NMR (600 MHz, J/Hz, $CDCl_3$): 2.79 (ddd, J = 5.1, 13.9, 13.9, Ha-1), 1.82 (br d, J = 13.9, Hb-1), 2.59 (ddd, J = 4.0, 5.1, 16.8, Ha-2), 2.50 (ddd, J = 5.5, 13.9, 16.8, Hb-2), 6.60 (s, H-4), 6.19 (s, H-7), 2.09 (m, Ha-11), 1.83 (m, Hb-11), 2.18 (ddd, J = 4.4, 13.2, 13.6, Ha-12), 1.75 (br d, J = 13.6, Hb-12), 1.97 (m, Ha-15), 1.65 (m, Hb-15), 1.94 (m, Ha-16), 1.46 (m, Hb-16), 2.01 (m, H-17), 0.77 (s, CH_3-18), 1.37 (s, CH_3-19), 2.11 (m, H-20), 1.05 (d, J = 6.6, CH_3-21), 5.20 (dd, J = 8.4, 15.0, H-22), 5.29 (dd, J = 7.7, 15.0, H-23), 1.88 (m, H-24), 1.49 (m, H-25), 0.84 (d, J = 6.9, CH_3-26), 0.85 (d, J = 6.9, CH_3-27), 0.93 (d, J = 6.9, CH_3-28), 4.22 (br s, OH-9 or OH-14), 2.46 (br s, OH-9a or OH-14a) [1]

^{1}H NMR (200 MHz, J/Hz, $CDCl_3$): 6.61 (s, H-4), 6.20 (s, H-7), 0.78 (s, CH_3-18), 1.39 (s, CH_3-19), 1.07 (d, J = 6.5, CH_3-21), 5.12–5.34 (m, H-22), 5.12–5.34 (m, H-23), 0.85 (d, J = 6.5, CH_3-26), 0.87 (d, J = 6.5, CH_3-27), 0.94 (d, J = 6.5, CH_3-28) [2]

^{13}C NMR (150 MHz, $CDCl_3$) [1]:

Table 1

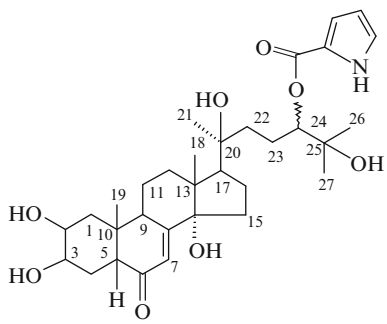
C-1	27.7	C-11	27.6	C-21	21.3
2	34.3	12	27.7	22	135.4
3	200.1	13	46.4	23	133.4
4	125.5	14	87.0	24	43.0
5	155.4	15	31.9	25	33.2
6	188.1	16	26.3	26	20.0
7	129.1	17	50.2	27	19.7
8	163.4	18	16.4	28	17.7
9	74.4	19	22.9		
10	44.1	20	40.0		

References

1. N. Kawahara, S. Sekita, M. Satake, Phytochemistry **38**, 947 (1995)
2. N.V. Kovganko, S.N. Sokolov, Chem. Nat. Comp. **35**, 320 (1999)

Canescensterone

CAS Registry Number: 162666-15-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Vitex canescens* [1]
$C_{32}H_{47}O_8N$: 573.3301
Mp: 152–153°C (EtOAc–MeOH) [1]
$[\alpha]_D^{26}$ + 18.8° (c 0.09, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3412, 1683, 1643 [1]
UV λ_{max}^{MeOH} nm (log ε): 240 sh (4.10), 259 (4.18) [1]
EI-MS m/z: 444 $[M + H–COC_4H_4N–2H_2O]^+$ (2), 426 (2), 411 (3), 393 (2), 363 (1), 345 (3), 327 (5), 309 (1), 391 (1), 211 (6), 210 (6), 209 (5), 193 (4), 192 (1), 191 (4), 183 (4), 182 (1), 143 (81), 125 (100), 111 (88), 109 (15), 107 (26), 94 (72), 93 (82), 67 (21), 66 (19), 65 (23) [1]
ES-MS m/z: 597 $[M + H + Na]^+$ (8), 596 $[M + Na]^+$ (25) [1]
^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.15 (br d, J = 8.6, Ha-2), 4.23 (br s, He-3), 3.00 (dd, J = 13.4, 3.8, H-5), 6.19 (d, J = 2.0, H-7), 3.53 (m, H-9), 2.90 (t, J = 9.4, H-17), 1.04 (s, CH_3-18), 1.02 (s, CH_3-19), 1.50 (s, CH_3-21), 5.58 (br d, J = 8.9, H-24), 1.42 (s, CH_3-26), 1.44 (s, CH_3-27), 13.30 (br s, H′-1), 7.28 (m, H′-3), 6.40 (m, H′-4), 7.28 (m, H′-5) [1]
^{13}C NMR (75.5 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-12	31.7	C-23	25.0
2	68.1	13	47.3	24	80.6
3	68.0	14	84.3	25	71.7
4	32.4	15	31.4	26	27.3
5	51.3	16	21.9	27	26.9
6	203.5	17	53.0	COO	161.9
7	121.5	18	17.8	C-2′	123.9
8	166.1	19	24.3	C-3′	115.9
9	34.3	20	74.0	C-4′	110.2
10	38.5	21	25.6	C-5′	124.1
11	20.9	22	41.7		

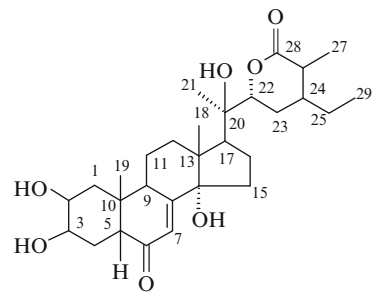
Pharm./Biol.: *Musca domestica* assay: 84% (20-hydroxyecdysone-100%) [1].

References

1. A. Suksamrarn, C. Sommechai, P. Charulpong, B. Chitkul, Phytochemistry **38**, 473 (1995)

Capitasterone

CAS Registry Number: 20835-65-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Cyathula capitata* [1]
$C_{29}H_{44}O_7$: 504.3087
Mp: 234–235°C [1]
IR (KBr) ν_{max} cm^{-1}: 1730, 1644 [1]
UV λ_{max}^{EtOH} nm: 242 [1]
EI-MS m/z: 504 $[M]^+$, 363, 345, 327, 141 $[M-363]^+$ [1]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 5.06 (ddd, Ha-2), 5.34 (ddd, He-3), 5.89 (d, H-7), 3.12 (ddd, Ha-9), 1.13 (s, CH_3-18), 1.07 (s, CH_3-19), 1.47 (s, CH_3-21), 4.20 (dd, H-22), 1.31 (d, CH_3-26), 0.72 (t, CH_3-27) [1]

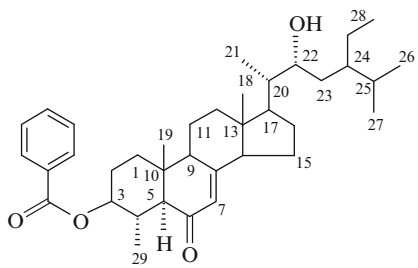
Pharm./Biol.: *Sarcophaga* biotest: high activity [1].

References

1. T. Takemoto, K. Nomoto, Y. Hikino, H. Hikino, Tetrah. Lett. **47**, 4929 (1968)

Carpesterol

CAS Registry Number: 31077-78-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Solanum xanthocarpum* [1]

$C_{37}H_{54}O_4$: 562.4022

Mp: 251°C (acetone-EtOH) [1, 2]

$[\alpha]_D^{27}$ + 67° (c, 0.716) [1, 2]

IR ($CHCl_3$) ν_{max} cm^{-1}: 3590, 1710, 1677, 1632, 1607, 1587 [2]

UV λ_{max}^{EtOH} nm (ε): 233 (19400) [2]

EI-MS m/z: 562 $[M]^+$ (9), 544 $[M\text{-}H_2O]^+$ (16), 529 $[M\text{-}H_2O\text{–}CH_3]$ + (10), 501 (10), 440 $[M\text{-}PhCOOH]^+$ (65), 422 (22), 403 (19), 312 (100), 297 (18), 257 (69), 109 (45), 105 (88) [2]

ORD (c, 0.014, MeOH): $[\varphi]_{600}$ + 400, $[\varphi]_{350}$ + 11500, $[\varphi]_{295}$ − 24500, $[\varphi]_{261}$ − 44500, $[\varphi]_{230}$ + 47600 [2]

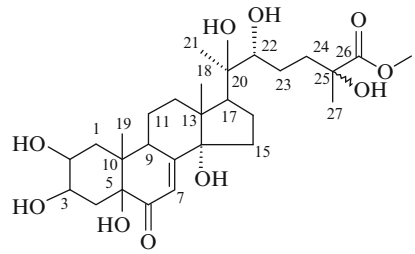
^{1}H NMR (C_5D_5N): 4.71 (br, H-3), 5.71 (s, H-7), 3.76 (br d, H-22), Ar: 7.30–8.20 (m, 5H) [2]

References

1. Y.H. Tsay, J.V. Silverton, J.A. Beisler, Y. Sato, J. Am. Chem. Soc. **92**, 7005 (1970)
2. J.A. Beisler, Y. Sato, J. Org. Chem. **36**, 3946 (1971)

Carthamasterone A

CAS Registry Number: 203513-39-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum carthamoides* [1]

$C_{28}H_{44}O_{10}$: 540.2934

Mp: 170–172°C (MeOH-EtOAc) [1]

$[\alpha]_D^{26}$ + 18.8° (c 0.09, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3405, 1710, 1674, 1202, 1138 [1]

UV λ_{max}^{EtOH} nm (log ε): 245 (4.01) [1]

EI-MS m/z: 494 (0.2), 478 (0.2), 477 (0.6), 459 (40), 446 (1), 441 (1), 425 (11), 422 (11), 409 (13), 379 (37), 361 (60), 343 (60), 326 (100), 325 (80), 317 (37), 316 (60), 99 (82), 81 (60) [1]

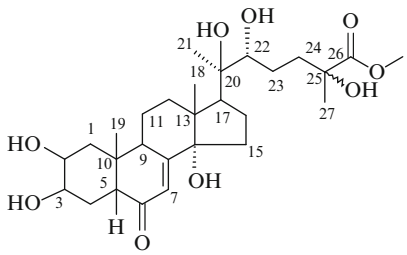
^{1}H NMR (100 MHz, C_5D_5N): 4.0–4.3 (m, Ha-2), 4.0–4.3 (m, He-3), 6.26 (br m, H-7), 3.58 (m, H-9), 1.20 (s, CH_3-18), 1.15 (s, CH_3-19), 1.59 (s, CH_3-21), 3.88 (m, H-22), 1.49 (s, CH_3-27), 3.75 (s, $COOCH_3$) [1]

References

1. N.Sh. Ramazanov, E.S. Maksimov, Z. Saatov, A.U. Mamathanov, N.D. Abdullaev, Chem. Nat. Comp. **33**, 301 (1997)

Carthamasterone B

CAS Registry Number: 86583-59-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum carthamoides* [1]

$C_{28}H_{44}O_9$: 524.2985

Mp: 179–182°C (MeOH-EtOAc) [1]

IR (KBr) ν_{max} cm^{-1}: 3400, 1710, 1670, 1204, 1140 [1]

UV λ_{max}^{EtOH} nm (log ε): 245 (4.00) [1]

EI-MS m/z: 460 $[M\text{-}2H_2O\text{–}CO]^+$ (7.1), 458 (4), 442 (71), 429 (22), 427 (34), 425 (28), 424 (28), 411 (22), 409 (22), 391 (20), 363 (75), 345 (82), 344 (69), 328 (84), 327 (85), 301 (42), 300 (100), 285 (42), 267 (47), 159 (85), 143 (88), 141 (99), 123 (85), 114 (95), 105 (88) [1]

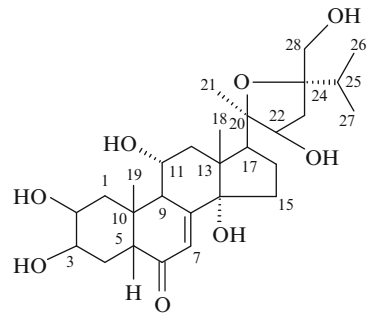
^{1}H NMR (100 MHz, C_5D_5N): 4.0–4.3 (m, Ha-2), 4.0–4.3 (m, He-3), 6.24 (br s, H-7), 3.58 (m, H-9), 1.20 (s, CH_3-18), 1.07 (s, CH_3-19), 1.59 (s, CH_3-21), 3.88 (m, H-22), 1.49 (s, CH_3-27), 3.88 (s, $COOCH_3$) [1]

References

1. N.Sh. Ramazanov, E.S. Maksimov, Z. Saatov, N.D. Abdullaev, Chem. Nat. Comp. **33**, 303 (1997)

Carthamoleusterone

CAS Registry Number: 1042045-39-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{28}H_{44}O_8$: 508.3036

$[\alpha]_D^{20}$ + 213° (c 0.02, EtOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3390, 1658, 1051, 1037 [1]

ESI-MS m/z: 509 $[M + H]^+$, 491 $[M + H\text{–}H_2O]^+$, 473 $[M + H\text{–}2H_2O]^+$, 455 $[M + H\text{–}3H_2O]^+$, 437 $[M + H\text{–}4H_2O]^+$, 419 $[M + H\text{–}5H_2O]^+$, 345, 299, 281, 173, 155, 137 [1]

HR-ESI-MS m/z: for $C_{28}H_{44}O_8Na$ $[M + Na]^+$ calcd. 531.2934, found 531.2943 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 2.60 (dd, J = 4.0, 12.8, Ha-1), 1.37 (dd, J = 11.8, 12.8, He-1), 4.01 (ddd, J = 3.0, 4.0, 11.8, Ha-2), 3.95 (q, J = 3.0, He-3), 1.77 (Ha-4), 1.69 (He-4), 2.33 (dd, J = 4.0, 13.2, H-5), 5.82 (dd, J = 0.7, 2.6, H-7), 3.15 (dd, J = 2.6, 9.2, Ha-9), 4.06 (ddd, J = 5.7, 9.2, 10.9, He-11), 2.24 (dd, J = 10.9, 12.2, Ha-12), 2.14 (dd, J = 5.7, 12.2, He-12), 1.89 (m, Ha-15), 1.54 (He-15), 2.07 (Ha-16), 2.28 (Hb-16), 2.66 (dd, J = 8.2, 9.8, H-17), 0.850 (s, CH_3-18), 1.053 (s, CH_3-19), 1.226 (s, CH_3-21), 3.82 (br d, J = 0.5, 5.6, H-22), 2.34 (dd, J = 5.6, 14.3, Ha-23), 1.87 (dd, J = 0.5, 14.3, Hb-23), 1.81 (H-25), 0.924 (d, J = 7.1, CH_3-26), 0.985 (d, J = 7.0, CH_3-27), 3.62 (d, J = 10.8, Ha-28), 3.54 (d, J = 10.8, Hb-28) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

C-1	39.80	C-11	69.66	C-21	27.60
2	68.94	12	43.87	22	82.62

(*continued*)

Table 1 (continued)

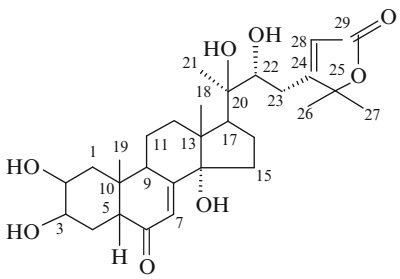
3	68.55	13	49.0	23	41.33
4	33.40	14	84.65	24	89.56
5	52.79	15	32.31	25	40.37
6	206.91	16	23.33	26	18.12
7	122.65	17	52.19	27	18.60
8	166.17	18	19.04	28	64.41
9	42.93	19	24.59		
10	39.11	20	89.72		

References

1. M. Budesinsky, K. Vokas, J. Harmatha, J. Cvacka, Steroids **73**, 502 (2008)

Carthamosterone

CAS Registry Number: 114805-00-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Klaseopsis chinensis* [1], *Leuzea carthamoides* [2, 3]

$C_{29}H_{42}O_8$: 518.2879

IR (KBr) ν_{max} cm^{-1}: 1745 [2], 3400, 1730, 1652 [3]

UV λ_{max}^{MeOH} nm: 210, 242 [2]

CI-MS m/z: 519 $[M + H]^+$, 501, 483, 393, 375, 363, 345 [2]

HR-MS m/z: 519, 2637 $[M + H]^+$ [3]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.80 (dd, Ha-1), 1.44 (dd, Hb-1), 3.83 (ddd, Ha-2), 3.95 (dq, He-3), 1.73 (Ha-4), 1.70 (He-4), 2.39 (dd, H-5), 5.82 (d, H-7), 3.15 (ddd, Ha-9), 1.83 (Ha-11), 1.72 (He-11), 2.15 (Ha-12), 1.90 (He-12), 1.99 (Ha-15), 1.62 (Hb-15), 1.74 (Ha-16), 2.06 (Hb-16), 2.36 (dd, H-17), 0.91 (s, CH_3-18), 0.97 (s, CH_3-19), 1.27 (s, CH_3-21), 3.71 (dd, H-22), 2.58 (ddd, Ha-23), 2.28 (ddd, Hb-23), 1.49 (s, CH_3-26), 1.49 (s, CH_3-27), 5.93 (t, C = CH-28) [3]

^{13}C NMR (125.7 MHz, CD_3OD) [3]:

Table 1

C-1	37.33	C-11	21.52	C-21	21.08
2	68.70	12	32.46	22	75.49
3	68.44	13	49.0	23	30.65
4	32.82	14	85.28	24	174.91
5	51.75	15	31.83	25	89.74
6	206.35	16	21.63	26	25.02
7	122.29	17	50.43	27	24.87
8	167.56	18	18.02	28	115.46
9	35.06	19	24.41	29	178.79
10	39.26	20	77.41		

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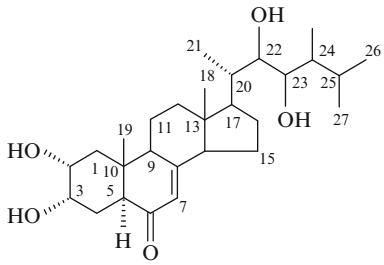
2. J.P. Girault, R. Lafont, E. Varga, Zs. Hajdu, I. Herke, K. Szendrei, Phytochemistry **27**, 737 (1988)
3. K. Vokac, M. Budesinsky, J. Harmata, Coll. Czech. Chem. Comm. **67**, 124 (2002)

Castasterone

CAS Registry Number: 80736-41-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Castanea* [1], *Dolichos lablab, Pharbitis purpurea, Phaseolus vulgaris, Pinus thunbergii* [2, 3]
$C_{28}H_{48}O_5$: 464.3501
Mp: 259–261°C ($CH_3CN–H_2O$) [2]
EI-MS m/z: 403 (0.4), 385 (0.3), 393 (3), 375 (2), 357 (2), 364 (100), 363 (35), 362 (36), 346 (42), 345 (59), 327 (36), 315 (7), 305 (5), 287 (17), 269 (10), 263 (11), 245 (13), 227 (5), 155 (5) [2]
FAB-MS m/z: 465 $[M + H]^+$ (base peak), 447 $[M + H–H_2O]^+$, 429 $[M + H–2H_2O]^+$, 393 $[C_{23}H_{37}O_5]^+$, 364 $[C_{27}H_{36}O_4]^+$, 155 $[C_8H_{11}O_3]^+$ [2]
CD (c, MeOH): $[\theta]_{292} - 5.475 \times 10^3$ [3]
^{1}H NMR (400 MHz, J/Hz, $CDCl_3$): 3.77 (br, H-2), 4.06 (br, H-3), 2.69 (dd, J = 13.0, 4.0, H-5), 0.69 (s, CH_3-18), 0.76 (s, CH_3-19), 3.56 (d, J = 9.0, H-22), 3.72 (d, J = 9.0, H-23), 0.85, 0.91, 0.95, 0.97 (s, 4 CH_3) [2]
Pharm./Biol.: *Rice-lamina* inclination test: activity [3].

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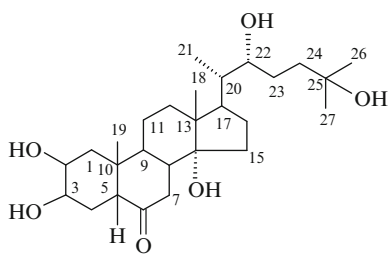
Cheilanthone A

CAS Registry Number: 26152-93-2



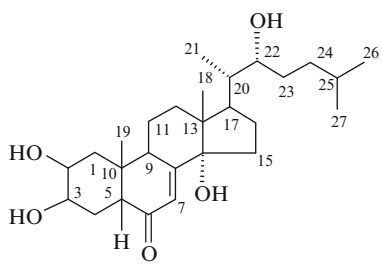
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Cheilanthes tenuifolia* [1]
$C_{27}H_{46}O_6$: 466.3294
Mp: 235–238°C [1]
IR (KBr) ν_{max} cm^{-1}: 1684 [1]
EI-MS m/z: 448 $[M-H_2O]^+$, 430, 412, 394, 379, 332, 302, 99, 81 [1]
^{1}H NMR (J/Hz, C_5D_5N): 0.83 (s, CH_3-18), 1.01 (s, CH_3-19), 1.24 (d, J = 6.0, CH_3-21), 1.36 (s, CH_3-26), 1.36 (s, CH_3-27) [1]
Pharm./Biol.: *Calliphora stygia* bioassay: up to 0.6 μg inactive [1].

References

1. A. Faux, M.N. Galbraith, D.H.S. Horn, E.J. Middleton, J.A. Thompson, J. Chem. Soc. Chem. Comm. **4**, 243 (1970).

Cheilanthone B

CAS Registry Number: 26130-75-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Cheilanthes tenuifolia* [1], *Ch. mysurensis* [2]
$C_{27}H_{46}O_5$: 450.3345
Mp: 225–228°C [1], 234–235°C [2]
$[\alpha]_D^{20}$ − 25.9° (c, MeOH) [2]
IR (KBr) ν_{max} cm^{-1}: 1684 [1], 3636 [2]
EI-MS m/z: 450 $[M]^+$, 432, 414, 396, 381, 332, 302 [1], 450 $[M]^+$ (2.5), 432 $[M-H_2O]^+$ (9.5), 417 (1),

414 $[M\text{-}2H_2O]^+$ (7), 399 (1.5), 396 $[M\text{-}3H_2O]^+$ (1), 381 $[M\text{-}3H_2O\text{–}CH_3]^+$ (0.5), 350 $[M\text{-}C_{22}\text{–}C_{27}]^+$ (3.5), 332 $[M\text{-}C_{22}\text{–}C_{27}\text{–}H_2O]^+$ (21), 302 $[M\text{-}C_{20}\text{–}C_{27}]^+$ (25), 101 (5.5), 83 (61), 69 (57), 55 (100), 41 (78) [2]

^{1}H NMR (J/Hz, C_5D_5N): 0.85 (s, CH_3-18), 1.03 (s, CH_3-19), 1.24 (d, J = 6.0, CH_3-21), 0.84 (d, J = 6.0, CH_3-26), 0.84 (d, J = 6.0, CH_3-27) [1]

Pharm./Biol.: *Calliphora stygia*: up to 0.6 µg inactive [1].

References

1. A. Faux, M.N. Galbraith, D.H.S. Horn, E.J. Middleton, J.A. Thompson, J. Chem. Soc. Chem. Comm. **4**, 243 (1970)
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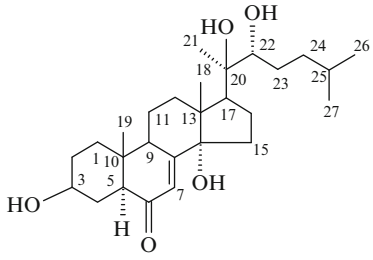
Cyanosterone A

CAS Registry Number: 476645-89-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotis arachnoidea* [1]

$C_{27}H_{44}O_5$: 448.3188

Mp: 272–274°C [1]

$[\alpha]_D^{20}$ + 12.7° (c, MeOH) [1]

UV λ_{max}^{MeOH} nm: 242.8 [1]

ESI-MS m/z: 449 $[M + H]^+$ [1]

^{1}H NMR (J/Hz, C_5D_5N): 3.80 (m, H-3), 2.21 (m, H-5), 6.20 (br s, H-7), 3.03 (ddd, H-9), 1.23 (s, CH_3-18), 0.92 (s, CH_3-19), 1.59 (s, CH_3-21), 0.82 (d, J = 3.3, CH_3-26), 0.82 (d, J = 3.3, CH_3-27) [1]

^{13}C NMR (C_5D_5N):

Table 1

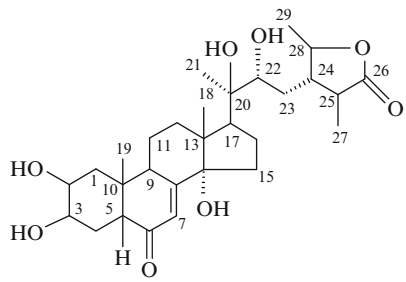
C-1	37.3	C-10	38.7	C-19	13.1
2	30.3	11	21.1	20	76.8
3	70.1	12	31.9	21	21.6
4	31.5	13	47.9	22	76.8
5	53.9	14	83.9	23	30.0
6	200.2	15	31.7	24	37.2
7	122.9	16	21.4	25	28.2
8	165.1	17	50.1	26	23.3
9	46.6	18	17.9	27	22.4

References

1. C.Y. Tan, Z. Li, X. Li, J. Asian Nat. Prod. Res. **5**, 237 (2003)

Cyasterone

CAS Registry Number: 17086-76-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga australis, A. bracteosa* [1], *A. chamapitys* [2], *A. chameacistus* [3], *A. chia* [4], *A. decumbens* [5], *A. japonica* [6], *A. incise* [5], *A. iva* [7–9], *A. linearifolia* [1], *A. macrosperma* var. *breviflora* [10], *A. multiflora* [11], *A. nipponensis* [5, 12], *A. remota* [3], *A. reptans* [13], *A. reptans var. atropurpurea* [14], *A. taiwanensis* [15], *A. turkestanica* [16], *Cyathyla*

capitata [17, 18], *C. officinalis* [19], *Eriophyton wallchii* [20], *Pteris cretica* [5]

$C_{29}H_{44}O_8$: 520.3036

Mp: 160–162°C [4, 5], 158–160°C (MeOH) [16], 164–166°C [17, 18], 162–164°C (MeOH) [19]

$[\alpha]_D^{27}$ + 61.3° (c 1.00, H_2O) [4], $[\alpha]_D^{20}$ + 60.0 ± 3° (c 1.00, Pyridine) [16], $[\alpha]_D$ + 64.5° (c 8.6, Pyridine) [17, 18]

IR (KBr) ν_{max} cm^{-1}: 3450, 1750, 1650 [4, 18], 3450, 1750, 1660 [5], 3450, 1752, 1660 [16]

UV λ_{max}^{EtOH} nm: 243 (log ε 4.10) [4], 243 (ε 12000) [5], 245 (log ε 4.05) [16], 243 (log ε 4.11) [18]

UV λ_{max}^{MeOH} nm (log ε): 241.4 (4.11) [19]

EI-MS m/z: 520 $[M]^+$ (0.4), 505 $[M\text{-}CH_3]^+$(0.2), 502 $[M\text{-}H_2O]^+$ (18.6), 487 $[M\text{-}CH_3\text{–}H_2O]^+$ (1), 484 $[M\text{-}2H_2O]^+$ (16), 469 $[M\text{-}CH_3\text{–}2H_2O]^+$ (7), 466 $[M\text{-}3H_2O]^+$ (13), 451 $[M\text{-}CH_3\text{–}3H_2O]^+$ (7), 448 $[M\text{-}4H_2O]^+$ (4), 433 $[M\text{-}CH_3\text{–}4H_2O]^+$ (8), 430 (1), 363 (7), 345 (29), 327 (30), 300 (17), 201 (9), 183 (28), 157 (45) [4, 18], 520, 502, 484, 469, 466, 451, 448, 433, 415, 363, 345, 327, 300, 183, 157 [16]

FAB-HR-MS m/z: for $C_{31}H_{51}O_{11}$ $[M + H]^+$ calcd. 647.3431, found 647.3425 [19]

CD (c, 0.100, dioxane): $[\theta]_{338}$ + 4.3x10^3 [17, 18]

ORD (c, 0.100, dioxane): $[\varphi]_{359}^{peak}$ + 3400, $[\varphi]_{308}^{trough}$ − 3100 [18]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.16 (Ha-2), 4.22 (He-3), 3.01 (H-5), 6.31 (H-7), 3.59 (H-9), 2.65 (H-12), 2.86 (H-17), 1.24 (s, CH_3-18), 1.07 (s, CH_3-19), 1.57 (s, CH_3-21), 3.94 (H-22), 1.36 (s, CH_3-27), 4.03 (dd, J = 6.0, 9.3, H-28), 1.31 (d, J = 6.0, CH_3-29) [12]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 6.15 (H-7), 1.11 (s, CH_3-18), 0.94 (s, CH_3-19), 1.44 (s, CH_3-21), 1.24 (d, J = 6.0, CH_3-27), 1.24 (d, J = 6.0, CH_3-29) [16]

^{1}H NMR (J/Hz, C_5D_5N): 3.80–4.10 (m, H-2), 4.12 (br s, H-3), 6.28 (d, J = 2.0, H-7), 3.50 (br q, J = 3.5, H-9), 1.19 (s, CH_3-18), 1.06 (s, CH_3-19), 1.51 (s, CH_3-21), 3.80–4.10 (m, H-22), 1.33 (d, J = 6.0, CH_3-27), 3.80–4.10 (m, H-28), 1.33 (d, J = 6.0, CH_3-29) [18]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.94 (Ha-1), 2.15 (dd, J = 4.2, 13.5, He-1), 4.16 (br d, J = 10.1, Ha-2), 4.22 (br s, He-3), 1.81 (Ha-4), 2.04 (He-4), 3.01 (dd, J = 3.4, 13.7, H-5), 6.28 (d, J = 2.1, H-7), 3.61 (br t, J = 8.8, H-9), 1.78 (Ha-11), 1.93 (He-11), 2.65 (td, J = 4.8, 12.8, Ha-12), 2.07 (He-12), 1.80 (Ha-15), 2.22 (Hb-15), 2.48 (m, Ha-16), 2.07 (Hb-16), 2.87 (t, J = 9.2, H-17), 1.25 (s, CH_3-18), 1.08 (s, CH_3-19), 1.58 (s, CH_3-21), 3.95 (br d, J = 9.8, H-22), 1.73 (Ha-23), 1.94 (Hb-23), 2.23 (H-24), 2.39 (dq, J = 7.1, 10.9, H-25), 4.03 (dq, J = 6.1, 9.3, H-28), 1.37 (d, J = 7.1, CH_3-27), 1.33 (d, J = 6.1, CH_3-29) [19]

^{13}C NMR (75 MHz, C_5D_5N) [12]: **^{13}C NMR** ($CDCl_3$) [13]:

Table 1

C-1	39.0 (t)	C-16	21.3 (t)	C-1	37.9	C-16	21.0
2	68.1 (d)	17	50.0 (d)	2	68.0	17	50.0
3	68.0 (d)	18	17.9 (q)	3	68.0	18	17.8
4	32.5 (t)	19	24.5 (q)	4	32.0	19	24.4
5	51.4 (d)	20	76.8 (s)	5	51.3	20	76.7
6	203.4 (s)	21	21.0 (q)	6	203.7	21	21.1
7	121.8 (d)	22	73.9 (d)	7	122.2	22	73.9
8	165.8 (s)	23	34.4 (t)	8	166.1	23	34.4
9	34.5 (d)	24	46.6 (d)	9	34.8	24	48.1
10	38.7 (s)	25	42.4 (d)	10	38.6	25	42.2
11	21.1 (t)	26	179.2 (s)	11	21.3	26	179.3
12	32.0 (t)	27	15.9 (q)	12	31.8	27	15.8
13	48.2 (s)	28	79.8 (d)	13	48.7	28	79.8
14	84.1 (s)	29	19.3 (q)	14	84.1	29	19.3
15	31.9 (t)			15	32.4		

^{13}C NMR (125 MHz, C_5D_5N) [20]:

Table 2

C-1	38.0	C-11	21.0	C-21	21.0
2	68.1	12	32.1	22	74.1
3	68.0	13	48.2	23	34.5
4	32.5	14	84.1	24	48.8
5	51.4	15	31.9	25	42.5
6	203.4	16	21.4	26	179.1
7	121.8	17	50.1	27	15.9
8	165.7	18	17.9	28	79.9
9	34.5	19	24.5	29	19.4
10	38.7	20	76.8		

Pharm./Biol.: *Chilo dipping* biotest: activity [5], *Musca domestica* bioassay: show that the activity of cyasterone is of the same order as that of 20-hydroxyecdysone [17], *Sarcophaga* bioassay: show activity as that of 20-hydroxyecdysone [18], showed potential antitumor-promoting activities on

Epstein-Barr virus early antigen (EBV-EA) induction [21], *Galleria mellonella* bioassay: ED_{50} = 3.75 μg/g, *Sarcophaga bullata* bioassay: ED_{50} = 10.4 μg/g, *Dermestes vulpinus* bioassay: ED_{50} = 21.0 μg/g [22], *Drosophila melanogaster* B_{II} bioassay: EC_{50} = 1.2, 5.3 × 10^{-8} M [23, 24].

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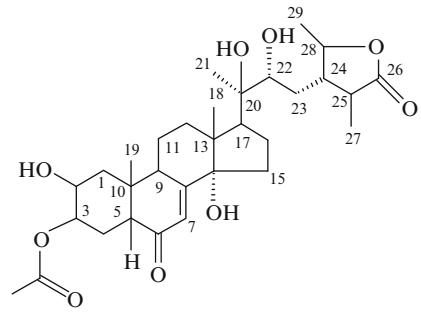
Cyasterone-3-Acetate

CAS Registry Number: 164220-24-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{31}H_{46}O_9$: 562.3142

TSP-MS m/z: 580 $[M + NH_4]^+$ (88), 563 $[M + H]^+$ (51), 562 $[M]^+$ (100), 545 $[M + H–H_2O]^+$ (69), 520 $[M + NH_4–CH_3COOH]^+$ (27), 502 $[M-CH_3COOH]^+$ (38) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.29 (br m, Ha-2), 5.50 (br m, He-3), 2.67 (dd, J = 4.2, 13.2, H-5), 6.28 (d, J = 2.4, H-7), 3.59 (br t, H-9), 2.87 (br t, J = 9.0, H-17), 1.25 (s, CH_3-18), 1.09 (s, CH_3-19), 1.58 (s, CH_3-21), 3.95 (br, H-22), 2.38 (dq, J = 6.9, 11.1, H-25), 1.37 (d, J = 6.9, CH_3-27), 4.01 (dq, J = 6.0, 9.3, H-28), 1.31 (d, J = 6.0, CH_3-29), 1.97 (s, CH_3COO -3) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	38.74	C-11	21.09	C-21	21.01
2	66.10	12	31.91	22	73.99
3	71.29	13	48.17	23	34.52
4	29.65	14	84.11	24	48.70
5	51.95	15	32.01	25	42.46
6	202.13	16	21.36	26	179.18
7	121.65	17	49.66	27	15.94
8	166.21	18	17.91	28	79.83
9	34.41	19	24.28	29	19.35
10	38.62	20	76.77	CH_3COO CH_3COO	21.09, 170.57

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.3 \times 10^{-7}$M [2, 3].

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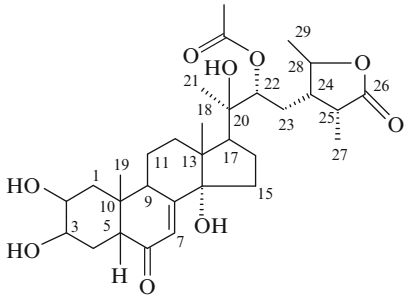
Cyasterone-22-Acetate

CAS Registry Number: 67883-31-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga nipponensis* [1], *A. taiwanensis* [2], *A. turkestanica* [3]

$C_{31}H_{46}O_9$: 562.3141

Mp: 212–214°C [2], 212–215°C (acetone-hexane) [3]

$[\alpha]_D^{25}$ + 111.7° (c 0.01, $CHCl_3$) [2]

$[\alpha]_D^{29}$ + 96 ± 2° (c 0.56, MeOH) [3]

IR (KBr) ν_{max} cm^{-1}: 3382, 1769, 1735, 1655, 1259, 1188, 1042 [2], 3440, 1745, 1655 [3]

UV λ_{max}^{MeOH} nm (log ε): 241 (4.02) [2]

UV λ_{max}^{EtOH} nm (log ε):, 240 (4.07) [3]

EI-MS m/z: 544 $[M\text{-}H_2O]^+$ (1), 526 $[M\text{-}2H_2O]^+$ (2), 516 $[M\text{-}H_2O\text{–}CO]^+$ (1), 508 $[M\text{-}3H_2O]^+$ (1), 498 $[M\text{-}2H_2O\text{–}CO]^+$ (12), 484 $[M\text{-}AcOH\text{–}H_2O]^+$ (16), 466 $[M\text{-}AcOH\text{–}2H_2O]^+$ (85), 456 (16), 451 (14), 448 (8), 433 (11), 377 (5), 371 (12), 363 (3), 360 (10), 359 (16), 353 (10), 345 (5), 327 (8), 301 (10), 300 (13), 299 (11), 250 (10), 249 (11), 183 (22), 139 (19), 69 (42), 60 (14), 43 (100) [3]

FAB-MS m/z: 563 $[M + H]^+$ (5), 545 (6), 544 (2), 526 (3), 517 (2), 508 (3), 498 (2), 484 (2), 466 (2), 456 (2), 451 (3), 448 (4), 433 (3), 377 (4), 371 (26), 363 (7), 360 (3), 353 (5), 345 (5), 327 (5), 301 (7), 300 (5), 299 (6), 250 (7), 249 (11), 183 (15), 139 (33), 119 (100) [2]

HR-FAB-MS m/z: for $C_{31}H_{47}O_9$ $[M + H]^+$ calcd. 563.3220, found 563.3218 [2]

CD (c, MeOH): Δε = +1.27 (340 nm), Δε = −0.66 (288 nm) [3]

CD (dioxane): $[\theta]_{361} + 2.822x10^3$, $[\theta]_{260} + 2.515x10^3$, a = +53 [3]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.15 (dm, J = 13.8, Ha-2), 4.21 (br s, He-3), 3.01 (dd, J = 3.6, 12.2, H-5), 6.26 (d, J = 2.1, H-7), 3.58 (br m, H-9), 2.63 (H-12), 2.83 (t, J = 8.4, H-17), 1.18 (s, CH_3-18), 1.06 (s, CH_3-19), 1.57 (s, CH_3-21), 5.47 (br d, J = 10.5, H-22), 1.44 (d, J = 7.2, CH_3-27), 3.96 (dq, J = 6.0, 8.7, H-28), 1.32 (d, J = 6.0, CH_3-29), 2.04 (s, CH_3COO -22) [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 2.32–2.12 (m, Ha-1), 2.04–1.60 (m, He-1), 4.23 (br s, Ha-2), 4.16 (br d, J = 9.2, He-3), 2.04–1.60 (m, H-4), 3.02 (dd, J = 3.2, 12.8, H-5), 6.27 (d, J = 2.0, H-7), 3.60 (t, J = 8.4, H-9), 2.04–1.60 (m, H-11), 2.68–2.57 (m, Ha-12), 2.04–1.60 (m, He-12), 2.32–2.12 (m, Ha-15), 2.04–1.60 (m, Hb-15), 2.68–2.57 (m, Ha-16), 2.32–2.12 (m, Hb-16), 2.84 (t, J = 9.2, H-17), 1.19 (s, CH_3-18), 1.07 (s, CH_3-19), 1.58 (s, CH_3-21), 5.47 (d, J = 10.4, H-22), 2.04–1.60 (m, H-23), 2.04–1.60 (m, H-24), 2.32–2.12 (m, H-25), 1.45 (d, J = 7.2, CH_3-27), 4.00 (qd, J = 6.4, 6.4, H-28), 1.33 (d, J = 6.4, CH_3-29), Other: 2.06 (s, CH_3COO -22), 6.15 (br s, OH-2) [2]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.05 (s, Ha-2), 4.05 (He-3), 6.12 (s, H-7), 3.44 (m, Ha-9), 0.95 (s, CH_3-18), 1.06 (s, CH_3-19), 1.47 (s, CH_3-21), 1.21 (s, CH_3-27), 3.90 (m, H-28), 1.32 (s, CH_3-29), 1.94 (s, CH_3COO) [3]

^{13}C NMR (75 MHz, C_5D_5N) [1]: **^{13}C NMR** (100 MHz, C_5D_5N) [2]:

Table 1

C-1	37.9 (t)	C-16	21.0 (t)	C-1	38.0	C-16	21.6
2	68.1 (d)	17	50.3 (d)	2	68.1	17	50.3

(*continued*)

Table 1 (continued)

3	68.0 (d)	18	17.8 (q)	3	68.1	18	17.9
4	32.0 (t)	19	24.4 (q)	4	32.5	19	24.5
5	51.3 (d)	20	76.1 (s)	5	51.4	20	76.2
6	203.3 (s)	21	21.2 (q)	6	203.4	21	21.8
7	121.9 (d)	22	76.8 (d)	7	122.0	22	76.9
8	165.5 (s)	23	29.9 (t)	8	165.6	23	33.3
9	34.3 (d)	24	48.0 (d)	9	34.4	24	48.2
10	38.7 (s)	25	42.7 (d)	10	38.8	25	42.8
11	21.5 (t)	26	178.7 (s)	11	21.1	26	178.7
12	31.8 (t)	27	15.6 (q)	12	32.1	27	15.7
13	48.2 (s)	28	79.2 (d)	13	48.1	28	79.3
14	84.1 (s)	29	18.9 (q)	14	84.2	29	19.0
15	32.4 (t)	$\underline{CH_3COO}$	21.7 (q)	15	31.9	$\underline{CH_3COO}$	21.3
		$\underline{CH_3COO}$	170.8 (s)			$\underline{CH_3COO}$	170.9

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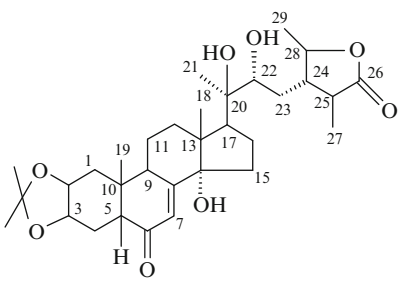
2. Y.Y. Chan, T.Sh. Wu, C.S. Kuoh, A.G. Damu, Chem. Pharm. Bull. **53**, 836 (2005)
3. B.Z. Usmanov, Y.V. Rashkes, N.K. Abubakirov, Chem. Nat. Comp. **14**, 514 (1978)

Cyasterone-2,3-Acetonide

CAS Registry Number: 860303-32-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyathula officinalis* [1]

$C_{32}H_{48}O_8$: 560.3349

Mp: 241–243°C [1]

$[\alpha]_D^{25}$ + 30.9° (c 0.11, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3456, 1752, 1643 [1]

UV λ_{max}^{MeOH} nm (log ε): 243 (3.95) [1]

ESI-MS m/z: 559 $[M-H]^-$; 583 $[M + Na]^+$, 1143 $[2M + Na]^+$ [1]

HR-ESI-MS m/z: for $C_{32}H_{47}O_8$ $[M-H]^-$calcd. 559.3270, found 559.3251 [1]

^{1}H NMR (J/Hz, C_5D_5N/Me_2CO-d_6): 4.16 (m, Ha-2), 4.18 (br s, He-3), 2.27 (d, J = 11.6, H-5), 5.84 (d, J = 2.0, H-7), 3.03 (t, J = 8.4, H-9), 2.18 (q, J = 10.8, Ha-16), 2.56 (t, J = 9.2, H-17), 1.00 (s, CH_3-18), 0.98 (s, CH_3-19), 1.45 (s, CH_3-21), 3.70 (d, J = 10.0, H-22), 2.42 (dq, J = 10.8, 6.8, H-25), 1.26 (d, J = 6.8, CH_3-27), 4.10 (dq, J = 9.6, 6.4, H-28), 1.38 (d, J = 6.4, CH_3-29), Other: 1.27 and 1.31 (s, 2,3-iPr) [1]

^{13}C NMR (C_5D_5N/Me_2CO-d_6) [1]: **^{13}C NMR** ($CDCl_3$) [1]:

Table 1

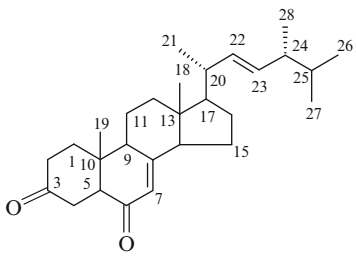
C-1	37.9	C-16	20.5	C-1	37.6	C-16	20.3
2	72.5	17	49.7	2	72.1	17	48.9
3	72.1	18	17.5	3	71.6	18	17.4
4	26.8	19	23.6	4	26.7	19	23.6
5	51.5	20	76.6	5	50.8	20	77.0
6	201.7	21	21.0	6	202.6	21	20.4
7	121.2	22	74.0	7	121.7	22	73.2
8	164.4	23	34.1	8	162.6	23	33.7
9	34.9	24	48.2	9	34.4	24	47.7
10	38.2	25	42.3	10	37.8	25	42.3
11	21.0	26	178.6	11	20.5	26	179.1
12	31.3	27	15.4	12	31.3	27	15.7
13	49.0	28	79.8	13	48.2	28	80.1
14	84.1	29	19.2	14	84.5	29	19.6
15	31.9	2,3-iPr	28.5, 26.3, 108.1	15	31.7	2,3-iPr	28.5, 26.4, 108.4

References

1. R. Zhou, B.G. Li, G.L. Zhang, J. Asian Nat. Prod. Res. **7**, 245 (2005)

Cyathisterone

CAS Registry Number: 159813-67-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Calvatia cyathiformis* [1]

$C_{28}H_{42}O_2$: 410.3185

Mp: 200–203°C (n-hexane) [1]

$[\alpha]_D^{25}$ + 12° (c 0.17, $CHCl_3$) [1]

IR (KBr) ν_{max} cm^{-1}: 1720, 1660 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (4.45) [1]

EI-MS m/z: 410 $[M]^+$ (14), 285 $[M\text{-}C_9H_{17}]^+$ (12), 259 (23), 109 (43) [1]

HR-MS m/z: for $C_{28}H_{42}O_2$ $[M + H]^+$ calcd. 410.3185, found 410.3193 [1]

^{1}H NMR (300 MHz, J/Hz, $CDCl_3$): 2.56 (dd, J = 4.0, 15.5, Ha-4), 2.60 (dd, J = 12.5, 15.5, He-4), 2.66 (dd, J = 4.0, 12,5, H-5), 5.78 (br t, J = 2.2, H-7), 0.65 (s, CH_3-18), 1.07 (s, CH_3-19), 1.05 (d, J = 6.6, CH_3-21), 5.17 (dd, J = 7.7, 15.3, H-22), 5.27 (dd, J = 7.8, 15.3, H-23), 0.83 (d, J = 6.8, CH_3-26), 0.84 (d, J = 6.7, CH_3-27), 0.92 (d, J = 6.8, CH_3-28) [1]

^{13}C NMR (75 MHz, $CDCl_3$) [1]:

Table 1

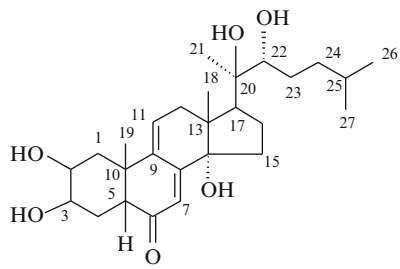
C-1	38.3 (t)	C-11	22.1 (t)	C-21	21.2 (q)
2	37.4 (t)	12	38.8 (t)	22	135.4 (d)
3	211.7 (s)	13	44.7 (s)	23	133.1 (d)
4	37.2 (t)	14	56.0 (d)	24	43.0 (d)
5	54.8 (d)	15	22.7 (t)	25	33.2 (d)
6	199.0 (s)	16	28.0 (t)	26	20.0 (q)
7	123.3 (d)	17	56.3 (d)	27	19.7 (q)
8	164.4 (s)	18	12.7 (q)	28	17.7 (q)
9	49.9 (d)	19	12.9 (q)		
10	38.5 (s)	20	40.4 (d)		

References

1. N. Kawahara, S. Sekita, M. Satake, Phytochemistry **37**, 213 (1994)

Dacryhainansterone (5-Deoxykaladasterone)

CAS Registry Number: 83921-17-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Asparagus filicinus* [1], *Dacrydium pierrei* [2], *Leuzea carthamoides* [3, 4], *Serratula coronata* [5]

$C_{27}H_{42}O_6$: 462.2981

Mp: 242–245°C [4]

IR (KBr) ν_{max} cm^{-1}: 3200–3550, 2940, 2860, 1620, 1600, 1450, 1445, 1365, 1355, 1290, 1245, 1125, 1105, 1095, 1040, 1020 [4]

UV λ_{max}^{EtOH} nm: 298, 235 [3, 4]

CI-MS m/z: 463 $[M + H]^+$, 445, 427, 361, 343, 325 [3]; 462 $[M]^+$ [4]

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.70 (Ha-1), 2.10 (Hb-1), 3.72 (m, Ha-2), 3.84 (m, He-3), 1.60 (Ha-4), 1.78 (He-4), 2.40 (H-5), 5.75 (br s, H-7), 6.3 (ddd, J = 6.5, 2.0, 2.0, Ha-11), 2.72 (br d, J = 18.0, Ha-12), 2.42 (He-12), 2.05 (Ha-16), 1.75 (Hb-16), 2.45 (H-17), 0.89 (s, CH_3-18), 1.10 (s, CH_3-19), 1.18 (s, CH_3-21), 3.33 (dd, J = 11.0, 2.0, H-22), 1.35 (Ha-23), 1.55 (Hb-23), 1.55 (H-25), 0.91 (d, J = 6.5, CH_3-26), 0.94 (d, J = 6.5, CH_3-27) [4]

^{13}C NMR (100 MHz, CD_3OD) [5]:

Table 1

C-1	36.2	C-10	39.4	C-19	30.0
2	67.4	11	132.4	20	76.2
3	66.9	12	37.7	21	19.3
4	35.0	13	47.0	22	76.6
5	50.2	14	83.1	23	29.1
6	204.0	15	30.0	24	36.0
7	117.8	16	20.3	25	27.8
8	162.2	17	49.1	26	21.3
9	145.0	18	16.7	27	21.9

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 5.2 \times 10^{-10}$M [6–8].

References

1. J. Wu, H. Wang, W. Ye, X. Zuo, S. Zhao. Zhongguo yaoke Daxue Xuebao **37**, 487 (2006)
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3. J.P. Girault, R. Lafont, E. Varga, Zs. Hajdu, I. Herke, K. Szendei, Phytochemistry **27**, 737 (1988)
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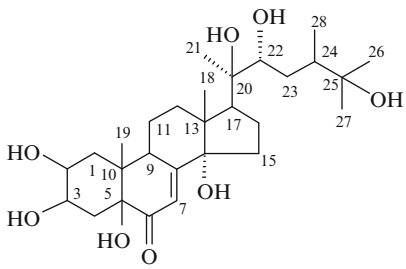
8. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

Dacrysterone

CAS Registry Number: 50299-45-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Dacrydium intermedium* [1]

$C_{28}H_{46}O_8$: 510.3192

Mp: 283–285°C [1]

IR (KBr) ν_{max} cm^{-1}: 1690 [1]

UV λ_{max}^{EtOH} nm (ε): 240 (11000) [1]

EI-MS m/z: 492 $[M\text{-}H_2O]^+$ (1), 474 (2), 456 (3), 438 (3), 379 (50), 361 (47), 343 (23), 325 (25), 189 (20), 140 (22), 131 (13), 113 (100), 105 (26), 95 (66), 93 (20), 91 (25), 85 (28), 83 (23),81 (23), 70 (95) [1]

CD (c, 0.02, dioxane): $[\theta]_{370}$ =0, $[\theta]_{328}$ +9282, $[\theta]_{275–285}$ =0, $[\theta]_{253}$ −16700, $[\theta]_{240}$ =0 [1]

^{1}H NMR (J/Hz, C_5D_5N): 1.22 (s, CH_3-18), 1.15 (s, CH_3-19), 1.56 (s, CH_3-21), 1.32 (s, CH_3-26), 1.32 (s, CH_3-27), 1.07 (d, J = 6, CH_3-28) [1]

^{13}C NMR (C_5D_5N) [2]:

Table 1

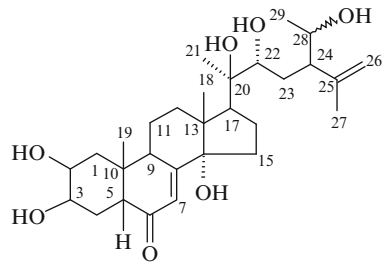
C-1	34.7	C-11	21.2	C-21	21.5
2	67.9	12	31.6	22	74.7
3	69.7	13	48.1	23	34.5
4	35.8	14	84.0	24	41.7
5	79.7	15	32.0	25	72.1
6	200.7	16	22.0	26	26.4
7	119.8	17	49.8	27	28.2
8	166.8	18	17.8	28	15.3
9	38.2	19	17.0		
10	44.7	20	76.9		

References

1. G.B. Russel, J.G. Fraser, Aust. J. Chem. **26**, 1805 (1973)
2. J.W. Blunt, G.A. Lane, M.H.G. Munro, G.B. Russel, Aust. J. Chem. **32**, 779 (1979)

Decumbesterone A

CAS Registry Number: 234772-53-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga decumbens* [1]

$C_{29}H_{46}O_7$: 506.3243

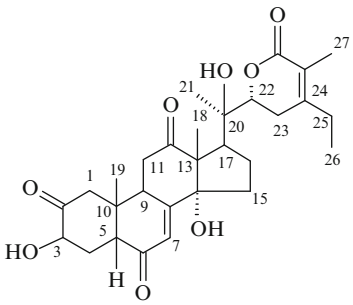
Pharm./Biol.: Cytotoxity bioassay: Showed strong inhibitory effects on *Epstein-Barr* virus early antigen induction [1].

References

1. M. Takasaki, H. Tokuda, H. Nishino, T. Konoshima, J. Nat. Prod. **62**, 972 (1999)

2-Dehydroajugalactone

CAS Registry Number: 179308-45-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{29}H_{38}O_8$: 514.2566

IR (KBr) ν_{max} cm^{-1}: 3427, 1716, 1684 [1]

TSP-MS m/z: 532 $[M + NH_4]^+$ (100), 515 $[M + H]^+$ (38), 514 $[M]^+$ (39), 497 $[M + H–H_2O]^+$ (48) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 2.44 (Ha-1), 1.88 (He-1), 4.59 (dd, J = 11.1, 7.5, He-3), 2.46 (Ha-4), 1.87 (He-4), 3.00 (dd, J = 13.5, 4.3, H-5), 6.39 (d, J = 2.7, H-7), 3.73 (ddd, J = 9.3, 9.2, 2.7, H-9), 2.88 (cs, 2H, Hab-11), 2.58 (Ha-16), 2.04 (Hb-16), 3.43 (br t, J = 9.0, H-17), 1.50 (s, CH_3-18), 1.24 (s, CH_3-19), 1.66 (s, CH_3-21), 4.44 (dd, J = 13.0, 3.5, H-22), 2.47 (Ha-23), 2.22 (dd, J = 17.4, 3.0, Hb-23), 1.87 (s, CH_3-27), 1.86 (Ha-28), 0.68 (t, J = 7.5, CH_3-29) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

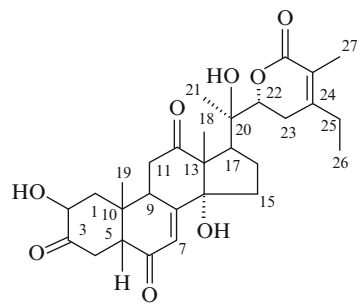
C-1	48.9	C-11	36.4	C-21	22.1
2	209.4	12	209.2	22	83.1
3	74.6	13	61.6	23	30.0
4	35.7	14	88.8	24	154.3
5	55.1	15	31.9	25	121.1
6	199.6	16	21.0	26	161.2
7	122.9	17	43.9	27	12.2
8	166.8	18	17.4	28	27.0
9	38.3	19	22.3	29	11.5
10	44.2	20	74.9		

References

1. M.P. Calcagno, F. Camps, J. Coll, E. Male, F.S. Baeza, Tetrahedron **52**, 10137 (1996)

3-Dehydroajugalactone

CAS Registry Number: 179308-44-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{29}H_{38}O_8$: 514.2566

IR (KBr) ν_{max} cm^{-1}: 3427, 1750–1600 [1]

TSP-MS m/z: 532 $[M + NH_4]^+$ (77), 515 $[M + H]^+$ (56), 514 $[M]^+$ (100), 497 $[M + H–H_2O]$ (63) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.87 (m, Ha-2), 2.78 (dd, J = 13.4, 5.5, H-5), 6.41 (d, J = 2.7, H-7), 4.41 (m, H-9), 3.01 (cs, Ha-11), 3.01 (cs, Hb-11), 3.51 (t, J = 8.6, H-17), 1.55 (s, CH_3-18), 1.19 (s, CH_3-19), 1.70 (s, CH_3-21), 4.46 (dd, J = 12.9, 3.3, H-22), 2.44 (Ha-23), 2.23 (m, Hb-23), 1.87 (s, CH_3-27), 1.87 (Ha-28), 0.67 (t, J = 7.5, CH_3-29) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

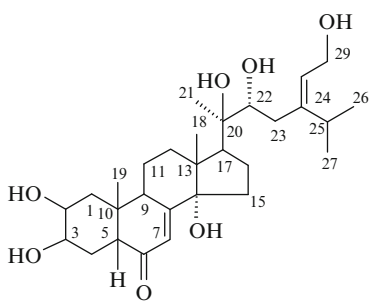
C-1	38.5	C-11	36.8	C-21	22.1
2	71.7	12	208.4	22	83.1
3	209.7	13	61.7	23	30.1
4	45.4	14	89.1	24	154.2
5	57.5	15	32.0	25	121.2
6	198.2	16	21.0	26	163.1
7	122.5	17	43.9	27	12.2
8	166.8	18	17.4	28	27.1
9	37.4	19	22.1	29	11.5
10	39.9	20	74.9		

References

1. M.P. Calcagno, F. Camps, J. Coll, E. Male, F.S. Baeza, Tetrahedron **52**, 10137 (1996)

24(28)-Dehydroamarasterone B

CAS Registry Number: 196213-11-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{29}H_{46}O_7$: 506.3243

Mp: amorphous [1]

UV λ_{max}^{EtOH} nm: 243 [1]

CI-MS m/z: 524 $[M + H + NH_3]^+$, 507 $[M + H]^+$, 489 $[M + H–H_2O]^+$, 471$[M + H–2H_2O]^+$, 453 $[M + H–3H_2O]^+$, 380 $[M + H + NH_3\text{-}C_{22}–C_{29}]^+$, 363 $[M + H–C_{22}–C_{29}]^+$, 345 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.40 (t, J = 13.0, Ha-1), 1.85 (He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.34 (t, H-5), 5.99 (d, J = 2.5, H-7), 3.11 (m, H-9), 1.75 (Ha-11), 1.85 (He-11), 1.73 (Ha-12), 1.95 (He-12), 1.65 (Ha-15), 2.05 (m, Hb-15), 1.95 (Ha-16), 1.85 (Hb-16), 2.39 (t, H-17), 0.88 (s, CH_3-18), 1.00 (s, CH_3-19), 1.27 (s, CH_3-21), 3.72 (d, J = 10.0, Hb-22), 2.41 (Ha-23), 1.95 (Hb-23), 2.87 (sp, J = 6.6, H-25), 1.04 (d, J = 6.6, CH_3-26), 1.04 (d, J = 6.6, CH_3-27), 5.45 (t, J = 7.0, H-28), 4.23 (m, Ha and Hb-29) [1]

^{13}C NMR (100 MHz, D_2O) [1]:

Table 1

C-1	36.4	C-11	21.0	C-21	20.6
2	68.3	12	32.0	22	75.7
3	68.2	13	48.5	23	34.7
4	32.3	14	86.3	24	147.4
5	51.4	15	31.2	25	30.4
6	209.3	16	21.0	26	21.7
7	122.1	17	50.2	27	22.2
8		18	18.1	28	124.3
9	34.9	19	24.2	29	58.7
10	39.1	20	79.0		

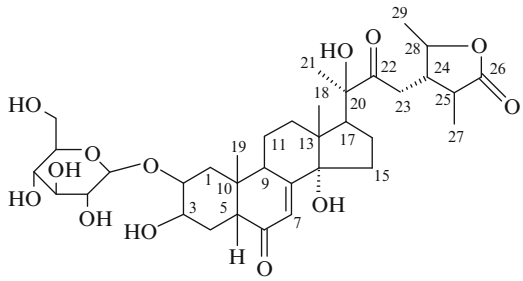
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 5.2 \times 10^{-7}$M [1–3].

References

1. U.A. Baltaev, L. Dinan, J.P. Girault, R. Lafont, Phytochemistry **46**, 103 (1997)
2. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
3. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

22-Dehydrocyasterone-2-Glucoside

CAS Registry Number: 948294-71-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga nipponensis* [1]

$C_{35}H_{52}O_{13}$: 680.3407

Mp: amorphous [1]

IR (KBr) ν_{max} cm^{-1}: 3481, 2867, 2915, 1742, 1711, 1657, 1444, 1036, 878 [1]

ES-MS m/z: 703.3 $[M + 23]^+$, 715.3 [M + 35] [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.95 (t, J = 12.9, Ha-1), 2.20 (He-1), 4.27 (br d, J = 11.0, Ha-2), 4.35 (br s, He-3), 1.77 (Ha-4), 2.06 (dt, J = 3.9, 14.4, He-4), 2.95 (dd, J = 4.0, 13.5, H-5), 6.22 (d, J = 2.2, H-7), 3.50 (br t, J = 8.0, H-9), 1.62 (Ha-11), 1.77 (He-11), 1.90 (Ha-12), 2.55 (td, J = 4.6, 13.3, He-12), 2.13 (Ha-15), 1.88 (Hb-15), 1.88 (Ha-16), 2.17 (Hb-16), 3.18 (t, J = 8.0, H-17), 1.09 (s, CH_3-18), 0.99 (s, CH_3-19), 1.66 (s, CH_3-21), 3.13 (dd, J = 5.8, 18.5, Ha-23), 3.19 (dd, J = 5.6, 18.5, Hb-23), 2.41 (ddt, J = 5.8, 8.8, 11.0, H-24), 2.48 (dq, J = 7.0, 11.0, H-25), 1.26 (d, J = 7.0, CH_3-27), 4.22 (dq, J = 6.1, 8.8, H-28), 1.33 (d, J = 6.1, CH_3-29), Other: β-D-Glcp′: 4.98 (d, J = 8.0, H-1), 4.05 (dd, J = 8.0, 8.8, H-2), 4.24 (H-3), 4.25 (H-4), 3.96 (ddd, J = 2.4, 5.1, 9.0, H-5), 4.38 (dd, J = 5.2, 11.7, Ha-6), 4.53 (dd, J = 2.4, 11.7, Hb-6) [1]

^{13}C NMR (100.62 MHz, C_5D_5N) [1]:

Table 1

C-1	35.95	C-13	48.01	C-25	42.08
2	75.71	14	83.89	26	178.56

(*continued*)

Table 1 (continued)

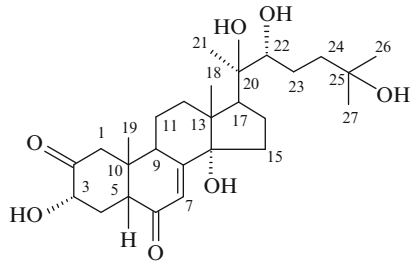
3	64.56	15	31.71	27	14.68
4	31.20	16	21.53	28	79.79
5	51.29	17	51.56	29	19.86
6	202.90	18	17.62	Glc′-1	101.67
7	121.97	19	24.12	2	75.44
8	165.36	20	81.28	3	78.60
9	34.29	21	25.54	4	71.51
10	38.70	22	215.04	5	78.74
11	20.79	23	39.11	6	62.62
12	31.86	24	45.95		

References

1. J. Coll, Y.A. Tandron, X. Zeng, Steroids **72**, 270 (2007)

2-Dehydro-3-epi-20-Hydroxyecdysone

CAS Registry Number: 220855-34-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Froelichia floridana* [1, 2]

$C_{27}H_{42}O_7$: 478.2930

UV λ_{max}^{EtOH} nm (log ε): 242 (4.106) [1]

LSI-MS m/z: 569 $[M\text{-}H + glycerol]^-$, 477 $[M\text{-}H]^-$ [1]

^{1}H NMR (MHz, J/Hz, C_5D_5N): 2.35 (d, J = 13.7, Ha-1), 2.70 (d, J = 13.7, He-1), 4.54 (dd, J = 11.0, 7.2, Ha-3), 2.00 (m, Ha-4), 2.40 (m, He-4), 2.80 (dd, J = 13.7, 3.9, H-5), 6.17 (d, J = 2.3, H-7), 3.25

(m, H-9), 1.70 (Ha-11), 1.88 (He-11), 2.05 (Ha-12), 2.45 (He-12), 1.95 (Ha-15), 2.10 (Hb-15), 2.46 (Ha-16), 2.15 (Hb-16), 2.90 (t, J = 9.7, H-17), 1.15 (s, CH_3-18), 1.06 (s, CH_3-19), 1.52 (s, CH_3-21), 3.83 (t, J = 9.4, H-22), 1.72 (Ha-23), 2.14 (Hb-23), 2.25 (Ha-24), 1.82 (Hb-24), 1.36 (s, CH_3-26), 1.36 (s, CH_3-27) [1]

^{13}C NMR (MHz, C_5D_5N) [1]:

Table 1

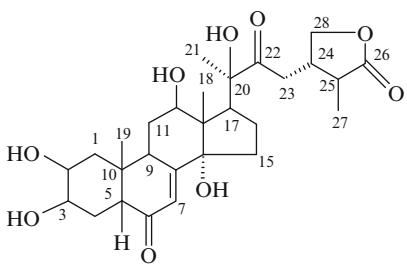
C-1	49.0	C-10	42.7	C-19	22.7
2	210.0	11	20.6	20	76.5
3	74.6	12	31.5	21	21.4
4	36.0	13	48.0	22	77.3
5	55.6	14	83.1	23	27.3
6		15	31.3	24	42.4
7	120.9	16	21.1	25	69.3
8		17	49.7	26	29.9
9	35.8	18	17.6	27	29.8

References

1. S.D. Sarker, V. Sik, H.H. Rees, L. Dinan, Phytochemistry **49**, 2311 (1998)
2. S. Charoensuk, B. Yingyongnarongkul, A. Suksamrarn, Tetrahedron **56**, 9313 (2000)

22–Dehydro-12-Hydroxycyasterone

CAS Registry Number: 171741-95-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{29}H_{42}O_9$: 534.2828

IR (KBr) ν_{max} cm^{-1}: 3405, 1757, 1708, 1658 [1]

TSP-MS m/z: 579 $[M + HCOO]^-$, 561 $[M + HCOO-H_2O]^-$ [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 2.34–1.86 (Ha-1), 2.02 (He-1), 4.16 (m, Ha-2), 4.22 (He-3), 2.34–1.86 (Ha-4), 1.74 (t, J = 14.0, He-4), 3.04 (dd, J = 13.0, 3.5, H-5), 6.30 (d, J = 2.0, H-7), 3.78 (m, H-9), 2.50–2.34 (Ha-11), 1.92 (He-11), 5.08 (Ha-12), 2.19 (Ha-15), 1.95 (Hb-15), 2.83 (m, Ha-16), 2.25 (Hb-16), 3.42 (t, J = 9.5, H-17), 0.84 (s, CH_3-18), 1.08 (s, CH_3-19), 1.58 (s, CH_3-21), 3.57 (dd, J = 19.0, 6.0, Ha-23), 3.31 (dd, J = 19.0, 6.0, Hb-23), 2.50–2.34 (Ha-24), 2.53 (dq, J = 11.0, 7.0, H-25), 1.31 (d, J = 7.0, CH_3-27), 4.24 (dq, J = 8.5, 6.0, H-28), 1.41 (d, J = 6.5, CH_3-29) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-11	29.7	C-21	28.8
2	68.0	12	71.0	22	218.4
3	67.9	13	51.8	23	42.0
4	32.4	14	85.9	24	45.8
5	51.2	15	31.6	25	42.2
6	203.3	16	23.0	26	178.6
7	122.3	17	59.3	27	14.7
8	163.1	18	12.1	28	79.8
9	34.5	19	24.3	29	20.2
10	38.8	20	79.0		

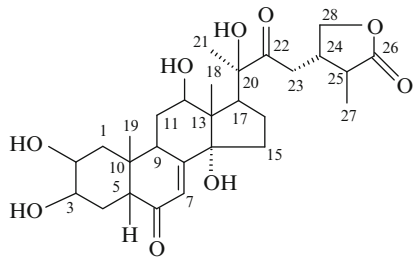
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.3 \times 10^{-6}$M [2, 3].

References

1. M.P. Calcagno, F. Camps, J. Coll, E. Male, F.S. Baeza, Tetrahedron **51**, 12119 (1995)
2. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
3. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

22–Dehydro-12-Hydroxy-29-Norcyasterone

CAS Registry Number: 171741-97-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{28}H_{40}O_9$: 520.2672

IR (KBr) ν_{max} cm^{-1}: 3394, 1754, 1705, 1652 [1]

TSP-MS m/z: 565 $[M + HCOO]^-$, 547 $[M + HCOO–H_2O]^-$ [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 2.30–1.85 (Ha-1), 1.98 (He-1), 4.15 (m, Ha-2), 4.23 (He-3), 2.30–1.85 (Ha-4), 1.74 (t, J = 15.0, He-4), 3.05 (dd, J = 13.0, 3.5, H-5), 6.30 (d, J = 2.0, H-7), 3.75 (m, H-9), 2.46 (m, Ha-11), 2.30–1.85 (He-11), 5.04 (He-12), 2.30–1.85 (Ha-15), 2.30–1.85 (Hb-15), 2.81 (m, Ha-16), 2.30–1.85 (Hb-16), 3.39 (t, J = 9.5, H-17), 0.77 (s, CH_3-18), 1.10 (s, CH_3-19), 1.56 (s, CH_3-21), 3.63 (dd, J = 19.0, 3.5, Ha-23), 3.30 (dd, J = 19.0, 10.0, Hb-23), 2.65 (m, Ha-24), 2.33 (dq, J = 11.0, 7.0, H-25), 1.18 (d, J = 7.0, CH_3-27), 4.78 (t, J = 8.5, Ha-28), 3.84 (t, J = 8.5, Hb-28) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-11	29.7	C-21	28.7
2	67.9	12	70.9	22	219.0
3	67.8	13	51.9	23	42.8
4	32.3	14	85.9	24	39.7
5	51.2	15	31.6	25	39.2
6	203.3	16	22.9	26	179.4
7	122.3	17	59.3	27	13.8
8	163.1	18	12.2	28	71.4
9	34.5	19	24.3		
10	38.8	20	78.9		

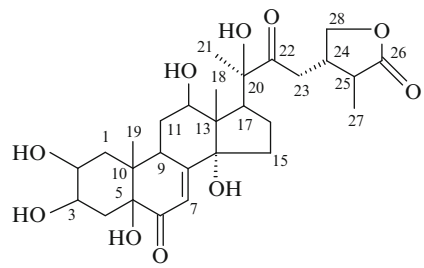
(*continued*)

References

1. M.P. Calcagno, F. Camps, J. Coll, E. Male, F.S. Baeza, Tetrahedron **51**, 12119 (1995)

22–Dehydro-12-Hydroxy-29-Norsengosterone

CAS Registry Number: 171741-98-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{28}H_{40}O_{10}$: 536.2621

IR (KBr) ν_{max} cm^{-1}: 3416, 1759, 1709, 1674 [1]

TPS-MS m/z: 537 $[M + H]^+$, 519 $[M + H–H_2O]^+$, 501 $[M + H–2H_2O]^+$, 483 $[M + H–3H_2O]^+$, 465 $[M + H–4H_2O]^+$ [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 2.30–1.85 (Hae-1), 4.25 (m, Ha-2), 4.19 (m, He-3), 2.30–1.85 (Hae-4), 6.33 (d, J = 3.5, H-7), 3.82 (m, H-9), 2.49 (m, Ha-11), 2.30–1.85 (He-11), 5.02 (Ha-12), 2.30–1.85 (Hab-15), 2.81 (m, Ha-16), 2.30–1.85 (Hb-16), 3.38 (t, J = 9.5, H-17), 0.76 (s, CH_3-18), 1.20 (s, CH_3-19), 1.56 (s, CH_3-21), 3.64 (dd,

J = 19.0, 3.5, Ha-23), 3.30 (dd, J = 19.0, 10.0, Hb-23), 2.65 (m, Ha-24), 2.34 (dq, J = 11.0, 7.0, H-25), 1.19 (d, J = 7.0, CH_3-27), 4.78 (t, J = 8.5, Ha-28), 3.85 (t, J = 8.5, Hb-28) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	34.8	C-11	30.7	C-21	28.8
2	67.7	12	70.8	22	219.0
3	69.7	13	51.9	23	42.8
4	35.8	14	85.7	24	39.7
5	79.8	15	31.6	25	39.2
6	200.7	16	22.9	26	179.4
7	120.8	17	59.2	27	13.8
8	163.6	18	12.3	28	71.4
9	38.1	19	17.2		
10	45.2	20	78.9		

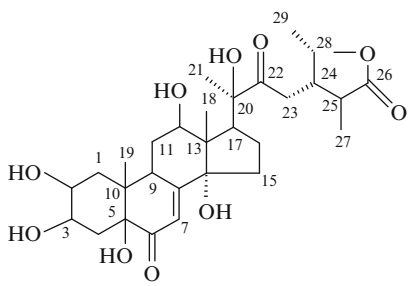
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.3 \times 10^{-5}$M [2, 3].

References

1. M.P. Calcagno, F. Camps, J. Coll, E. Male, F.S. Baeza, Tetrahedron **51**, 12119 (1995)
2. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
3. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

22–Dehydro-12-Hydroxysengosterone

CAS Registry Number: 171741-96-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{29}H_{42}O_{10}$: 550.2777

IR (KBr) ν_{max} cm^{-1}: 3405, 1755, 1706, 1674 [1]

TSP-MS m/z: 551 $[M + H]^+$, 533 $[M + H–H_2O]^+$, 515 $[M + H–2H_2O]^+$, 497 $[M + H–3H_2O]^+$, 479 $[M + H–4H_2O]^+$, 461 $[M + H–5H_2O]^+$ [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 2.30–1.90 (Ha-1), 2.05 (He-1), 4.25 (Ha-2), 4.17 (m, He-3), 2.30–1.90 (Ha-4), 1.98 (He-4), 6.33 (d, J = 2.5, H-7), 3.81 (m, H-9), 2.34 (Ha-11), 2.30–1.90 (He-11), 5.02 (He-12), 2.30–1.90 (Ha-15), 2.30–1.90 (Hb-15), 2.81 (m, Ha-16), 2.30–1.90 (Hb-16), 3.39 (t, J = 10.0, H-17), 0.83 (s, CH_3-18), 1.18 (s, CH_3-19), 1.56 (s, CH_3-21), 3.56 (dd, J = 19.0, 5.0, Ha-23), 3.32 (dd, J = 19.0, 6.0, Hb-23), 2.30–1.90 (Ha-24), 2.54 (dq, J = 11.0, 7.0, H-25), 1.31 (d, J = 7.0, CH_3-27), 4.25 (dq, J = 8.5, 6.0, H-28), 1.41 (d, J = 6.0, CH_3-29) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	34.8	C-11	30.7	C-21	28.9
2	67.8	12	70.8	22	218.5
3	69.7	13	51.9	23	42.0
4	35.8	14	85.8	24	45.8
5	79.8	15	31.6	25	42.2
6	200.7	16	23.0	26	178.7
7	120.8	17	59.2	27	14.7
8	163.6	18	12.1	28	79.8
9	38.1	19	17.2	29	20.3
10	45.1	20	79.0		

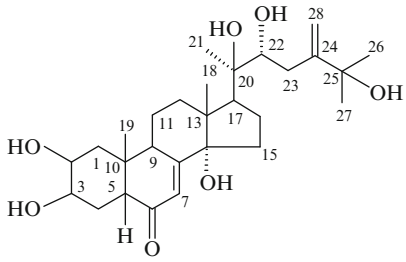
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 2.7 \times 10^{-6}$M [2, 3].

References

1. M.P. Calcagno, F. Camps, J. Coll, E. Male, F.S. Baeza, Tetrahedron **51**, 12119 (1995)
2. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
3. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

24(28)-Dehydromakisterone A

CAS Registry Number: 68556-61-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga iva* [1], *Chenopodium album* [2], *Cucubalis baccifer* [3], *Diploclisia glaucescens* [4], *Leuzea carthamoides* [5], *L. chalcedonica, L. wilfordii* [6], *Rhaponticum carthamoides* [7], *Rh. integrifolium* [8], *Silene frivaldszkyana* [9], *S. italica* ssp. *nemoralis* [10], *S. roemeri* [11], *Spinacea oleracea* [12], *Vitex leptobotrys* [13]

$C_{28}H_{44}O_7$: 492.3087

Mp: 239–248°C (MeOH) [2], 245–247°C (EtOAc-MeOH) [7], 244–246°C (MeOH) [8]

$[\alpha]_D^{20}$ + 54.4 ± 2° (c 0.37, MeOH) [8]

IR (KBr) ν_{max} cm^{-1}: 3300–3500, 1665 [8]

UV λ_{max}^{EtOH} nm: 242 [3], 4.245 (log ε 4.15) [8]

EI-MS m/z: 474 $[M\text{-}H_2O]^+$(3), 456 (11), 438 (15), 363 (66), 345 (100), 327 (47), 309 (13), 300 (26), 173 (17), 113 (37), 111 (55), 97 (52), 95 (63), 93 (35), 83 (91), 71 (62), 69 (62) [8]

CI-MS m/z: 493 $[M + H]^+$ [4]

CD (c, 0.08, MeOH): $\Delta\varepsilon = +1.7$ (338 nm), $\Delta\varepsilon = -4.3$ (248 nm) [8]

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.43 (Ha-1), 1.79 (Hb-1), 3.84 (m, Ha-2), 3.95 (m, He-3), 1.65 (Ha-4), 1.75 (He-4), 2.38 (dd, J = 12.0, 5.0, H-5), 5.81 (d, J = 2.5, H-7), 3.16 (m, Ha-9), 1.66 (Ha-11), 1.79 (He-11), 2.13 (Ha-12), 1.87 (He-12), 1.98 (Ha-15), 1.62 (Hb-15), 2.00 (Ha-16), 1.82 (Hb-16), 2.39 (H-17), 0.90 (s, CH_3-18), 0.97 (s, CH_3-19), 1.24 (s, CH_3-21), 3.60 (dd, J = 10.4, 1.8, Hb-22), 2.18 (Ha-23), 2.42 (Hb-23), 1.32 (s, CH_3-26), 1.38 (s, CH_3-27), 5.13 (CH_2-28), 4.95 (CH_2-28) [5]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 3.75–4.20 (m, H-2), 3.75–4.20 (m, H-3), 6.08 (br s, H-7), 3.45 (m, H-9), 1.08 (s, CH_3-18), 0.95 (s, CH_3-19), 1.46 (s, CH_3-21), 3.75–4.20 (m, H-22), 1.40 (s, CH_3-26), 1.46 (s, CH_3-27), 5.14, 4.97 (br s, CH_2-28) [8]

^{13}C NMR (CD_3OD) [3]: **^{13}C NMR** (22.3 MHz, C_5D_5N) [5]:

Table 1

C-1	39.28	C-15	32.85	C-1	38.1 (t)	C-15	32.1 (t)
2	68.52	16	21.55	2	68.1 (d)	16	21.5 (t)
3	68.72	17	50.49	3	68.1 (d)	17	50.1 (d)
4	32.51	18	18.05	4	32.5 (t)	18	17.9 (q)
5	51.80	19	24.40	5	51.4 (d)	19	24.5 (q)
6	206.46	20	77.81	6	203.3 (s)	20	76.8 (s)
7	122.16	21	21.55	7	121.7 (d)	21	21.6 (q)
8	167.90	22	78.01	8	166.0 (s)	22	78.0 (d)
9	34.61	23	34.61	9	34.6 (d)	23	34.9 (t)
10	37.20	24	155.32	10	38.7 (s)	24	156.2 (s)
11	21.55	25	73.62	11	21.2 (t)	25	72.2 (s)
12	31.78	26	31.78	12	31.9 (t)	26	30.2 (q)
13	48.49	27	32.51	13	48.2 (s)	27	30.9 (q)
14	85.28	28	110.38	14	84.2 (s)	28	109.6 (t)

Pharm./Biol.: *Galleria mellonela* assay (in vivo): 12.5 µg/g, *Sarcophaga bullata* assay (in vivo): 10.4 µg/g [14], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.0 \times 10^{-9}$M [15–17].

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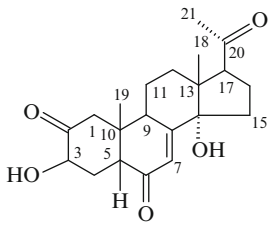
2-Dehydropoststerone

CAS Registry Number: 864678-05-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Chenopodium album* [1]

$C_{21}H_{28}O_5$: 360.1936

IR (KBr) ν_{max} cm^{-1}: 3510–3350, 1704, 1664 [1]

EI-MS m/z: 360 $[M]^+$, 345 $[M\text{-}CH_3]^+$, 342 $[M\text{-}H_2O]^+$, 317 $[M\text{-}CH_3CO]^+$ [1]

^{1}H NMR (J/Hz, CD_3OD): 1.30 (m, Ha-1), 1.98 (m, He-1), 4.05 (br s, He-3), 1.65 (m, Ha-4), 1.80 (m, He-4), 2.50 (dd, J = 3.9, 11.7, H-5), 5.86 (s, H-7), 3.10 (m, H-9), 2.31 (m, Ha-11), 1.92 (m, He-11), 2.28 (m, Ha-12), 1.80 (m, He-12), 2.10 (m, Ha-15), 1.61 (m, Hb-15), 2.33 (m, Ha-16), 1.99 (m, Hb-16), 3.30 (t, J = 8.8, H-17), 0.64 (s, CH_3-18), 0.99 (s, CH_3-19), 2.16 (s, CH_3-21) [1]

^{13}C NMR (CD_3OD) [1]:

Table 1

C-1	36.3	C-8	162.9	C-15	32.4
2	209.3	9	32.2	16	21.0
3	64.8	10	41.2	17	58.7
4	22.2	11	21.4	18	17.2
5	50.8	12	30.5	19	23.9
6	204.3	13	48.0	20	209.3
7	121.7	14	84.8	21	32.1

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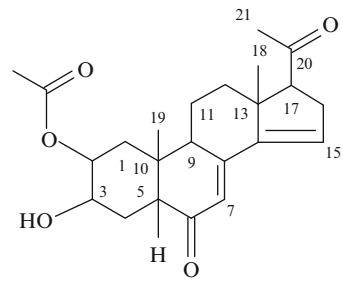
14,15-Dehydropoststerone-2-Acetate

CAS Registry Number: 1236073-69-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotus longifolia* [1]

$C_{23}H_{30}O_5$: 386.2093

CI-MS m/z: 404 $[M + NH_4]^+$, 387 $[M + H]^+$, 344 $[M + NH_4\text{–}CH_3COOH]^+$ [1]

^{1}H NMR (J/Hz, D_2O): 1.56 (t, J = 13.0, Ha-1), 1.99 (He-1), 5.05 (m, Ha-2), 4.21 (m, He-3), 1.78 (Ha-4), 1.89 (He-4), 2.42 (H-5), 6.25 (d, J = 2.2, H-7), 2.92 (m, H-9), 1.80 (Ha-11), 1.97 (He-12), 1.91 (Ha-12), 2.36 (He-12), 6.21 (br s, H-15), 2.43 (Ha-16), 2.84 (dd, J = 18.5, 11.2, Hb-16), 3.34 (t, J = 9.9, H-17), 0.85 (s, CH_3-18), 1.017 (s, CH_3-19), 2.296 (s, CH_3-21), 2.13 (s, CH_3COO-2) [1]

^{13}C NMR (D_2O) [1]:

Table 1

C-1	35.1	C-9	41.3	C-17	67.6
2	74.4	10	41.6	18	21.1
3	68.2	11	23.1	19	25.5
4	n.d.	12	40.7	20	219.1
5	52.7	13	50.8	21	33.2
6	n.d.	14	149.6	$\underline{CH_3}COO$	23.4
7	122.9	15	133.8	$CH_3\underline{COO}$	175.7
8	n.d.	16	n.d.		

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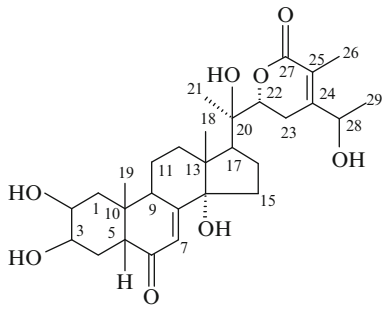
24,25-Dehydroprecyasterone

CAS Registry Number: 145075-79-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga iva* [1], *Ajuga reptans* var. *reptans* [2]

$C_{29}H_{42}O_8$: 518.2879

Mp: 275–277°C [2]

$[\alpha]_D^{25}$ + 7° (c 0.1, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 1695, 1652 [1]

UV λ_{max}^{MeOH} nm (log ε): 243 (4.013) [2]

CI-MS m/z: 536 $[M + H + NH_3]^+$, 519 $[M + H]^+$, 501 $[M + H\text{-}H_2O]^+$ [1]

^{1}H NMR (J/Hz, CD_3OD): 3.83 (m, H-2), 3.95 (m, H-3), 5.80 (d, J = 2.5, H-7), 3.15 (m, H-9), 0.89 (s, CH_3-18), 0.96 (s, CH_3-19), 1.33 (s, CH_3-21), 4.13 (dd, J = 3.0, 13.0, H-22), 1.84 (d, J = 1.0, CH_3-26), 4.90 (H-28), 1.29 (d, J = 6.0, CH_3-29) [1]

^{1}H NMR (J/Hz, D_2O): 1.40 (Ha-1), 1.85 (He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.36 (H-5), 5.99 (d, J = 2.5, H-7), 3.12 (m, H-9), 1.70 (Ha-11), 1.80 (He-11), 1.95 (Ha-16), 1.75 (Hb-16), 2.60 (H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.33 (s, CH_3-21), 4.34 (dd, J = 4.5, 11.5, H-22), 2.40 (Ha-23), 2.55 (br s, Hb-23), 1.83 (br s, CH_3-26), 4.93 (d, J = 6.0, H-28), 1.32 (d, J = 6.0, CH_3-29) [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.43 (dd, J = 13.5,12.4, Ha-1), 1.80 (He-1), 3.85 (ddd, J = 12.1, 4.3, 3.3, Ha-2), 3.96 (q, J = 2.8, He-3), 1.71 (Ha-4), 1.77 (He-4), 2.39 (dd, J = 13.0, 4.5, H-5), 5.82 (d, J = 2.6, H-7), 3.17 (ddd, J = 11.5, 7.1, 2.6, H-9), 1.71 (Ha-11), 1.82 (He-11), 2.03 (Ha-16), 1.79 (Hb-16), 2.50 (H-17), 0.90 (s, CH_3-18), 0.97 (s, CH_3-19), 1.34 (s, CH_3-21), 4.14 (dd, J = 13.5, 3.2, H-22), 2.33 (ddq, J = 18.1, 13.5, 2.5, Ha-23), 2.56 (dd, J = 18.1, 3.1, Hb-23), 1.86 (d, J = 2.2, CH_3-26), 4.84 (q, J = 6.6, H-28), 1.30 (d, J = 6.6, CH_3-29) [2]

^{13}C NMR (125 MHz, CD_3OD) [2]:

Table 1

C-1	37.5	C-11	21.63	C-21	21.58
2	68.8	12	32.6	22	84.4
3	68.7	13	48.8	23	25.2
4	33.0	14	85.3	24	158.3
5	51.9	15	31.9	25	121.0
6	206.6	16	21.7	26	169.3
7	122.4	17	50.6	27	12.0
8	167.9	18	18.3	28	67.0
9	35.2	19	24.5	29	21.3
10	39.4	20	76.6		

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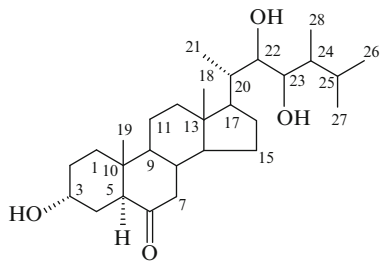
2-Deoxycastasterone

CAS Registry Number: 87734-68-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Typha latifolia* [1], *Pinus thunbergii* [2]
$C_{28}H_{48}O_4$: 448.3552
Mp: 227–230°C ($CHCl_3$–MeOH) [1]
EI-MS m/z: 448 $[M]^+$ [1]
FAB-MS m/z: 471 $[M + Na]^+$ (100) [1]
HR-MS m/z: for $C_{28}H_{48}O_4$ found 448.3548 [1]
CD (c, CH_2Cl_2): $\Delta\varepsilon = -2.2$ (294 nm) [1]
^{1}H NMR (360 MHz, J/Hz, CD_3OD): 3.56 (m, Ha-2), 4.17 (br s, He-3), 1.72 (H-4), 2.76 (H-5), 2.01(Ha-7), 2.31 (He-7), 1.80 (H-8), 0.69 (s, CH_3-18), 0.76 (s, CH_3-19), 0.85 (d, CH_3-21), 0.92 (d, CH_3-26), 0.95 (d, CH_3-27), 0.97 (s, CH_3-28) [1]
Pharm./Biol.: Plant growth promoting activity [1].

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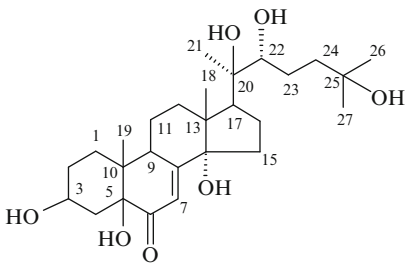
2-Deoxy-5β,20-Dihydroxyecdysone

CAS Registry Number: 623924-84-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Diploclisia glauscens* [1]
$C_{27}H_{44}O_7$: 480.3087
Mp: 128–130°C [1]
$[\alpha]_D^{25}$ + 62.4° (c 0.34, MeOH) [1]
UV λ_{max}^{EtOH} nm: 241 [1]
HR-MS m/z: for $C_{27}H_{45}O_6$ $[M + H]^+$ calcd. 481.3124, found 481.3165 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.57 (br d, J = 14.1, Ha-1), 2.17 (m, He-1), 1.87 (m, Ha-2), 1.87 (m, He-2), 4.02 (m, He-3), 1.75 (br d, J = 14.4, Ha-4), 1.97 (br d, J = 14.4, He-4), 6.27 (d, J = 2.5, H-7), 3.60 (m, H-9), 1.79 (m, Ha-11), 1.88 (m, He-11), 2.61 (m, Ha-12), 2.07 (m, He-12), 2.61 (m, Ha-15), 1.90 (m, Hb-15), 2.47 (m, Ha-16), 2.07 (m, Hb-16), 3.00 (t, J = 9.0, H-17), 1.22 (s, CH_3-18), 1.11 (s, CH_3-19), 1.60 (s, CH_3-21), 3.88 (br d, J = 8.5, H-22), 1.87 (m, Ha-23), 2.17 (m, Hb-23), 1.82 (m, Ha-24), 2.28 (m, Hb-24), 1.37 (s, CH_3-26), 1.37 (s, CH_3-27) [1]
^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

C-1	24.94	C-10	42.37	C-19	17.24
2	29.11	11	21.76	20	76.76
3	65.81	12	32.02	21	21.62
4	36.48	13	48.09	22	77.50
5	80.23	14	84.01	23	27.41
6	209.31	15	31.60	24	42.57
7	119.66	16	21.32	25	69.47
8	167.33	17	49.95	26	29.92
9	37.03	18	17.80	27	30.07

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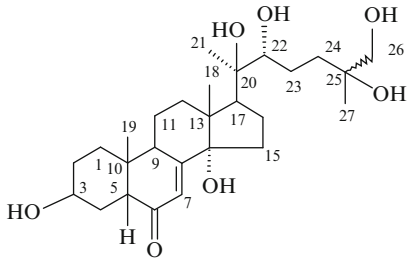
2-Deoxy-20,26-Dihydroxyecdysone

CAS Registry Number: 397248-04-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotis longifolia* [1], *Silene pseudotites* [2, 3]
$C_{27}H_{44}O_7$: 480.3087
CI-MS m/z: 498 $[M + H + NH_3]^+$, 481 $[M + H]^+$, 480 $[M]^+$, 463 $[M + H–H_2O]^+$ [1]; 498 $[M + H + NH_3]^+$ (81), 481 $[M + H]^+$ (54), 480 $[M]^+$ (100), 463 $[M + H–H_2O]^+$ (10.5), 445 $[M + H–2H_2O]^+$ (4) [3]
^{1}H NMR (J/Hz, D_2O): 4.10 (br s, H-3), 2.39 (br dd, J = 3.4, 12.5. H-5), 5.96 (d, J = 2.2, H-7), 3.15 (br s, H-9), 2.33 (t, J = 9.7, H-17), 0.863 (s, CH_3-18), 0.976 (br s, CH_3-19), 1.235 (s, CH_3-21), 3.44 (d, J = 10.5, H-22), 3.45 (s, CH_2OH-26), 1.161 (s, CH_3-27) [2, 3]

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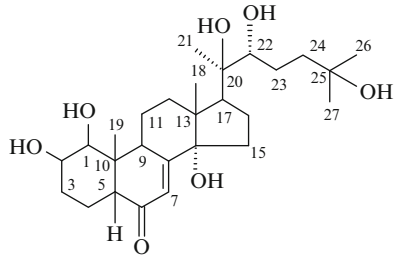
3-Deoxy-1β,20-Dihydroxyecdysone

CAS Registry Number: 460731-05-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Diploclisia glaucescens* [1]
$C_{27}H_{44}O_7$: 480.3087
Mp: 152–155°C (MeOH) [1]
$[\alpha]_D^{25}$ + 63.3° (c 0.72, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3450, 1660, 1640 [1]
UV λ_{max}^{EtOH} nm: 241 [1]
FAB-MS m/z: 481 $[M + H]^+$, 463 $[M + H–H_2O]^+$, 445 $[M + H–2H_2O]^+$, 427 $[M + H–3H_2O]^+$ [1]
HR-MS m/z: for $C_{27}H_{45}O_7$ $[M + H]^+$ calcd. 481.3123, found 481.3165 [1]
^{1}H NMR (400 MHz, J/Hz, CD_3OD): 3.72 (d, J = 2.4, Ha-1), 3.95 (m, Ha-2), 1.62 (m, Ha-3), 1.73 (m, He-3), 1.52 (m, Ha-4), 1.63 (m, He-4), 2.29 (dd, J = 11.6, 5.6, H-5), 5.78 (d, J = 2.4, H-7), 3.14 (td, J = 8.0, 2.0, H-9), 1.70 (m, Ha-11), 1.90 (m, He-12), 2.00 (m, Ha-15), 1.70 (m, Hb-16), 2.39 (t, J = 9.2, H-17), 0.89 (s, CH_3-18), 1.03 (s, CH_3-19), 1.19 (s, CH_3-21), 3.30 (m, H-22), 1.26 (m, Ha-23), 1.28 (m, Hb-23), 1.79 (m, Ha-24), 1.44 (m, Hb-24), 1.18 (s, CH_3-26), 1.18 (s, CH_3-27) [1]
^{13}C NMR (100 MHz, CD_3OD) [1]:

Table 1

C-1	73.78	C-10	43.65	C-19	20.16
2	68.94	11	21.93	20	77.91
3	27.64	12	32.56	21	21.05
4	25.62	13	49.00	22	78.44
5	52.12	14	85.08	23	27.37
6	206.14	15	31.78	24	42.39
7	121.70	16	21.39	25	71.30
8	167.14	17	50.58	26	28.97
9	35.76	18	18.03	27	29.69

Pharm./Biol.: Showed 40% potency of 20-hydroxyecdysone in the spiracle index assay using the fourth instar larvae of the silkworm *Bombyx mori* [1].

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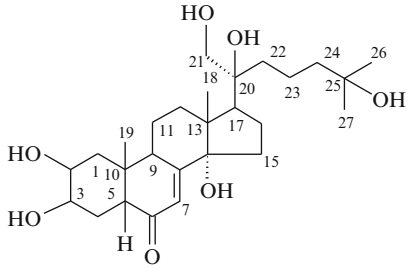
22-Deoxy-20,21-Dihydroxyecdysone

CAS Registry Number: 229644-40-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Rhagodia baccata* [1]
$C_{27}H_{44}O_7$: 480.3087
UV λ_{max}^{EtOH} nm: 242 [1]
LSI-MS m/z: 479 $[M-H]^-$ [1]
^{1}H NMR (J/Hz, C_5D_5N): 1.91 (Ha-1), 2.15 (He-1), 4.16 (m, Ha-2), 4.21 (m, He-3), 1.84 (Ha-4), 2.05 (He-4), 2.97 (H-5), 6.23 (d, J = 2.4, H-7), 3.58 (m, H-9), 1.71 (Ha-11), 1.89 (He-11), 2.60 (ddd, J = 5.0, 13.0, 13.0, Ha-12), 2.00 (He-12), 2.15 (Ha-15), 1.96 (Hb-15), 2.47 (Ha-16), 2.19 (Hb-16), 3.10 (dd, J = 9.5, 9.5, H-17), 1.20 (s, CH_3-18), 1.05 (s, CH_3-19), 4.25 (d, J = 10.7, Ha-21), 4.05 (d, J = 10.7, Hb-21), 1.65–2.10 (m, Ha-22), 1.65–2.10 (m, Hb-22), 1.65–2.10 (m, Ha-23), 1.65–2.10 (m, Hb-23), 1.65–2.10 (m, Ha-24), 1.65–2.10 (m, Hb-24), 1.31 (s, CH_3-26), 1.31 (s, CH_3-27) [1]
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 2.0 \times 10^{-7}$M [1].

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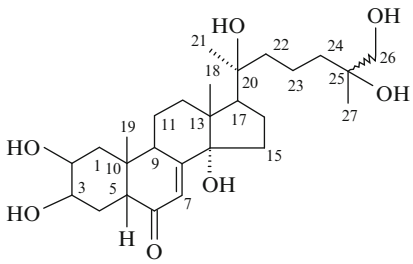
1. L. Dinan, S.D. Sarker, P. Bourne, P. Whiting, V. Sik, H. Rees, Arch. Insect Biochem. Physiol. **41**, 18 (1999)

22-Deoxy-20,26-Dihydroxyecdysone

CAS Registry Number: 128552-88-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Silene nutans* [1]
$C_{27}H_{44}O_7$: 480.3087
CI-MS m/z: 498 $[M + H + NH_3]^+$, 481 $[M + H]^+$, 463, 445, 427, 391, 363, 345 [1]; 498 $[M + H + NH_3]^+$, 481 $[M + H]^+$, 463, 445, 427, 409, 320, 303 [2]
^{1}H NMR (250 MHz, J/Hz, D_2O): 3.99 (m, Ha-2), 4.07 (m, He-3), 2.35 (t-like, H-5), 5.97 (d, J = 2.5, H-7), 3.09 (m, Ha-9), 2.30 (H-17), 0.82 (s, CH_3-18), 1.00 (s, CH_3-19), 1.30 (d, J = 6.0, CH_3-21), 3.45 (s, CH_2OH-26), 1.17 (s, CH_3-27) [1]
^{1}H NMR (250 MHz, J/Hz, D_2O): 3.98 (m, Ha-2), 4.06 (m, He-3), 5.97 (d, J = 2.5, H-7), 3.09 (m, Ha-9), 0.82 (s, CH_3-18), 0.99 (s, CH_3-19), 1.30 (s, CH_3-21), 3.45 (s, CH_2OH-26), 1.17 (s, CH_3-27) [2]

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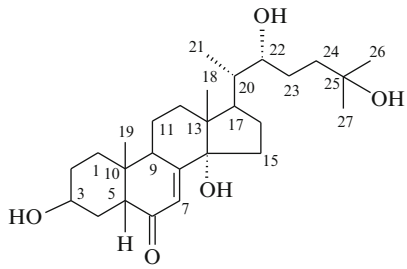
2. J.P. Girault, M. Bathori, E. Varga, K. Szendrei, R. Lafont, J. Nat. Prod. **53**, 279 (1990)

2-Deoxy-α-Ecdysone

CAS Registry Number: 31575-91-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Blechnum minus, B. penna-marina, B. vulcanicum* [1–3], *Cheilantes seiberi* [4], *Microsorum maximum, M. scolopendria* [5], *M. membranifolium* [6], *Silene brahuica* [7], *S. claviformis* [8], *S. fridvaldszkyana*, *S. gigantea* L., *S. graminifolia* [9], *S. latifolia* [10], *S. otites* [11], *S. praemixta* [12], *S. pseudotites, S. roemeri*

[13, 14], *S. scabrifolia* [15], *S. tomentella* [16], *S. wallichiana* [17, 18], *Trianthema galericulata* [4]

$C_{27}H_{44}O_5$: 448.6400

Mp: 231–232°C [2], 235–236°C (EtOH–H_2O) [12, 17], 233–235°C (EtOAc) [19]

$[\alpha]_D^{23}$ + 93.3 ± 3° (c 1.5, MeOH) [12, 17], $[\alpha]_D^{20}$ + 41° (c 0.6, dioxane) [19]

IR (KBr) ν_{max} cm^{-1}: 3450, 1650 [2], 3440, 1645 [11], 3400, 1651 [19]

UV λ_{max}^{EtOH} nm: 244 (ε 12900) [2], 245 (log ε 4.12) [12], 243 (log ε 4.1) [19]

EI-MS m/z: 448 $[M]^+$, 430 $[M\text{-}H_2O]^+$, 412 $[M\text{-}2H_2O]^+$, 361, 332, 314, 284, 99, 81 [2], 448 $[M]^+$, 430 (13), 415 (14), 412 (11), 402 (16), 397 (16), 379 (3), 361 (7), 343 (6), 332 (33), 314 (28), 303 (3), 299 (16), 285 (12), 284 (12), 263 (38), 235 (26), 234 (50), 233 (32), 215 (10), 99 (100), 81 (63) [12], 448 $[M]^+$ (3), 430 $[M\text{-}H_2O]^+$ (37), 415 $[M\text{-}H_2O\text{–}CH_3]^+$ (51), 412 (42), 402 (61), 397 (61), 379 (12), 361 (18), 343 (16), 332 (87), 314 (74), 303 (8), 299 (15), 285 (45), 263 (100) [19]

LSI-MS m/z: 447 $[M\text{-}H]^-$, 429 $[M\text{-}H\text{-}H_2O]^-$ [14]

^{1}H NMR (250 MHz, J/Hz, C_5D_5N): 4.10 (H-3), 2.96 (H-5), 6.20 (d, J = 1.5, H-7), 3.49 (H-9), 0.73 (s, CH_3-18), 1.05 (s, CH_3-19), 1.30 (d, J = 6.5, CH_3-21), 4.05 (H-22), 1.38 (s, CH_3-26), 1.38 (s, CH_3-27) [3]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.14 (m, H-3), 6.22 (d, J = 2.0, H-7), 3.52 (m, H-9), 0.75 (s, CH_3-18), 1.07 (s, CH_3-19), 1.31 (d, J = 6.6, CH_3-21), 4.08 (br d, J = 9.2, H-22), 1.40 (s, CH_3-26), 1.40 (s, CH_3-27) [7]

^{1}H NMR (100 MHz, C_5D_5N): 4.00 (m, H-3), 6.13 (br s, H-7), 0.61 (s, CH_3-18), 0.95 (s, CH_3-19), 1.17 (s, CH_3-21), 4.00 (m, H-22), 1.26 (s, CH_3-26), 1.26 (s, CH_3-27) [17]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.01 (H-3), 5.98 (d, J = 2.5, H-7), 3.37 (d, J = 3.0, H-9), 0.62 (s, CH_3-18), 0.96 (s, CH_3-19), 1.32 (d, J = 6.0, CH_3-21), 4.01 (H-22), 1.28 (s, CH_3-26), 1.28 (s, CH_3-27) [19]

^{13}C NMR (62.9 MHz, C_5D_5N) [3]: **^{13}C NMR** (75 MHz, C_5D_5N) [7]:

Table 1

C-1	33.2	C-15	31.7	C-1	29.3	C-15	31.5
2	29.1	16	26.7	2	28.7	16	26.5
3	64.1	17	48.3	3	64.2	17	48.1
4	29.5	18	15.8	4	32.7	18	15.8
5	51.6	19	24.3	5	51.3	19	24.1
6	203.2	20	43.0	6	203.8	20	42.7
7	121.3	21	13.6	7	121.1	21	13.4
8	166.0	22	73.9	8	166.4	22	74.0
9	34.3	23	25.5	9	34.4	23	25.2
10	37.0	24	42.5	10	36.8	24	42.0
11	21.3	25	69.7	11	21.4	25	70.0
12	31.7	26	30.0	12	31.5	26	29.9
13	48.1	27	30.2	13	47.9	27	29.6
14	84.0			14	84.1		

Pharm./Biol.: *Calliphora* bioassay: Showed activity approximately equal to that of α-ecdysone [2, 20], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 5.0 \times 10^{-5}$M [21–23], *Galleria mellonella* bioassay: ED_{50} = 15.6 µg/g, *Sarcophaga bullata* bioassay: ED_{50} = 31.25 µg/g [24].

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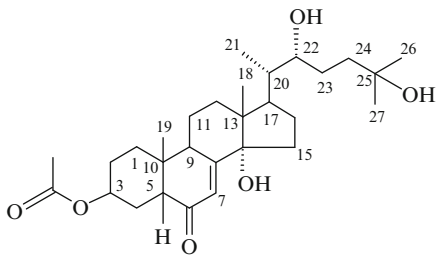
2-Deoxyecdysone-3-Acetate

CAS Registry Number: 105888-75-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene scabrifolia* [1]

$C_{29}H_{46}O_6$: 490.3294

Mp: 216–218°C (EtOH–H_2O) [1]

$[\alpha]_D^{20}$ + 131.9 ± 2° (c 0.90, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3340–3475, 1735, 1665, 1250 [1]

UV λ_{max}^{EtOH} nm (log ε): 245 (4.00) [1]

EI-MS m/z: 490 $[M]^+$ (0.2), 473 (2), 454 (27), 444 (2), 439 (2), 412 (3), 397 (2), 384 (3), 379 (4), 374 (25), 356 (27), 341 (31), 327 (27), 326 (34), 305 (27), 281 (7), 276 (8), 275 (6), 267 (7), 266 (7), 251 (27), 217 (27), 216 (27), 215 (17), 99 (100), 81 (65) [1]

CD (c, 0.12, MeOH): Δε = +2.11 (330 nm), Δε = −2.30 (253 nm) [1]

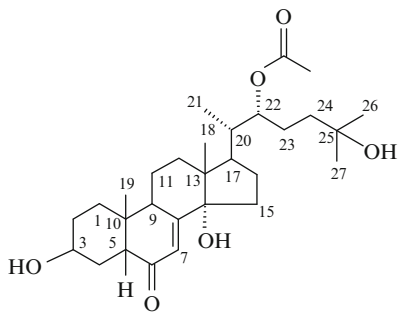
^{1}H NMR (100 MHz, C_5D_5N): 4.87 (m, H-3), 6.00 (s, H-7), 3.25 (m, H-9), 0.57 (s, CH_3-18), 0.87 (s, CH_3-19), 1.12 (s, CH_3-21), 4.00 (m, H-22), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27), 1.85 (s, CH_3COO -3) [1]

References

1. Z. Saatov, M.B. Gorovits, N.K. Abubakirov, Chem. Nat. Comp. **22**, 409 (1986)

2-Deoxyecdysone-22-Acetate

CAS Registry Number: 76026-42-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brachuica* [1], *S. otites* [2]

$C_{29}H_{46}O_6$: 490.3294

Mp: 146–148°C (MeOH–H_2O) [1]

$[\alpha]_D^{20}$ + 50.2 ± 2° (c 0.15, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3445, 1730, 1665, 1255 [1]

EI-MS m/z: 490 $[M]^+$ (21), 472 (11), 462 (14), 457 (31), 454 (42), 444 (20), 430 (14), 412 (22), 403 (13), 397 (36), 394 (35), 384 (36), 379 (16), 331 (14), 314 (14), 313 (13), 303 (14), 302 (14), 285 (46), 284 (100), 269 (25), 251 (25), 234 (91), 233 (90), 109 (46), 99 (46), 81 (48), 69 (46) [1]

CI-MS m/z: 508 $[M + H + NH_3]^+$, 491 $[M + H]^+$, 473 $[M + H– H_2O]^+$, 455, 431, 413, 397, 396 [2]

HR-MS m/z: for $C_{29}H_{47}O_6$ $[M + H]^+$ calcd. 491.3289, found 491.3372 [2]

^{1}H NMR (J/Hz, C_5D_5N): 3.93 (m, H-3), 6.02 (br s, H-7), 3.30 (m, H-9), 0.62 (s, CH_3-18), 0.90

(s, CH_3-19), 1.01 (d, J = 6.0, CH_3-21), 5.14 (m, H-22), 1.20 (s, CH_3-26), 1.20 (s, CH_3-27), 1.95 (s, CH_3COO-22) [1]

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 3.98 (m, He-3), 2.33 (dd, J = 12.0, 3.0, H-5), 5.80 (d, J = 2.5, H-7), 3.20 (H-9), 0.70 (s, CH_3-18), 0.96 (s, CH_3-19), 0.98 (d, J = 6.5, CH_3-21), 4.87 (d, H-22), 1.18 (s, CH_3-26), 1.19 (s, CH_3-27), 2.04 (s, CH_3COO-22) [2]

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.4 \times 10^{-6}$M [3–6].

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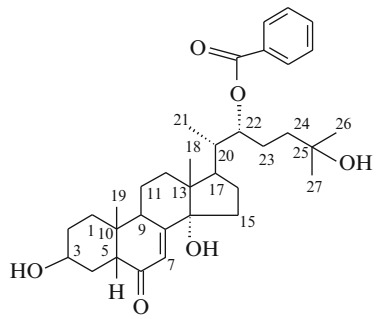
2-Deoxyecdysone-22-Benzoate

CAS Registry Number: 114317-61-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene wallichiana* [1]

$C_{34}H_{48}O_6$: 552.3450

Mp: 182–185°C (MeOH–H_2O) [1]

$[\alpha]_D^{20}$ + 141.1 ± 2° (c 0.40, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3400–3440, 1740, 1665, 1610, 1290, 710 [1]

UV λ_{max}^{EtOH} nm (log ε): 234 (4.09) [1]

EI-MS m/z: 552 $[M]^+$ (4), 534 (7), 524 (15), 519 (4), 506 (16), 476 (1.7), 430 (3), 412 (23), 402 (22), 397 (24), 394 (23), 384 (41), 379 (11), 369 (11), 351 (10), 332 (7), 331 (11), 303 (2), 285 (41), 284 (66), 233 (82), 122 $[C_7H_6O_2]^+$ (22), 105 $[C_7H_5O]^+$ (100), 99 (59), 81 (59), 77 $[C_7H_5]^+$ (59), 69 (59), 51 (10) [1]

CD (c, 0.10, MeOH): Δε = +3.08 (221 nm), Δε = −8.90 (242 nm), Δε = +1.67 (332 nm) [1]

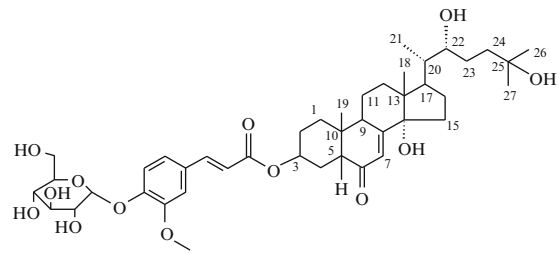
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 3.96 (m, H-3), 6.08 (br s, H-7), 0.63 (s, CH_3-18), 0.90 (s, CH_3-19), 1.13 (d, J = 6.0, CH_3-21), 5.47 (d, J = 7.5, H-22), 1.20 (s, CH_3-26), 1.20 (s, CH_3-27), Ar: 7.40 (3H), 8.19 (2H) [1]

References

1. Z. Saatov, M.B. Gorovits, N.K. Abubakirov, Chem. Nat. Comp. **23**, 708 (1987)

2-Deoxyecdysone-3-[4-(1-β-D-Glucopyranosyl)]-Ferulate

CAS Registry Number: 1019196-07-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Microsorum membranifolium* [1]
$C_{43}H_{62}O_{13}$: 786.4190
UV λ_{max}^{EtOH} nm: 240, 394, 317 [1]
FAB-MS m/z: 825 $[M + K]^+$, 809 $[M + Na]^+$, 787 $[M + H]^+$, 769 $[M + H–H_2O]^+$, 751 $[M + H–2H_2O]^+$, 625 [M + H-sugar]$^+$, 607 [M + H-sugar-H_2O]$^+$, 431, 413, 395, 377 [1]
^{1}H NMR (J/Hz, CD_3OD): 1.46 (Ha-1), 1.76 (He-1), 1.87 (Ha-2), 1.94 (He-2), 5.16 (m, He-3), 1.77 (Ha-4), 1.87 (He-4), 2.41 (dd, J = 4.2, 12.6, H-5), 5.85 (d, J = 2.0, H-7), 3.27 (m, Ha-9), 1.67 (Ha-11), 1.78 (He-11), 2.13 (dt, J = 4.5, 13.0, Ha-12), 1.78 (He-12), 1.98 (Ha-15), 1.62 (He-15), 1.98 (Ha-16), 1.51 (Hb-16), 2.06 (H-17), 0.745 (s, CH_3-18), 1.01 (s, CH_3-19), 1.77 (H-20), 0.957 (d, J = 6.6, CH_3-21), 3.61 (br d, J = 10.1, H-22), 1.33 (Ha-23), 1.55 (Hb-23), 1.79 (Ha-24), 1.42 (Hb-24), 1.20 (s, CH_3-26), 1.21 (s, CH_3-27), Other: Ferulate″: 7.31 (s, H-2), 7.19 (H-5); β-D-Glcp′: 4.98 (d, J = 7.3, H-1), 3.53 (dd, J = 7.5, 9.0, H-2), 3.48 (t, J = 9.0, H-3), 3.43 (dd, J = 8.6, 9.5, H-4), 3.45 (ddd, J = 2.2, 5.2, 9.5, H-5), 3.70 (dd, J = 5.0, 12.0, Ha-6), 3.89 (dd, J = 1.8, 12.2, Hb-6) [1]
^{13}C NMR (CD_3OD) [1]:

Table 1

C-1	30.1	C-15	31.6	Ferulate-1″	130.4
2	26.3	16	26.9	2″	112.3
3	69.4	17	48.6	3″	150.7
4	30.3	18	15.9	4″	149.5
5	53.1	19	24.2	5″	117.1
6	205.6	20	43.3	6″	123.4
7	121.5	21	13.0	8″	117.5
8		22	75.0	9″	168.0
9	37.4	23	25.2	Glc′-1	102.1
10	37.4	24	42.2	2	74.85
11	21.5	25	71.1	3	77.6
12	32.0	26	29.0	4	71.29
13	48.2	27	29.3	5	78.06
14	85.4	CH_3O	56.7	6	62.2

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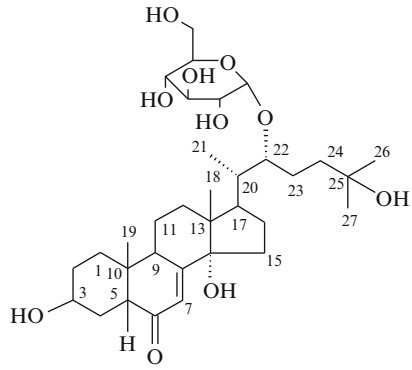
2-Deoxyecdysone-22-Glucoside

CAS Registry Number: 627511-32-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Silene pseudotites* [1, 2]
$C_{33}H_{54}O_{10}$: 610.3717
CI-MS m/z: 628 $[M + H + NH_3]^+$ (100), 611 $[M + H]^+$ (18), 610 $[M]^+$ (41), 593 $[M + H–H_2O]^+$ (7) [1, 2]
^{1}H NMR (J/Hz, D_2O): 4.10 (br s, He-3), 2.41 (dd, J = 3.2, 12.3, H-5), 5.97 (d, J = 2.1, H-7), 3.14 (br m, H-9), 2.18 (m, H-17), 0.74 (s, CH_3-18), 0.99 (br s, CH_3-19), 0.956 (d, J = 6.8, CH_3-21), 3.73 (br d, J = 10.5, H-22), 1.238 (s, CH_3-26), 1.243 (s, CH_3-27), Other: β-D-Glcp′: 4.53 (d, J = 8.0, H-1), 3.29 (dd, J = 8.1, 9.1, H-2), 3.48 (t, J = 9.3, H-3), 3.38 (t, J = 9.3, H-4), 3.45 (m, H-5), 3.70 (dd, J = 6.2, 12.4, Ha-6), 3.89 (dd, J = 2.3, 12.3, Hb-6) [1, 2]
^{13}C NMR (C_5D_5N): 101.8 (C-1′) [1, 2]

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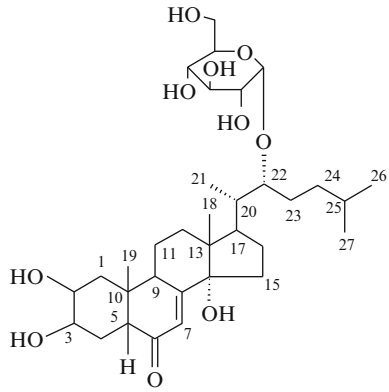
25-Deoxyecdysone-22-Glucoside

CAS Registry Number: 130690-20-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Microsorum scolopendria* [1]

$C_{33}H_{54}O_{10}$: 610.3717

CI/D-MS m/z: 610 $[M + NH_4–H_2O]^+$, 593 $[M + H–H_2O]^+$, 448 $[M + NH_4\text{-sugar}]^+$, 431 $[M + H\text{-sugar}]^+$, 415 $[M + H–H_2O\text{-sugar}]^+$, 350, 332, 226, 164, 136 [1]

^{1}H NMR (J/Hz, D_2O): 1.38 (Ha-1), 1.88 (He-1), 3.99 (Ha-2), 4.07 (He-3), 1.75 (Ha-4), 1.75 (He-4), 2.34 (t, H-5), 5.98 (d, J = 2.5, H-7), 3.10 (Ha-9), 1.70 (Ha-11), 1.84 (He-11), 1.87 (Ha-12), 1.87 (He-12), 1.62 (Ha-15), 2.05 (Hb-15), 1.95 (Ha-16), 1.87 (Hb-16), 1.87 (H-17), 2.14 (H-20), 0.737 (s, CH_3-18), 1.00 (s, CH_3-19), 0.936 (d, J = 6.6, CH_3-21), 3.73 (d, J = 10.0, Hb-22), 1.28 (m, Ha-23), 1.46 (Hb-23), 1.49 (Ha-24), 1.49 (Hb-24), 1.56 (H-25), 0.887 (d, J = 6.6, CH_3-26), 0.899 (d, J = 6.6, CH_3-27), Other: β-D-Glcp′: 4.52 (d, J = 8.2, H-1), 3.28 (dd, J = 9.8, 9.8, H-2), 3.47 (t, J = 9.0, H-3), 3.37 (t, J = 9.4H-4), 3.43 (m, H-5), 3.69 (dd, J = 6.2, 12.3, Ha-6), 3.87 (dd, J = 1.8, 12.3, Hb-6) [1]

^{13}C NMR (D_2O) [1]:

Table 1

C-1	37.7	C-12	33.0	C-23	
2	69.9	13	49.4	24	38.0
3	69.9	14	86.8	25	30.6
4	33.9	15	32.8	26	24.6
5	53.2	16		27	25.4
6		17	50.1	Glc′-1	107.4
7	123.5	18	17.8	2	76.6
8		19	25.8	3	78.9
9	36.5	20	42.9	4	72.7
10	41.8	21	15.5	5	78.6
11	22.8	22	89.9	6	63.3

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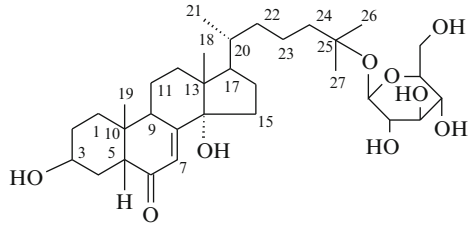
2,22-Deoxyecdysone-25-Glucoside

CAS Registry Number: 1140954-72-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Froelichia floridana* [1]

$C_{33}H_{54}O_9$: 594.3767

Mp: amorphous [1]

$[\alpha]_D^{21}$ + 14° (c 0.43, MeOH) [1]

UV λ_{max}^{MeOH} nm: 247 [1]

HR-ESI-MS m/z: for $C_{33}H_{54}O_9Na$ $[M + Na]^+$ calcd. 617.3666, found 617.3250 [1]

^{1}H NMR (600 MHz, J/Hz, DMSO-d_6): 1.43 (m, Ha-1), 1.62 (m, He-1), 1.65 (m, Ha-2), 1.80 (m, He-2), 3.98 (br s, He-3), 1.31 (m, Ha-4), 1.57 (m, Ha-4), 2.42 (dd, J = 12.1, 4.0, H-5), 5.81 (s, H-7), 3.34 (m, H-9), 1.53 (m, Ha-11), 1.74 (m, He-11), 2.08 (m, Ha-12), 1.77 (m, He-12), 1.58 (m, Ha-15), 1.95 (m, Hb-15), 2.06 (m, Ha-16), 1.42 (Hb-16), 1.97

(t, J = 9.5, H-17), 0.71 (s, CH_3-18), 0.97 (s, CH_3-19), 1.50 (m, H-20), 0.96 (d, J = 6.4, CH_3-21), 1.45 (m, Ha-22), 1.02 (m, Hb-22), 1.62 (m, Ha-23), 1.47 (m, Hb-23), 1.56 (m, Ha-24), 1.46 (m, Hb-24), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27), Other: β-D-Glcp′: 4.45 (d, J = 7.8, H-1), 3.13 (m, H-2), 3.36 (m, H-3), 3.30 (m, H-4), 3.24 (m, H-5), 3.82 (dd, J = 11.7, 2.3, Ha-6), 3.65 (m, Hb-6) [1]

^{13}C NMR (150 MHz, DMSO-d_6) [1]:

Table 1

C-1	29.9	C-12	32.4	C-23	21.8
2	29.0	13	48.3	24	43.7
3	65.6	14	86.1	25	79.2
4	33.4	15	31.9	26	26.9
5	52.5	16	28.0	27	27.1
6	207.0	17	52.0	Glc′-1	98.8
7	121.8	18	16.4	2	75.4
8	168.6	19	24.5	3	78.4
9	37.7	20	37.0	4	71.9
10	43.4	21	19.6	5	77.7
11	21.8	22	38.0	6	63.0

Pharm./Biol.: Human DNA Topoisomerase I test: not active [1].

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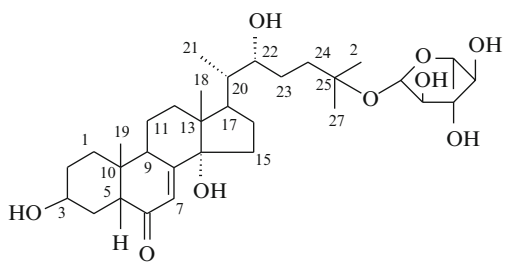
2-Deoxyecdysone-25-Rhamnoside

CAS Registry Number: 1019196-09-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Microsorum membranifolium* [1]

$C_{33}H_{54}O_9$: 594.3768

UV λ_{max}^{EtOH} nm: 242 [1]

CI-MS m/z: 612 $[M + NH_4]^+$, 595 $[M + H]^+$, 594 $[M]^+$, 577 $[M + H\text{-}H_2O]^+$, 559 $[M + H\text{-}2H_2O]^+$, 448 $[M + NH_4\text{-sugar}]^+$, 431 $[M + H\text{-sugar}]^+$, 413 $[M + H\text{-sugar-}H_2O]^+$, 395 $[M + H\text{-sugar-}2H_2O]^+$, 164 $[sugar]^+$ [1]

^{1}H NMR (J/Hz, CD_3OD): 1.46 (Ha-1), 1.64 (He-1), 1.66 (Ha-2), 1.82 (He-2), 3.98 (m, He-3), 1.57 (Ha-4), 1.79 (He-4), 2.42 (dd, J = 4.0, 12.3, H-5), 5.81 (br d, J = 2.4, H-7), 3.22 (m, Ha-9), 1.64 (Ha-11), 1.74 (He-11), 2.09 (m, Ha-12), 1.77 (He-12), 1.98 (Ha-15), 1.64 (He-15), 1.96 (Ha-16), 1.51 (Hb-16), 2.03 (H-17), 0.73 (s, CH_3-18), 0.97 (s, CH_3-19), 1.76 (H-20), 0.94 (d, J = 6.6, CH_3-21), 3.59 (br d, J = 10.6, H-22), 1.31 (Ha-23), 1.58 (Hb-23), 1.84 (Ha-24), 1.50 (Hb-24), 1.23 (s, CH_3-26), 1.25 (s, CH_3-27), Other: β-D-Rhap′: 4.95 (br d, J = 1.5, H-1), 3.68 (m, H-2), 3.69 (m, H-3), 3.34 (t, J = 9.3, H-4), 3.77 (dq, J = 6.3, 9.3, H-5), 1.235 (d, J = 6.3, CH_3-6) [1]

^{13}C NMR (CD_3OD) [1]:

Table 1

C-1	29.3	C-12	32.4	C-23	24.8
2	28.9	13	48.2	24	40.5
3	65.2	14	84.9	25	77.9
4	32.8	15	31.5	26	26.4
5	52.1	16	27.0	27	26.7
6	206.3	17	49.1	Glc′-1	97.1
7	121.5	18	15.9	2	73.8
8	168.6	19	24.2	3	72.6
9	37.5	20	43.3	4	74.2
10	37.5	21	13.0	5	69.7
11	21.8	22	75.3	6	17.7

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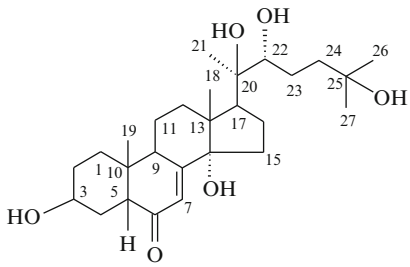
2-Deoxy-20-Hydroxyecdysone

CAS Registry Number: 17942-08-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Blechnum minus* [1], *B. pennamarina* [2], *Cheilantes seiberi* [3], *Coronaria flos-cuculi* [4], *Diploclisia glaucescens* [5], *Lychnis flos-cuculi* [6], *Microsorum membranifolium* [7], *M. scolopendria* [8], *Rhaponticum carthamoides* [9], *Serratula inermis* [10], *S. komarovii* [11], *Silene brachuica* [12], *S. chlorifolia* [13], *S. clavoformis* [14], *S. cretica, S. disticha* [13], *S. fridvaldszkyana*, *S. gigantea* L. [15], *S. italica* [13], *S. latifolia* [16], *S. linicola* [17], *S. otites* [18], *S. portensis* [13], *S. praemixta* [19], *S. pseudotites* [20], *S. roemeri* [21], *S. viridiflora* [22, 23], *S. wallichina* [24], *Stemmacantha uniflora* [25], *Trianthema galericulata* [3], *Vitex leptobortys* [26]

$C_{27}H_{44}O_6$: 464.3137

Mp: 254–256°C (EtOH–H_2O) [16], 215–218°C [27]

$[\alpha]_D^{22}$ + 82 ± 2° (c 0.5, MeOH) [17]

IR (KBr) ν_{max} cm^{-1}: 3370, 1645 [17], 3390, 2962, 1639, 1445, 1378, 1156, 1052, 1032, 949, 895, 872 [28]

UV λ_{max}^{EtOH} nm: 241 [27]

EI-MS m/z: 464 $[M]^+$ (1), 446 (3), 428 (10), 413 (8), 410 (14), 395 (6), 392 (6), 377 (5), 347 (35), 329 (90), 312 (33), 311 (28), 303 (9), 302 (11), 297 (13), 295 (14), 285 (30), 284 (35), 234 (15), 233 (15), 99 (100), 81 (73) [17]

FAB-MS m/z: 465 $[M + H]^+$, 447, 429, 411 [27]

FAB-HR-MS m/z: for $C_{27}H_{45}O_6$ $[M + H]^+$ calcd. 465.3215, found 465.3215 [28]

LSI-MS m/z: 463 $[M\text{-}H]^-$, 445 $[M\text{-}H\text{-}H_2O]^-$ [20]

^{1}H NMR (J/Hz, C_5D_5N): 4.12 (br s, H-3), 2.97 (m, H-5), 6.25 (d, J = 2.1, H-7), 3.54 (m, H-9), 3.03 (t, J = 9.0, H-17), 1.23 (s, CH_3-18), 1.05 (s, CH_3-19), 1.60 (s, CH_3-21), 3.88 (br d, J = 10.3, H-22), 1.36 (s, CH_3-26), 1.36 (s, CH_3-27) [28]

^{1}H NMR (J/Hz, CD_3OD): 3.98 (br s, H-3), 2.41 (dd, J = 4.2, 12.8, H-5), 5.79 (d, J = 2.1, H-7), 3.20 (m, H-9), 2.39 (t, J = 8.0, H-17), 0.88 (s, CH_3-18), 0.95 (s, CH_3-19), 1.19 (s, CH_3-21), 3.32 (dd, J = 1.5, 10.0, H-22), 1.18 (s, CH_3-26), 1.19 (s, CH_3-27) [28]

^{1}H NMR (J/Hz, D_2O): 1.38 (Ha-1), 1.85 (He-1), 1.38 (Ha-2), 1.65 (He-2), 4.11 (m, He-3), 1.62 (Ha-4), 1.75 (He-4), 2.40 (dd, J = 2.0, 12.0, H-5), 5.97 (d, J = 1.8, H-7), 3.16 (m, H-9), 1.71 (Ha-11), 1.84 (He-11), 1.96 (Ha-12), 1.70 (He-12), 2.07 (m, Ha-15), 1.65 (Hb-15), 1.90 (Ha-16), 1.80 (Hb-16), 2.34 (t, J = 9.3, H-17), 0.87 (s, CH_3-18), 0.98 (s, CH_3-19), 1.24 (s, CH_3-21), 3.43 (d, J = 10.0, H-22), 1.33 (Ha-23), 1.65 (Hb-23), 1.51 (d, J = 3.6, 12.5, Ha-24), 1.80 (Hb-24), 1.23 (s, CH_3-26), 1.24 (s, CH_3-27) [18]

^{13}C NMR (D_2O) [18]:

Table 1

C-1	28.6	C-10	37.1	C-19	24.1
2	28.0	11	21.0	20	78.9
3	65.7	12	31.9	21	20.6
4		13	48.3	22	78.3
5	52.3	14	86.1	23	27.0
6		15	31.1	24	41.6
7	121.8	16	21.0	25	72.5
8		17	50.3	26	28.3
9	37.1	18	18.0	27	29.2

^{13}C NMR (125 MHz, CD_3OD) [23]:

Table 2

C-1	29.9	C-10	37.8	C-19	24.5
2	29.0	11	22.0	20	78.1
3	65.6	12	32.9	21	21.2
4	33.5	13	49.4	22	78.6
5	52.5	14	85.6	23	27.5
6	206.7	15	31.8	24	42.5
7	122.1	16	21.7	25	71.5
8	168.6	17	50.7	26	29.1
9	34.9	18	18.2	27	29.8

Pharm./Biol.: *Galleria mellonella* bioassay: ED_{50} = 12.5 μg/g, *Sarcophaga bullata* bioassay: ED_{50} = 26.0 μg/g [29], *Drosophila melanogaster in vitro* bioassay: active [30], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 6.6 \times 10^{-7}$M [18, 31–33].

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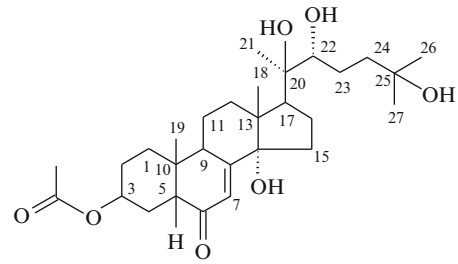
2-Deoxy-20-Hydroxyecdysone-3-Acetate

CAS Registry Number: 98149-16-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene praemixta* [1], *Silene otites* [2]

$C_{29}H_{46}O_7$: 506.3243
Mp: 150–152°C (MeOH–C_6H_6) [1]
$[\alpha]_D^{20}$ + 72.1 ± 2° (c 0.70, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}:3450, 1740, 1655, 1255 [1]
UV λ_{max}^{EtOH} nm (log ε): 246 (4.01) [1]
EI-MS m/z: 470 $[M\text{-}2H_2O]^+$ (1), 455 (8), 389 $[M\text{-}C_{22}\text{-}C_{27}]^+$ (100), 372 (96), 371 (96), 357 (23), 355 (22), 329 (88), 328 (85), 327 (24), 300 (95), 143 (96), 125 (96), 99 (97), 81 (96), 69 (96) [1]
CI-MS m/z: 524 $[M + H + NH_3]^+$, 507 $[M + H]^+$, 489 $[M + H\text{-}H_2O]^+$, 471 $[M + H\text{-}2H_2O]^+$, 453 $[M + H\text{-}3H_2O]^+$, 406 $[524\text{-}C_{22}\text{-}C_{27}]^+$, 363 $[507\text{-}C_{22}\text{-}C_{27}]^+$ [2]
CD (c, 0.10, MeOH): Δε = +1.43 (327 nm), Δε = −1.93 (253 nm) [1]
^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 5.03 (m, H-3), 6.23 (d, J = 2.4, H-7), 3.46 (m, H-9), 1.23 (s, CH_3-18), 1.02 (s, CH_3-19), 1.62 (s, CH_3-21), 3.91 (d, J = 9.2, H-22), 1.39 (s, CH_3-26), 1.39 (s, CH_3-27), 2.00 (s, CH_3COO-3) [1]
^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	29.5	C-11	21.5	C-21	21.5
2	25.6	12	31.5	22	77.5
3	68.3	13	48.5	23	27.4
4	29.7	14	84.3	24	42.6
5	52.1	15	32.2	25	69.5
6	201.8	16	21.5	26	30.0
7	121.2	17	50.1	27	30.0
8	166.5	18	17.8	$\underline{CH_3}COO$	21.1
				$CH_3\underline{COO}$	170.0
9	34.2	19	24.1		
10	36.6	20	76.8		

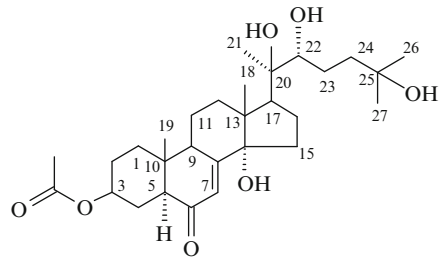
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.3 \times 10^{-6}$M [3].

References

1. Z. Saatov, M.B. Gorovits, N.D. Abdullaev, B.Z. Usmanov, N.K. Abubakirov, Chem. Nat. Comp. **21**, 56 (1985)
2. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, R. Lafont, J. Pharm. Biomed. Anal. **16**, 327 (1997)
3. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **41**, 1 (1999)

5α-2-Deoxy-20-Hydroxyecdysone-3-Acetate

CAS Registry Number: 188247-16-7



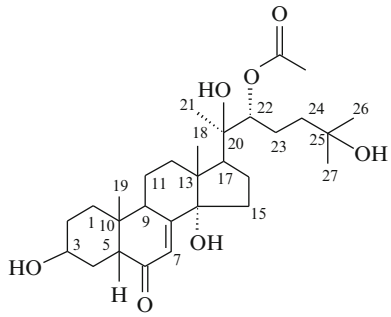
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Silene otites* [1]
$C_{29}H_{46}O_7$: 506.3243
Mp: 257–259°C (MeOH–$CHCl_3$) [2]
IR (KBr) ν_{max} cm^{-1}: 3420, 2958, 1735, 1712, 1656, 1464, 1381, 1237, 1135, 1029, 960, 902, 874, 835 [2]
EI-MS m/z: 389 $[M\text{-}C_6H_{13}O_2]^+$ (6), 371 (29), 329 (16), 327 (27), 311 (70), 293 (12), 285 (9), 267 (30), 161 (22), 143 (43), 125 (21), 117 (27), 107 (40), 99 (84), 91 (100) [2]
CI-MS m/z: 524 $[M + H + NH_3]^+$, 507 $[M + H]^+$, 489, 471, 453, 429, 406 [1]
FAB-MS m/z:, $C_{29}H_{45}O_7$ $[M\text{-}H]^-$ calcd. 505.3162, found 505.3165 [2]
^{1}H NMR (J/Hz, C_5D_5N): 4.78 (br m, H-3), 6.16 (d, J = 2.7, H-7), 2.99 (m, H-9), 3.00 (m, H-17), 1.19 (s, CH_3-18), 0.86 (s, CH_3-19), 1.58 (s, CH_3-21), 3.90 (d, J = 9.4, H-22), 1.38 (s, CH_3-26), 1.38 (s, CH_3-27), 2.00 (s, CH_3COO-3) [2]

References

1. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, R. Lafont, J. Pharm. Biomed. Anal. **16**, 327 (1997)
2. A. Suksamrarn, B. Yingyongnarongkul, Tetrahedron **53**, 3145 (1997)

2-Deoxy-20-Hydroxyecdysone-22-Acetate

CAS Registry Number: 117048-09-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene otites* [1]

$C_{29}H_{46}O_7$: 506.3243

IR (KBr) ν_{max} cm^{-1}: 3414, 2964, 1715, 1651, 1378, 1249, 1043, 949 [2]

CI-MS m/z: 507 $[M + H]^+$,489, 473, 471, 447, 429, 413, 411, 347, 329 [1]

HR-MS m/z: for $C_{29}H_{47}O_7$ $[M + H]^+$ calcd. 507.3321, found 507.3200 [1], for $C_{29}H_{47}O_7$ $[M + H]^+$ calcd. 507.3321, found 507.3320 [2]

^{1}H NMR (J/Hz, CD_3OD): 3.98 (m, He-3), 2.43 (dd, J = 4.0, 12.0, H-5), 5.79 (d, J = 2.5, H-7), 3.20 (m, H-9), 2.39 (m, H-17), 0.87 (s, CH_3-18), 0.95 (s, CH_3-19), 1.28 (s, CH_3-21), 4.87 (d, H-22), 1.15 (s, CH_3-26), 1.16 (s, CH_3-27), Other: 2.08 (s, CH_3COO-22) [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.12 (br s, He-3), 2.98 (m, H-5), 6.24 (d, J = 2.4, H-7), 3.53 (m, H-9), 3.01 (t, J = 8.8, H-17), 1.18 (s, CH_3-18), 1.04 (s, CH_3-19), 1.63 (s, CH_3-21), 5.50 (dd, J = 2.1, 10.6, H-22), 1.33 (s, CH_3-26), 1.34 (s, CH_3-27), Other: 2.02 (s, CH_3COO-22) [2]

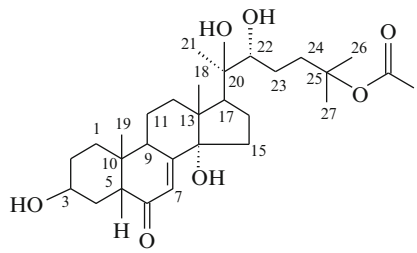
Pharm./Biol.: *Musca* bioassay: less active than 2-deoxy-20-hydroxyecdysone-3-acetate [2], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 2.4 \times 10^{-5}$M [3].

References

1. J.P. Girault, M. Bathori, E. Varga, K. Szendrei, R. Lafont, J. Nat. Prod. **53**, 279 (1990)
2. A. Suksamrarn, B. Yingyongnarongkul, Tetrahedron **52**, 12623 (1996)
3. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **41**, 1 (1999)

2-Deoxy-20-Hydroxyecdysone-25-Acetate

CAS Registry Number: 478809-55-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene wallichiana* [1]

$C_{29}H_{46}O_7$: 506.3243

Mp: 192–196°C (MeOH-H_2O) [1]

IR (KBr) ν_{max} cm^{-1}: 3378, 1721, 1255 [1]

EI-MS m/z: 410 $[M\text{-}CH_3COOH\text{-}2H_2O]^+$, 395, 392; 377, 336, 332, 331, 318, 287, 286, 285, 284, 237, 185, 144, 143, 99, 81, 69 [1]

^{1}H NMR (500.13 MHz, C_5D_5N): 4.15 (m, He-3), 6.20 (s, H-7), 3.56 (m, H-9), 1.27 (s, CH_3-18), 1.08 (s, CH_3-19), 1.61 (s, CH_3-21), 3.85 (m, H-22), 1.44 (s, CH_3-26), 1.51 (s, CH_3-27), 1.95 (CH_3COO) [1]

^{13}C NMR (125.27 MHz, C_5D_5N) [1]:

Table 1

C-1	29.19	C-11	21.61	C-21	22.33
2	29.51	12	31.67	22	77.53
3	64.18	13	46.73	23	27.00
4	32.40	14	84.43	24	39.42
5	51.85	15	32.01	25	82.44
6	203.41	16	21.70	26	26.21

(*continued*)

Table 1 (continued)

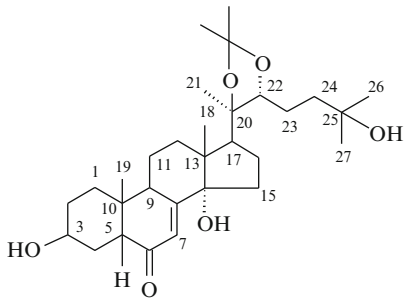
7	121.63	17	50.29	27	26.38
8	166.42	18	17.97	CH_3COO	21.21
9	33.32	19	24.47	CH_3COO	170.0
10	37.09	20	76.91		

References

1. N.Z. Mamadalieva, Z. Saatov, V.V. Kachala, A.S. Shashkov, Chem. Nat. Comp. **38**, 179 (2002)

2-Deoxy-20-Hydroxyecdysone-20,22-Acetonide

CAS Registry Number: 142735-52-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1], *S. viridiflora* [2]

$C_{30}H_{48}O_6$: 504.3450

Mp: amorphous [1]

$[\alpha]_D^{20}$ + 78.2 ± 2° (c 0.32, MeOH) [1], $[\alpha]_D^{25}$ + 14° (c 0.05, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3400–3500, 1670 [1]

UV λ_{max}^{MeOH} nm: 243 (log ε 3.7) [2]

EI-MS m/z: 504 (0.4) $[M]^+$, 489 (0.6), 486 (0.6), 471 (1.2), 453 (1.2), 429 (2), 411 (19), 405 (2), 393 (5), 347 (100), 329 (25), 285 (7.2), 234 (9), 233 (6), 201 (8), 143 (21), 125 (21), 102 (40), 99 (40), 81 (10) [1]

^{1}H NMR (100 MHz, C_5D_5N): 4.12 (m, He-3), 6.25 (br s, H-7), 3.47 (m, Ha-9), 1.05 (s, CH_3-18), 1.05 (s, CH_3-19), 1.56 (s, CH_3-21), 3.95 (m, H-22), 1.37 (s, CH_3-26), 1.37 (s, CH_3-27), Other; 1.37 and 1.48 (s, $(CH_3)_2C$) [1]

^{13}C NMR (125 MHz, CD_3OD) [2]:

Table 1

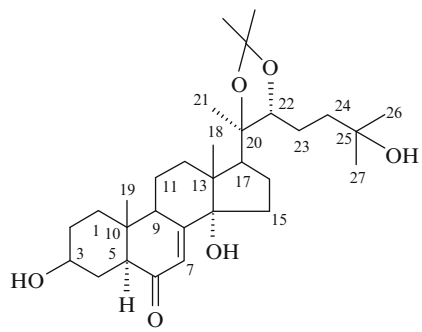
C-1	29.9	C-11	21.9	C-21	22.7
2	29.4	12	32.6	22	83.4
3	65.5	13	49.2	23	24.8
4	33.3	14	85.6	24	42.3
5	52.4	15	31.7	25	71.2
6	206.5	16	22.6	26	29.1
7	122.0	17	50.6	27	29.6
8	168.3	18	17.8	20,22-iPr	27.3
9	34.6	19	24.5		29.5
10	37.6	20	85.9		108.6

References

1. M.X. Djukharova, Z. Saatov, M.B. Gorovits, N.K. Abubakirov, Chem. Nat. Comp. **27**, 207 (1991)
2. A. Simon, N. Toth, G. Toth, Z. Kele, J. Groska, M. Bathori, Helv. Chim. Acta. **92**, 753 (2009)

5α-2-Deoxy-20-Hydroxyecdysone-20,22-Acetonide

CAS Registry Number: 188246-96-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *S. viridiflora* [1]
$C_{30}H_{48}O_6$: 504.3451
$[\alpha]_D^{25}$ + 57° (c 0.05, MeOH) [1]
UV λ_{max}^{MeOH} nm: 238 (log ε 3.4) [1]
ESI-MS m/z: 1031 $[2M + Na]^+$ (9), 544 $[M + H + K]^+$ (9), 528 $[M + H + Na]^+$ (14), 527 $[M + Na]^+$ (41), 504 $[M]^+$ (10), 487 $[M + H\text{-}H_2O]^+$ (39), 429 $[M + H\text{-}H_2O\text{-acetone}]^+$ (100), 413 (23), 391 (60), 333 (21) [1]
HR-ESI-MS m/z: for $C_{30}H_{48}NaO_6$ $[M + Na]^+$ calcd. 527.3349, found 527.3336 [1]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.87 (m, Ha-1), 1.38–1.43 (d, J = 12.5, He-1), 1.37–1.41 (m, Ha-2), 1.76–1.82 (m, He-2), 3.55 (tt, J = 11.0, 4.4, He-3), 1.365 (q, J = 12.0, Ha-4), 2.07–2.14 (m, He-4), 2.355 (dd, J = 12.2, 3.6, H-5), 5.83 (d, J = 2.8, H-7), 2.75 (ddd, J = 11.7, 7.2, 2.7, H-9), 1.75–1.82 (m, Ha-11), 1.60–1.66 (m, Hb-11), 2.07–2.16 (m, Ha-12), 1.78–1.86 (m, He-12), 1.615 (t, J = 13.0, Ha-15), 1.93–1.98 (m, Hb-15), 1.83–1.89 (m, Ha-16), 1.99–2.07 (m, Hb-16), 2.30 (dd, J = 9.1, 8.6, H-17), 0.826 (s, CH_3-18), 0.854 (s, CH_3-19), 1.175 (s, CH_3-21), 3.66–3.71 (m, H-22), 1.47–1.58 (m, Ha-23), 1.47–1.58 (m, Hb-23), 1.44–1.53 (m, Ha-24), 1.69–1.78 (m, Hb-24), 1.196 (s, CH_3-26), 1.205 (s, CH_3-27), Other: 1.32 and 1.39 (s, 20,22-iPr) [1]
^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

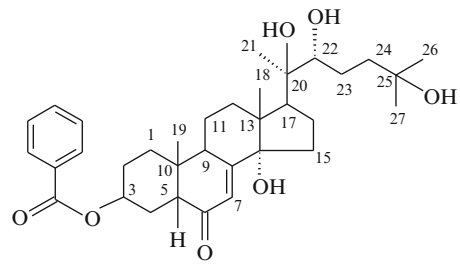
C-1	38.0	C-11	21.7	C-21	22.7
2	31.5	12	32.4	22	83.5
3	71.31	13	48.4	23	24.9
4	31.0	14	85.3	24	42.4
5	54.7	15	31.9	25	71.27
6	203.3	16	22.5	26	29.1
7	123.6	17	50.7	27	29.6
8	166.5	18	17.8	20,22-iPr	27.3
9	47.6	19	13.4		29.5
10	39.7	20	86.0		108.2

References

1. A. Simon, N. Toth, G. Toth, Z. Kele, J. Groska, M. Bathori, Helv. Chim. Acta. **92**, 753 (2009)

2-Deoxy-20-Hydroxyecdysone-3-Benzoate

CAS Registry Number: 345958-46-5



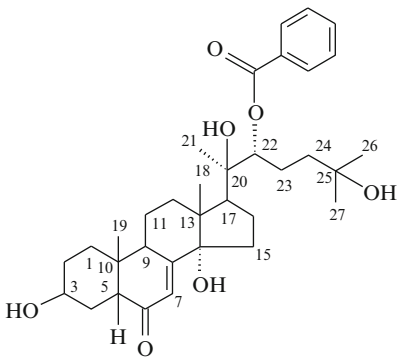
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Silene wallichiana* [1]
$C_{34}H_{48}O_7$: 568.3400
Mp: 210–212°C (EtOH–H_2O) [1]
$[\alpha]_D^{23}$ + 72.3 ± 2° (c 0.5, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3400–3440, 1733, 1665, 1610, 1290, 720 [1]
EI-MS m/z: 514 $[M\text{-}3H_2O]^+$, 410, 386, 347, 340, 338, 337, 329, 311, 303, 279, 256, 234, 233, 122, 105, 99, 83, 81, 77, 69 [1]
^{1}H NMR (C_5D_5N): 5.22 (br s, He-3), 6.12 (H-7), 3.40 (m, H-9), 1.12 (s, CH_3-18), 0.92 (s, CH_3-19), 1.50 (s, CH_3-21), 3.80 (m, H-22), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27), Other: Ar-H: 7.37 (3H), 8.12 (2H) [1]

References

1. N.Z. Mamadalieva, N.Sh. Ramazanov, L. Dinan, Z. Saatov, Chem. Nat. Comp. **36**, 513 (2000)

2-Deoxy-20-Hydroxyecdysone-22-Benzoate

CAS Registry Number: 128529-85-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene tatarica* [1]

$C_{34}H_{48}O_7$: 568.3400

IR (KBr) ν_{max} cm^{-1}: 3404, 2964, 1698, 1649, 1449, 1380, 1281, 1116, 1039, 946, 894, 754, 711 [2]

CI-MS m/z: 569 $[M + H]^+$, 551, 533, 447, 429, 411, 347, 329 [1]

HR-MS m/z: for $C_{34}H_{49}O_7$ $[M + H]^+$ calcd. 569.3477, found 569.3479 [2]

^{1}H NMR (J/Hz, CD_3OD): 3.98 (br m, He-3), 2.38 (dd, J = 5.0, 12.0, H-5), 5.81 (d, J = 2.5, H-7), 3.20 (m, H-9), 2.47 (t, J = 8.5, H-17), 0.89 (s, CH_3-18), 0.95 (s, CH_3-19), 1.42 (s, CH_3-21), 5.15 (dd, J = 2.0, 12.0, H-22), 1.15 (s, CH_3-26), 1.16 (s, CH_3-27), Other: C_6H_5COO: 7.48 (t, J = 7.0, H-3′, H-5′), 8.07 (t, J = 7.0, H-2′, H-6′), 7.60 (t, J = 7.0, H-4′) [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.13 (br s, He-3), 2.98 (m, H-5), 6.24 (d, J = 1.8, H-7), 3.55 (m, H-9), 3.11 (t, J = 9.1, H-17), 1.21 (s, CH_3-18), 1.05 (s, CH_3-19), 1.78 (s, CH_3-21), 5.79 (dd, J = 1.7, 10.5, H-22), 1.30 (s, CH_3-26), 1.31 (s, CH_3-27), Other: C_6H_5COO: 7.35 (m, H-3′, H-5′), 8.27 (m, H-2′, H-6′), 7.46 (m, H-4′) [2]

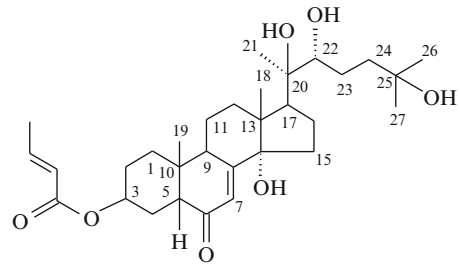
Pharm./Biol.: *Musca* bioassay: very low activity [2], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 6.3 \times 10^{-6}$M [3–5].

References

1. J.P. Girault, M. Bathori, E. Varga, K. Szendrei, R. Lafont, J. Nat. Prod. **53**, 279 (1990)
2. A. Suksamrarn, B. Yingyongnarongkul, Tetrahedron **52**, 12623 (1996)
3. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **41**, 1 (1999)
4. L. Dinan, R.E. Hormann, T. Fujimoto, J. Computer-Aided Mol. Design. **13**, 185 (1999)
5. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput Sci. **41**, 1587 (2001)

2-Deoxy-20-Hydroxyecdysone-3-Crotonate

CAS Registry Number: 200867-02-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene otites* [1]

$C_{31}H_{48}O_7$: 532.3400

CI-MS m/z: 550 $[M + H + NH_3]^+$, 533 $[M + H]^+$, 447 $[M + H\text{-crotonic acid}]^+$, 432 $[550\text{-}C_{22}\text{-}C_{27}]^+$, 417 $[M + H\text{-}C_{22}\text{-}C_{27}]^+$ [1]

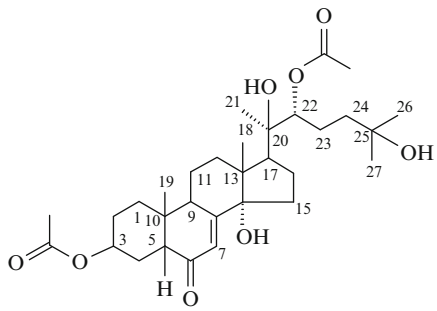
^{1}H NMR (J/Hz, $CDCl_3$): 5.13 (br s, He-3), 2.39 (dd, H-5), 5.85 (d, J = 2.5, H-7), 3.11 (m, H-9), 2.37 (H-17), 0.86 (s, CH_3-18), 0.98 (s, CH_3-19), 1.21 (s, CH_3-21), 3.44 (d, J = 10.0, H-22), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27), Other: 1.87 (dd, J = 1.6, 7.1, CH_3CH), 5.83 (dq, J = 6.0, 16.1, CH-a), 6.95 (dq, J = 7.1, 16.0, CH-b) [1].

References

1. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, R. Lafont, J. Pharm. Biomed. Anal. **16**, 327 (1997)

2-Deoxy-20-Hydroxyecdysone-3,22-Diacetate

CAS Registry Number: 102942-11-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene otites* [1]

$C_{31}H_{48}O_8$: 548.3349

CI-MS m/z: 566 $[M + H + NH_3]^+$, 549 $[M + H]^+$, 531 $[M + H\text{-}H_2O]^+$, 506 $[M + H + NH_3\text{-acetic acid}]^+$, 489 $[M + H\text{-acetic acid}]^+$, 471 $[489\text{-}H_2O]^+$, 453 $[489\text{-}2H_2O]^+$, 406, 389 [1]

^{1}H NMR (J/Hz, $CDCl_3$): 5.07 (br s, He-3), 2.37 (H-5), 5.84 (d, J = 2.5, H-7), 3.09 (m, H-9), 2.38 (H-17), 0.84 (s, CH_3-18), 0.97 (s, CH_3-19), 1.26 (s, CH_3-21), 4.85 (dd, J = 2.0, 11.0, H-22), 1.20 (s, CH_3-26), 1.22 (s, CH_3-27), Other: 2.04 (s, CH_3COO-3), 2.10 (s, CH_3COO-22) [1]

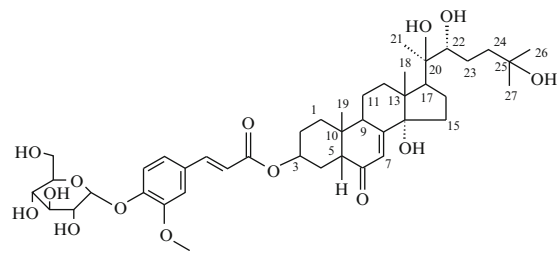
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: inactive [2].

References

1. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, R. Lafont, J. Pharm. Biomed. Anal. **16**, 327 (1997)
2. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **41**, 1 (1999)

2-Deoxy-20-Hydroxyecdysone-3-[4-(1-β-D-Glucopyranosyl)]-Ferulate

CAS Registry Number: 1019196-08-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Microsorum membranifolium* [1]

$C_{43}H_{62}O_{14}$: 802.4139

UV λ_{max}^{EtOH} nm: 240, 294, 317 [1]

FAB-MS m/z: 841 $[M + K]^+$, 825 $[M + Na]^+$, 803 $[M + H]^+$, 785 $[M + H\text{-}H_2O]^+$, 767 $[M + H\text{-}2H_2O]^+$, 749 $[M + H\text{-}3H_2O]^+$, 641 [M + H-sugar]$^+$, 623 $[M + H\text{-sugar-}H_2O]^+$, 605 $[M + H\text{-sugar-}2H_2O]^+$, 447, 429, 411, 393, 345, 329, 327, 309, 241 [1]

^{1}H NMR (J/Hz, CD_3OD): 1.46 (Ha-1), 1.76 (He-1), 1.87 (Ha-2), 1.94 (He-2), 5.18 (m, He-3), 1.77 (Ha-4), 1.87 (He-4), 2.40 (dd, J = 3.4, 12.0, H-5), 5.84 (d, J = 2.4, H-7), 3.27 (Ha-9), 1.68 (Ha-11), 1.76 (He-11), 2.15 (dt, J = 4.8, 13.8, Ha-12), 1.88 (He-12), 2.00 (Ha-15), 1.63 (He-15), 2.00 (Ha-16), 1.76 (Hb-16), 2.42 (t, J = 9.9, H-17), 0.907 (s, CH_3-18), 0.97 (s, CH_3-19), 1.203 (s, CH_3-21), 3.35 (H-22), 1.31 (Ha-23), 1.69 (Hb-23), 1.81 (Ha-24), 1.46 (Hb-24), 1.197 (s, CH_3-26), 1.211 (s, CH_3-27), Other: Ferulate″: 7.31 (s, H-2), 7.19 (H-5), 7.19 (H-6), 7.66 (d, J = 15.8, H-7), 6.50 (d, J = 15.8, H-8), 3.92 (s, CH_3O); β-D-Glcp′: 4.98 (d, J = 7.3, H-1), 3.53 (dd, J = 7.5, 9.0, H-2), 3.48 (t, J = 9.0, H-3), 3.43 (dd, J = 8.6, 9.5, H-4), 3.45 (ddd, J = 2.2, 5.2, 9.5, H-5), 3.70 (dd, J = 5.0, 12.0, Ha-6), 3.89 (dd, J = 1.8, 12.2, Hb-6) [1]

^{13}C NMR (CD_3OD) [1]:

Table 1

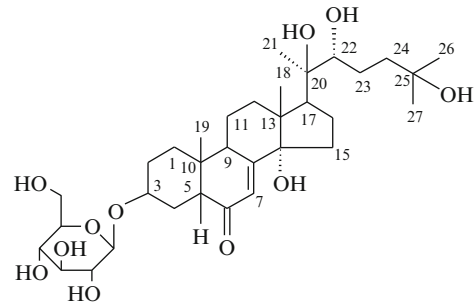
C-1	30.1	C-16	21.4	3″	150.7
2	26.3	17	50.5	4″	149.5
3	69.4	18	17.9	5″	117.1
4	26.3	19	24.2	6″	123.4
5	53.0	20	77.7	7″	145.8
6	206.1	21	20.8	8″	117.5
7	121.7	22	78.3	9″	168.0
8		23	27.3	Glc′-1	102.1
9	37.3	24	42.2	2	74.85
10	37.3	25	71.1	3	77.6
11	21.4	26	29.0	4	71.29
12	32.5	27	29.3	5	78.06
13	49.0	Ferulate-CH_3O	56.7	6	62.41
14	85.4	Ferulate-1″	130.4		
15	31.7	2″	112.3		

References

1. R. Ho, J.P. Girault, P.Y. Cousteau, J.P. Bianchini, P. Raharivelomanana, R. Lafont, J. Chrom. Sci. **46**, 102 (2008)

2-Deoxy-20-Hydroxyecdysone-3-Glucoside

CAS Registry Number: 136849-87-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Sida rhombifolia L.* [1], *Tinospora capillipes* [2]

$C_{33}H_{54}O_{11}$: 626.3666

Mp: 271–273°C [2]

$[\alpha]_D^{20}$ + 63.6° (c 0.28, MeOH) [2]

FAB-MS m/z: 649 $[M + Na]^+$, 665 $[M + K]^+$ [2]

^{13}C NMR (C_5D_5N) [2]:

Table 1

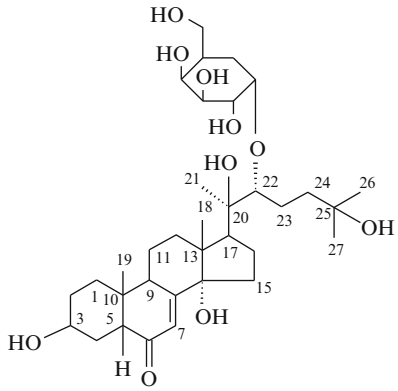
C-1	29.45	C-12	31.49	C-23	27.38
2	27.38	13	48.44	24	42.51
3	75.12	14	84.27	25	69.52
4	29.45	15	32.14	26	29.98
5	51.47	16	21.56	27	29.98
6	202.72	17	50.04	Glc′-1	103.19
7	121.32	18	17.77	2	72.35
8	166.26	19	23.91	3	78.18
9	34.45	20	76.48	4	71.63
10	36.61	21	21.56	5	78.48
11	21.56	22	77.48	6	62.78

References

1. A.N. Jadhav, R.S. Pawar, B. Avula, I.A. Khan, Chem. Biodivers. **4**, 2225 (2007)
2. C. Song, R. Xu, Chin. Chem. Lett. **2**, 13 (1991)

2-Deoxy-20-Hydroxyecdysone-22-Glucoside

CAS Registry Number: 478062-03-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene italica* ssp. *nemoralis* [1]

$C_{33}H_{54}O_{11}$: 624.3510

EI-MS m/z: 633 $[M + Li]^+$, 615 $[M\text{-}H_2O + Li]^+$, 471 $[M\text{-}Glu + Li]^+$, 459 $[M\text{-}Glu\text{-}H_2O + Li]^+$, 435 $[M\text{-}Glu\text{-}2H_2O + Li]^+$, 417 $[M\text{-}Glu\text{-}3H_2O + Li]^+$, 329 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.39 (Ha-1), 1.70 (He-1), 1.67 (Ha-2), 1.85 (He-2), 4.12 (m, He-3), 1.62 (Ha-4), 1.77 (He-4), 2.41 (dd, J = 2.5, 12.0, H-5), 5.97 (d, J = 2.2, H-7), 3.17 (m, H-9), 1.67 (Ha-11), 1.78 (He-11), 1.97 (Ha-12), 1.70 (He-12), 2.08 (m, Ha-15), 1.65 (Hb-15), 1.94 (Ha-16), 1.79 (Hb-16), 2.29 (t, J = 9.5, H-17), 0.88 (s, CH_3-18), 0.98 (s, CH_3-19), 1.29 (s, CH_3-21), 3.65 (br d, J = 7.0, H-22), 1.55 (m, Ha-23), 1.75 (Hb-23), 1.97 (Ha-24), 1.55 (Hb-24), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27), Other: β-D-Glcp′: 4.54 (d, J = 7.8, H-1), 3.38 (dd, J = 7.8, 9.0, H-2), 3.52 (t, J = 9.0, H-3), 3.46 (m, H-4), 3.46 (m, H-5), 3.93 (d, J = 12.5, Ha-6), 3.76 (dd, J = 5.0, 12.0, Hb-6) [2]

^{13}C NMR (125 MHz, D_2O) [2]:

Table 1

C-1	30.8	C-12	33.9	C-23	26.8
2	29.5	13	50.5	24	42.3
3	67.2	14	87.9	25	74.2
4	34.2	15	32.6	26	30.0
5	53.8	16	22.6	27	30.8
6		17	52.2	Glc′-1	105.8
7	123.3	18	19.5	2	76.1
8		19	25.6	3	78.4
9	39.1	20	79.9	4	72.3
10	39.1	21	23.4	5	78.5
11	22.7	22	90.6	6	63.0

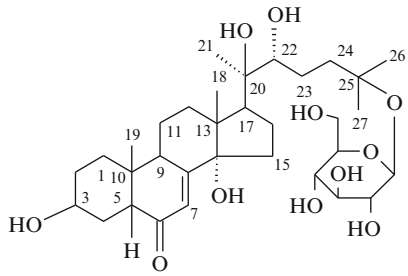
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 3.0 \times 10^{-6}$M [2].

References

1. M. Bathori, Z. Pongracz, G. Toth, A. Simon, L. Kandra, Z. Kele, R. Ohmacht, J. Chrom. Sci. **40**, 409 (2002)
2. A. Maria, J.P. Girault, Z. Saatov, J. Harmatha, L. Dinan, R. Lafont, J. Chrom. Sci. **43**, 149 (2005)

2-Deoxy-20-Hydroxyecdysone-25-Glucoside

CAS Registry Number: 1236075-32-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene fridvaldszkyana* [1]

$C_{33}H_{54}O_{11}$: 626.3666

UV λ_{max}^{EtOH} nm: 242 [1]

CI-MS m/z: 644 $[M + H + NH_3]^+$, 626 $[M]^+$, 610, 592, 482, 465, 447, 429, 411, 363, 345, 329 [1]

^{1}H NMR (J/Hz, D_2O): 1.35 (Ha-1), 1.68 (He-1), 1.87 (Ha-2), 1.69 (He-2), 4.14 (m, He-3), 1.63 (Ha-4), 1.76 (He-4), 2.42 (br d, J = 12.0, H-5), 5.99 (d, J = 2.4, H-7), 3.18 (m, H-9), 1.69 (Ha-11), 1.82 (He-11), 1.97 (Ha-12), 1.97 (He-12), 1.67 (Ha-15), 2.09 (Hb-15), 1.81 (Ha-16), 1.91 (Hb-16), 2.35 (t, J = 9.5, H-17), 0.88 (s, CH_3-18), 1.00 (s, CH_3-19), 1.25 (s, CH_3-21), 3.44 (d, J = 9.7, H-22), 1.73 (Ha-23), 1.39 (Hb-23), 1.86 (Ha-24), 1.61 (Hb-24), 1.30 (s, CH_3-26), 1.30 (s, CH_3-27), Other: β-D-Glcp′: 4.67 (d, J = 8.1, H-1), 3.23 (dd, J = 9.3, 8.1, H-2), 3.53 (t, J = 9.3, H-3), 3.37 (t, J = 9.3, H-4), 3.48 (m, H-5), 3.92 (dd, J = 12.5, 2.3, Ha-6), 3.70 (dd, J = 12.5, 6.6, Hb-6) [1]

^{1}H NMR (J/Hz, CD_3OD): 1.36 (Ha-1), 1.61 (He-1), 1.83 (Ha-2), 1.70 (He-2), 3.99 (He-3), 1.59 (Ha-4), 1.85 (He-4), 2.43 (dd, J = 12.5, 4.2, H-5), 5.81 (d, J = 2.1, H-7), 3.15 (m, H-9), 1.70 (Ha-11), 1.74 (He-11), 2.12 (Ha-12), 1.82 (He-12), 1.61 (Ha-15), 1.98 (Hb-15), 1.76 (Ha-16), 1.98 (Hb-16), 2.40 (m, H-17), 0.89 (s, CH_3-18), 0.96 (s, CH_3-19), 1.19 (s, CH_3-21), 3.36 (d, H-22), 1.75 (Ha-23), 1.46 (Hb-23), 1.96 (Ha-24), 1.51 (Hb-24), 1.27 (s, CH_3-26), 1.28 (s, CH_3-27), Other: β-D-Glcp′: 4.46 (d, J = 7.9, H-1), 3.17 (dd, J = 9.5, 8.1, H-2), 3.36 (H-3), 3.24 (H-4), 3.26 (H-5), 3.88 (dd, J = 11.6, 1.8, Ha-6), 3.65 (Hb-6) [1]

^{13}C NMR (D_2O) [1]:

Table 1

C-1	29.3	C-12	32.3	C-23	26.8
2	28.1	13	48.9	24	39.7
3	65.8	14	86.8	25	80.9
4	32.7	15	31.3	26	26.9
5	52.3	16	21.3	27	26.9
6	n.d.	17	50.3	Glc′-1	97.8
7	122.0	18	18.2	2	74.6
8	n.d.	19	24.2	3	77.1
9	36.7	20	78.2	4	71.2
10	37.7	21	20.6	5	77.1
11	21.3	22	78.2	6	62.3

^{13}C NMR (CD_3OD) [1]:

Table 2

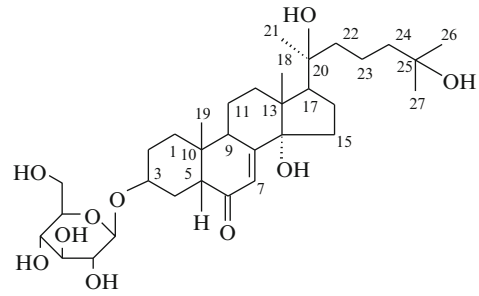
C-1	29.5	C-12	32.6	C-23	26.5
2	28.7	13	49.1 (q)	24	39.8
3	65.3	14	85.6 (q)	25	78.6
4	33.0	15	32.6	26	27.2
5	52.2	16	21.4	27	27.2
6	n.d.	17	50.3	Glc′-1	98.5
7	121.9	18	17.8	2	75.0
8	n.d.	19	24.2	3	78.0
9	37.6	20	77.6	4	71.7
10	37.6 (q)	21	20.8	5	77.6
11	21.4	22	78.5	6	62.8

References

1. L. Zibareva, V.I. Yeriomina, N. Munkhjargal, J.P. Girault, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **72**, 234 (2009)

2,22-Deoxy-20-Hydroxyecdysone-3-Glucoside

CAS Registry Number: 360049-27-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cucubalis baccifer* [1]

$C_{33}H_{54}O_{10}$: 610.3717

$[\alpha]_D^{28}$ + 49° (c 1.1, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3348, 1653 [1]

UV λ_{max}^{EtOH} nm: 244 [1]

FAB-MS m/z: 609 $[M-H]^-$ (100), 447 $[M-163]^-$ (12) [1]

^{1}H NMR (J/Hz, CD_3OD): 3.85 (d, J = 1.7, H-3), 5.80 (d, J = 1.8, H-7), 0.94 (s, CH_3-18), 0.84 (s, CH_3-19), 1.24 (s, CH_3-21), 1.18 (s, CH_3-26), 1.18 (s, CH_3-27), Other: β-D-Glcp′: 4.35 (d, J = 7.8, H-1) [1]

^{13}C NMR (CD_3OD) [1]:

Table 1

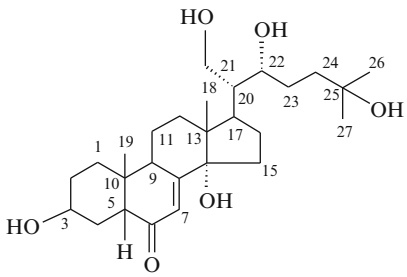
C-1	30.19	C-10	37.49	C-19	24.24
2	27.93	11	22.03	20	75.99
3	71.48	12	32.57	21	26.49
4	31.49	13	48.58	22	45.70
5	53.44	14	85.71	23	20.08
6	206.30	15	32.57	24	45.88
7	121.91	16	20.08	25	71.48
8	168.97	17		26	29.34
9		18	18.12	27	29.15

References

1. Y.X. Cheng, J. Zhou, N.H. Tan, Z.T. Ding, Acta Botanica Sinica **43**, 316 (2001)

2-Deoxy-21-Hydroxyecdysone

CAS Registry Number: 232280-38-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene otites* [1]

$C_{27}H_{44}O_6$: 464.3137

CI-MS m/z: 482 $[M + H + NH_3]^+$, 465 $[M + H]^+$, 452, 447 (base peak), 435, 429, 417, 411, 399, 393, 366, 349, 331, 313, 116 [1]

^{1}H NMR (250 MHz, J/Hz, D_2O): 1.36 (Ha-1), 1.85 (He-1), 1.36 (Ha-2), 1.68 (He-2), 4.10 (m, He-3), 1.62 (Ha-4), 1.76 (He-4), 2.40 (dd, J = 12.5, 2.0, H-5), 5.97 (d, J = 2, H-7), 3.14 (m, H-9), 1.66 (Ha-11), 1.81 (He-11), 1.91 (Ha-12), 1.75 (He-12), 2.09 (Ha-15), 1.64 (Hb-15), 1.97 (Ha-16), 1.62 (Hb-16), 2.07 (H-17), 0.77 (s, CH_3-18), 0.98 (s, CH_3-19), 1.92 (H-20), 3.90 (dd, J = 11.2, 4.1, Ha-21), 3.76 (dd, J = 11.2, 7.2, Hb-21), 3.78 (H-22), 1.53 (Ha-23), 1.67 (Hb-23), 1.48 (Ha-24), 1.82 (Hb-24), 1.236 (s, CH_3-26), 1.243 (s, CH_3-27) [1]

^{13}C NMR (D_2O) [1]:

Table 1

C-1	29.2	C-10	37.4	C-19	24.2
2		11	21.0	20	48.5
3	65.7	12	31.2	21	62.2
4		13	48.0	22	75.8
5	52.3	14	86.5	23	27.1
6		15	31.4	24	41.8
7	121.8	16	26.4	25	72.7
8		17	44.4	26	28.6
9	37.4	18	16.6	27	29.2

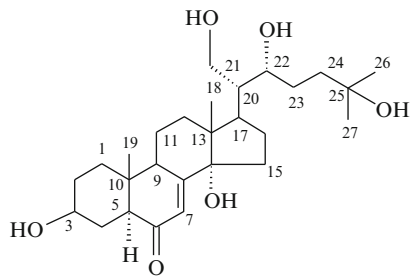
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.3 \times 10^{-6}$M [1].

References

1. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **41**, 1 (1999)

5α-2-Deoxy-21-Hydroxyecdysone

CAS Registry Number: 232280-39-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene otites* [1]

$C_{27}H_{44}O_6$: 464.3137

CI-MS m/z: 482 $[M + H + NH_3]^+$, 465 [M + H], 452, 447, 435, 429 (base peak), 417, 411, 399, 393, 366, 349, 331, 313, 116 [1]

^{1}H NMR (250 MHz, J/Hz, D_2O): 1.49 (Ha-1), 1.66 (He-1), 1.81 (Ha-2), 1.49 (He-2), 3.70 (m, He-3), 1.39 (Ha-4), 2.09 (He-4), 2.58 (dd, J = 12.1, 2.0, H-5), 5.99 (d, J = 2.0, H-7), 2.74 (m, H-9), 1.64 (Ha-11), 1.81 (He-11), 1.93 (Ha-12), 1.73 (He-12), 2.05 (Ha-15), 1.65 (Hb-15), 1.95 (Ha-16), 1.63 (Hb-16), 2.05 (H-17), 0.77 (s, CH_3-18), 0.87 (s, CH_3-19), 1.94 (H-20), 3.91 (dd, J = 11.4, 4.0, Ha-21), 3.77 (dd, J = 11.4, 7.0, Hb-21), 3.79 (H-22), 1.53 (Ha-23), 1.67 (Hb-23), 1.49 (Ha-24), 1.83 (Hb-24), 1.236 (s, CH_3-26), 1.243 (s, CH_3-27) [1]

^{13}C NMR (D_2O) [1]:

Table 1

C-1	37.1	C-10	39.6	C-19	13.1
2		11		20	48.5
3		12	30.8	21	62.0
4		13	47.4	22	75.3
5	54.2	14	86.1	23	27.1
6		15		24	41.6
7	123.4	16		25	72.7
8		17	44.4	26	28.6
9	46.9	18	16.5	27	29.2

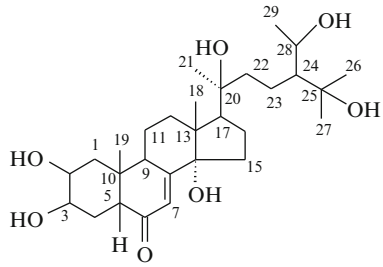
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 9.5 \times 10^{-5}$M [1].

References

1. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **41**, 1 (1999)

22-Deoxy-28-Hydroxymakisterone C

CAS Registry Number:1042045-42-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{29}H_{48}O_7$: 508.3400

$[\alpha]_D^{20}$ + 34.9° (c 0.16, EtOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3400, 1652, 1060 [1]

ESI-MS m/z: 509 $[M + H]^+$, 491 $[M + H\text{-}H_2O]^+$, 473 $[M + H\text{-}2H_2O]^+$, 455 $[M + H\text{-}3H_2O]^+$, 447 $[M + H\text{-}C_3H_8O]^+$, 429 $[M + H\text{-}C_3H_8O\text{-}H_2O]^+$, 411 $[M + H\text{-}C_3H_8O\text{-}2H_2O]^+$, 171, 153, 135 [1]

HR-ESI-MS m/z: for $C_{29}H_{48}O_7Na$ $[M + Na]^+$ calcd. 531.3298, found 531.3291 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.78 (Ha-1), 1.43 (He-1), 3.83 (ddd, J = 3.0, 4.2, 12.0, Ha-2), 3.95 (q, J = 3.0, He-3), 1.70 (Ha-4), 1.70 (He-4), 2.38 (dd, J = 4.4, 12.6, H-5), 5.81 (d, J = 2.5, H-7), 3.15 (ddd, J = 2.5, 7.0, 11.5, Ha-9), 1.80 (Ha-11), 1.69 (He-11), 2.11 (dt, J = 5.0, 13.0, 13.0, Ha-12), 1.83 (He-12), 1.95 (Ha-15), 1.62 (He-15), 1.86 (Ha-16), 1.92 (Hb-16), 2.27 (dd, J = 8.2, 9.8, H-17), 0.854 (s, CH_3-18), 0.963 (s, CH_3-19), 1.264 (s, CH_3-21), 1.68 (Ha-22), 1.47 (He-22), 1.28 (Ha-23), 1.06 (Hb-23), 1.23 (Ha-24), 1.233 (s, CH_3-26), 1.247 (s, CH_3-27), 3.90 (dq, J = 6.2, 6.2, 6.2, 9.0, H-28), 1.234 (d, J = 6.2, CH_3-29) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

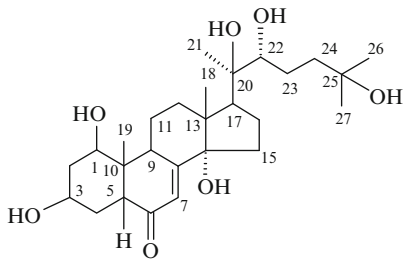
C-1	37.39	C-11	21.54	C-21	20.96
2	68.72	12	32.51	22	77.22
3	68.52	13	49.0	23	33.06
4	33.00	14	85.20	24	50.30
5	51.81	15	31.80	25	74.14
6	206.50	16	21.62	26	25.97
7	122.12	17	50.43	27	29.09
8	168.04	18	18.06	28	25.61
9	35.12	19	24.40	29	14.35
10	39.27	20	78.04		

References

1. M. Budesinsky, K. Vokas, J. Harmatha, J. Cvacka, Steroids **73**, 502 (2008)

2-Deoxyintegristerone A

CAS Registry Number: 117048-08-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene italica* ssp. *nemoralis* [1], *S. otites* [2, 3], *S. viridiflora* [4]

$C_{27}H_{44}O_7$: 480.3087

CI-MS m/z: 498 $[M + H + NH_3]^+$, 481 $[M + H]^+$, 463, 445, 427, 380, 363, 347, 345 [2]

^{1}H NMR (250 MHz, J/Hz, D_2O): 3.68 (br m, 20°C, He-1), 3.68 (dd, J = 4.0, 8.0, 80°C, He-1), 3.70 (br m, 20°C, He-3), 3.87 (br m, 80°C, He-3), 2.76 (br m, 20°C, H-5), 2.76 (dd, J = 4.0, 8.0, 80°C, H-5), 5.94 (d, J = 2.5, 80°C, H-7), 3.23 (br m, 20°C, H-9), 3.19 (m, 80°C, H-9), 2.36 (br m, 20°C, H-17), 2.34 (t, J = 8.5, 80°C, H-17), 0.85 (s, CH_3-18), 1.10 (s, CH_3-19), 1.22 (s, CH_3-21), 3.43 (dd, J = 11.0, 2.0, 80°C, H-22), 1.23 (s, CH_3-26), 1.24 (s, CH_3-27) [2]

^{13}C NMR (125 MHz, CD_3OD) [4]:

Table 1

C-1	72.6	C-10	42.3	C-19	20.0
2		11	21.7	20	78.1
3	68.7	12	32.5	21	21.1
4		13	49.1	22	78.6
5	47.8	14	85.5	23	27.5
6		15		24	42.5
7	122.3	16	21.7	25	71.5
8	168.0	17	50.7	26	29.1
9		18	18.2	27	29.8

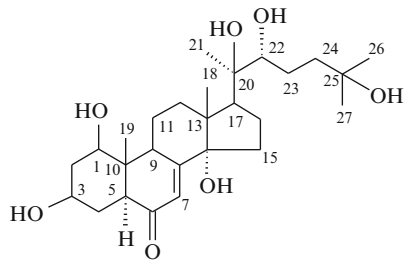
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 7.0 \times 10^{-6}$M [3].

References

1. M. Bathori, H. Kalasz, Z. Pongracz, I. Mathe, A. Kalman, G. Argay, Biomed. Chromatogr. **16**, 373 (2002)
2. J.P. Girault, M. Bathori, E. Varga, K. Szendrei, R. Lafont, J. Nat. Prod. **53**, 279 (1990)
3. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **41**, 1 (1999)
4. A. Simon, N. Toth, G. Toth, Z. Kele, J. Groska, M. Bathori, Helv. Chim. Acta. **92**, 753 (2009)

5α-2-Deoxyintegristerone A

CAS Registry Number: 482662-85-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene italica* ssp. *nemoralis* [1], *S. pseudotites* [2]

$C_{27}H_{44}O_7$: 480.3087

$[\alpha]_D^{26}$ + 4° (c 0.1, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3400, 1650 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (4.13) [1]

EI-MS m/z: 480 $[M + H + NH_3]^+$, 481 $[M + H]^+$, 463 $[M + H\text{-}H_2O]^+$, 445 $[M + H\text{-}2H_2O]^+$, 427 $[M + H\text{-}3H_2O]^+$, 409 $[M + H\text{-}4H_2O]^+$ [1, 2]

^{1}H NMR (J/Hz, CD_3OD): 3.655 (dd, J = 4.3, 11.8, Ha-1), 1.94 (Ha-2), 1.46 (He-2), 3.59 (tt, J = 4.6, 11.5, He-3), 2.055 (dm, Ha-4), 1.34 (q, J = 12.5, He-4), 2.31 (dd, J = 3.35, 12.5, H-5), 5.84 (d, J = 2.7, H-7), 2.955 (ddd, J = 2.6, 7.0, 11.7, H-9), 2.42 (dm, Ha-11), 1.69 (He-11), 2.115 (td, J = 4.8, 13.1, Ha-12), 1.77 (He-12), 1.535 (dd, J = 9.6, 10.5, Ha-15), 1.97 (Hb-15), 1.71 (Ha-16), 1.96 (Hb-16), 2.38 (dd, J = 8.1, 9.9, H-17), 0.895 (s, CH_3-18), 0.84 (s, CH_3-19), 1.184 (s, CH_3-21), 3.325 (dd, J = 1.7, 8.0, H-22), 1.29 (Ha-23), 1.67 (Hb-23), 1.42 (Ha-24),

1.80 (td, J = 4.8, 12.0, Hb-24), 1.19 (s, CH_3-26), 1.204 (s, CH_3-27) [1]

^{1}H NMR (J/Hz, D_2O): 3.744 (dd, J = 4.3, 11.9, Ha-1), 3.744 (tt, J = 4.7, 11.6, He-3), 2.543 (dd, J = 3.1, 12.5, H-5), 5.99 (d, J = 2.3, H-7), 2.95 (br s, H-9), 2.31 (t, J = 9.9, H-17), 0.863 (s, CH_3-18), 0.844 (s, CH_3-19), 1.224 (s, CH_3-21), 3.427 (d, J = 10.6, H-22), 1.224 (s, CH_3-26), 1.233 (s, CH_3-27) [2]

^{13}C NMR (CD_3OD) [1]:

Table 1

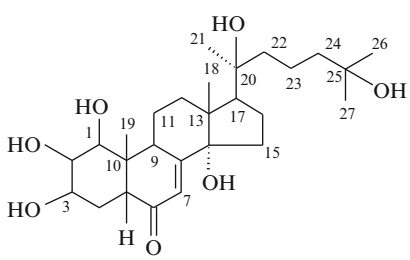
C-1	78.3	C-10	44.5	C-19	7.90
2	41.8	11	25.1	20	78.1
3	68.4	12	33.3	21	21.1
4	30.8	13	48.8	22	78.6
5	52.3	14	85.6	23	27.5
6	202.8	15	32.3	24	42.6
7	123.0	16	21.4	25	71.5
8	166.9	17	50.8	26	29.1
9	48.1	18	18.4	27	29.8

References

1. A. Simon, Z. Pongracz, G. Toth, M. Mak, I. Mathe, M. Bathori, Steroids **69**, 389 (2004)
2. Y. Meng, P. Whiting, L.N. Zibareva, G. Bertho, J.P. Girault, R. Lafont, L. Dinan, J. Chromatogr. A. **935**, 309 (2001)

22-Deoxyintegristerone A

CAS Registry Number: 128529-87-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene italica* ssp. *nemoralis* [1], *S. nutans* [2]

$C_{27}H_{44}O_7$: 480.3087

CI-MS m/z: 498, 481[M + H]$^+$, 463, 445, 427, 409, 391, 380, 361 [2]

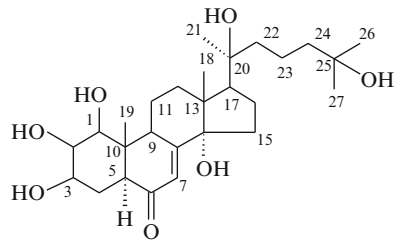
^{1}H NMR (250 MHz, J/Hz, D_2O): 3.92 (m, He-1), 4.03 (t, J = 3.2, Ha-2), 4.15 (m, He-3), 2.62 (t-like, H-5), 6.00 (d, J = 1.5, H-7), 3.04 (m, Ha-9), 2.30 (m, H-17), 0.83 (s, CH_3-18), 1.09 (s, CH_3-19), 1.30 (s, CH_3-21), 1.22 (s, CH_3-26), 1.22 (s, CH_3-27) [2]

References

1. M. Bathori, H. Kalasz, Z. Pongracz, I. Mathe, A. Kalman, G. Argay, Biomed. Chromatogr. **16**, 373 (2002)
2. J.P. Girault, M. Bathori, E. Varga, K. Szendrei, R. Lafont, J. Nat. Prod. **53**, 279 (1990)

5α-22-Deoxyintegristerone A

CAS Registry Number: 128529-88-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene nutans* [1]

$C_{27}H_{44}O_7$: 480.3087

CI-MS m/z: 498, 481[M + H]$^+$, 463, 445, 427, 409, 380, 363, 347 [1]

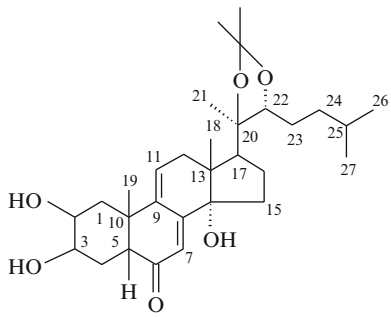
^{1}H NMR (250 MHz, J/Hz, D_2O): 3.73 (d, J = 3.5, Ha-1), 3.94 (m, He-2), 3.71 (m, He-3), 1.65 (Ha-4), 1.88 (He-4), 2.56 (dd, J = 11.0, 7.2, H-5), 6.00 (d, J = 2.5, H-7), 2.91 (m, Ha-9), 1.78 (Ha-11), 2.28 (m, He-11), 2.26 (Ha-12), 1.88 (He-12), 2.28 (m, H-17), 0.81 (s, CH_3-18), 0.93 (s, CH_3-19), 1.29 (s, CH_3-21), 1.22 (s, CH_3-26), 1.22 (s, CH_3-27) [1]

References

1. J.P. Girault, M. Bathori, E. Varga, K. Szendrei, R. Lafont, J. Nat. Prod. **53**, 279 (1990)

5-Deoxykaladasterone-20,22-Acetonide

CAS Registry Number: 393587-25-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum uniflorum* [1, 2]

$C_{30}H_{46}O_6$: 502.3294

Mp: 245–247°C [1]

UV λ_{max}^{MeOH} nm: 298 [1]

EI-MS m/z: 487 $[M\text{-}CH_3]^+$ (1.1), 469 $[M\text{-}CH_3\text{-}H_2O]^+$ (0.8), 444 (3.8), , 426 (9.1), 402 (5.6), 361 (5.3), 343 (11.3), 326 (15.1), 301 (24.4), 211 (13.8), 185 (100) [1]

FAB-MS m/z: 525 $[M + Na]^+$, 509 $[M + Li]^+$ [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.66 (d, J = 11.0, Ha-1), 2.12 (dd, J = 5.0, 11.0, He-1), 3.69 (m, Ha-2), 3.76 (m, He-3), 1.62 (m, Ha-4), 1.80 (m, He-4), 2.40 (H-5), 5.66 (br s, H-7), 6.22 (dd, J = 4.2, 6.0, Ha-11), 2.73 (br d, J = 17.6, Ha-12), 2.43 (br d, J = 17.6, He-12), 2.08 (Ha-16), 1.76 (Hb-16), 2.45 (H-17), 0.81 (s, CH_3-18), 1.06 (s, CH_3-19), 1.16 (s, CH_3-21), 3.81 (H-22), 1.35 (Ha-23), 1.55 (Hb-23), 1.52 (H-25), 0.88 (d, J = 6.7, CH_3-26), 0.89 (d, J = 6.7, CH_3-27), Other: 1.28 (CH_3-20), 1.35 (CH_3-22) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

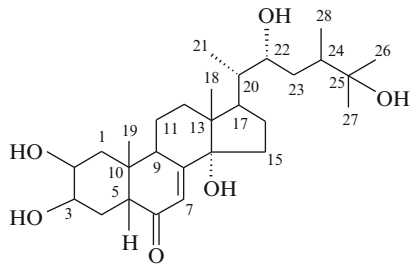
C-1	43.19	C-11	132.01	C-21	22.11
2	68.05	12	38.31	22	82.23
3	67.81	13	47.36	23	27.48
4	37.22	14	84.93	24	37.62
5	51.07	15	31.22	25	28.70
6	203.18	16	22.35	26	22.76
7	119.24	17	50.01	27	22.88
8	154.24	18	17.74	20,22-iPr	29.39
					29.68
9	141.14	19	27.08		106.81
10	37.13	20	83.16		

References

1. J.K. Cheng, Y.H. Zhang, Z.Y. Zhang, D.L. Cheng, G.L. Zhang, Chem. J. Chin. Univ. **23**, 2084 (2002)
2. Y.H. Zhang, H.Q. Wang, Pharmazie **56**, 828 (2001)

20-Deoxymakisterone A

CAS Registry Number: 93245-67-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Microsorum scolopendria* [1]

$C_{28}H_{46}O_6$: 478.3294

CI/D-MS m/z: 496 $[M + NH_4]^+$, 479 $[M + H]^+$, 461 $[M + H-H_2O]^+$, 443 $[M + H-2H_2O]^+$, 425 $[M + H-3H_2O]^+$, 240, 223, 180 [1]

^{1}H NMR (J/Hz, D_2O): 1.38 (t, J = 13.0, Ha-1), 1.88 (He-1), 3.99 (Ha-2), 4.07 (He-3), 1.75 (Ha-4), 1.75 (He-4), 2.34 (t, H-5), 5.96 (d, J = 2.4, H-7), 3.11 (Ha-9), 1.71 (Ha-11), 1.85 (He-11), 1.88 (Ha-12),

1.88 (He-12), 1.62 (Ha-15), 2.03 (Hb-15), 1.95 (Ha-16), 1.85 (Hb-16), 1.84 (H-17), 1.84 (H-20), 0.746 (s, CH_3-18), 1.00 (s, CH_3-19), 0.935 (d, J = 6.8, CH_3-21), 3.85 (d, J = 10.0, Hb-22), 1.13 (m, Ha-23), 1.56 (Hb-23), 1.66 (Ha-24), 1.179 (s, CH_3-26), 1.196 (s, CH_3-27), 0.935 (d, J = 6.8, CH_3-28) [1]

^{13}C NMR (D_2O) [1]:

Table 1

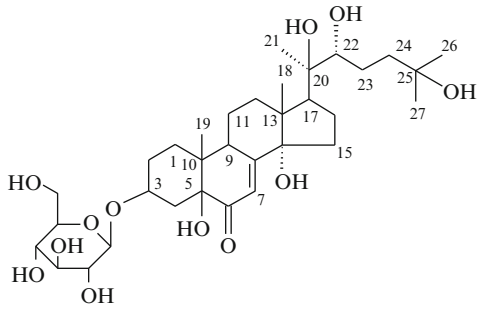
C-1	38.3	C-11		C-21	15.5
2	70.1	12	33.1	22	74.1
3	70.0	13	49.1	23	33.7
4	34.1	14	87.9	24	42.4
5	53.3	15	33.6	25	77.0
6	211.2	16		26	27.8
7	123.9	17	50.0	27	28.3
8		18	18.0	28	15.5
9	36.7	19	25.8		
10	40.8	20	44.6		

References

1. E. Snogan, I.L. Lechat, R. Ho, G. Bertho, J.P. Girault, S. Ortiga, A. Maria, R. Lafont, Phytochem. Anal. **18**, 441 (2007)

2-Deoxypolypodine B-3-β-D-Glucoside

CAS Registry Number: 397248-06-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene pseudotites* [1, 2]

$C_{33}H_{54}O_{12}$: 642.3615

CI-MS m/z: 480 $[M\text{-}Glu]^+$ (9), 463 $[M + H\text{-}Glu\text{-}H_2O]^+$ (40), 180 $[Glu]^+$ (46) [1, 2]

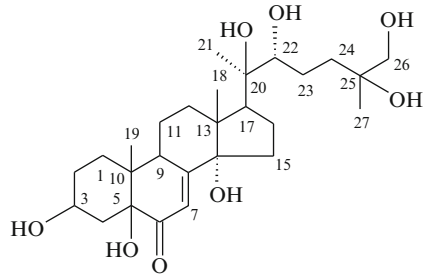
^{1}H NMR (J/Hz, D_2O): 4.31 (br s, He-3), 5.99 (d, J = 2.1, H-7), 3.243 (m, H-9), 2.32 (t, J = 9.3, H-17), 0.875 (s, CH_3-18), 0.905 (s, CH_3-19), 1.233 (s, CH_3-21), 3.44 (d, J = 10.5, H-22), 1.221 (s, CH_3-26), 1.233 (s, CH_3-27), Other: β-D-Glcp′: 4.56 (d, J = 8.0, H-1), 3.30 (dd, J = 8.0, 9.0, H-2), 3.51 (t, J = 9.3, H-3), 3.39 (t, J = 9.3, H-4), 3.45 (m, H-5), 3.71 (dd, J = 5.9, 12.4, Ha-6), 3.90 (dd, J = 2.0, 12.3, Hb-6) [1, 2]

References

1. Y. Meng, P. Whiting, L.N. Zibareva, G. Bertho, J.P. Girault, R. Lafont, L. Dinan, J. Chromatogr. A. **935**, 309 (2001)
2. N.Z. Mamadalieva, L.N. Zibareva, R. Lafont, L. Dinan, Z. Saatov, Chem. Nat. Comp. **40**, 574 (2004)

2-Deoxy-5,20,26-Trihydroxyecdysone

CAS Registry Number: 1039035-94-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *S. viridiflora* [1]

$C_{27}H_{44}O_8$: 496.3036

$[\alpha]_D^{25}$ + 41° (c 0.05, MeOH) [1]

UV λ_{max}^{MeOH} nm: 243 (log ε 4.02) [1]

ESI-MS m/z: 535 $[M + K]^+$ (100) [1]

HR-ESI-MS m/z: for $C_{27}H_{45}O_8$ $[M + H]^+$ calcd. 497.3102, found 497.3108 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 4.08 (br s, He-3), 5.85 (d, J = 2.2, H-7), 3.27 (m, H-9), 2.39 (t, J = 8.8, H-17), 0.90 (s, CH_3-18), 0.89 (s, CH_3-19), 1.19 (s, CH_3-21), 3.34 (m, H-22), 3.37 (Ha-26 and Hb-26), 1.14 (s, CH_3-27) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

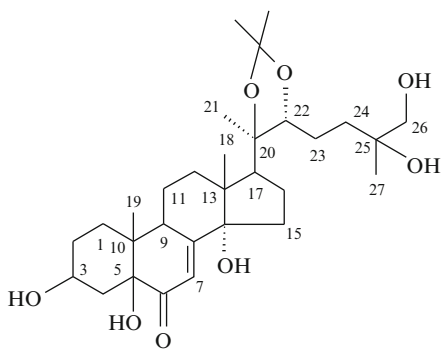
C-1	25.3	C-10	43.3	C-19	17.2
2		11		20	77.9
3	67.2	12	32.6	21	21.1
4		13	48.8	22	78.7
5	81.0	14	85.2	23	
6		15		24	37.2
7	120.7	16		25	73.6
8		17	50.5	26	70.8
9	37.9	18	18.2	27	23.6

References

1. N. Toth, A. Simon, G. Toth, Z. Kele, A. Hunyadi, M. Bathori, J. Nat. Prod. **71**, 1461 (2008)

2-Deoxy-5,20,26-Trihydroxyecdysone-20,22-Acetonide

CAS Registry Number: 1039036-00-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *S. viridiflora* [1]

$C_{30}H_{48}O_8$: 536.3349

$[\alpha]_D^{25}$ + 25° (c 0.05, MeOH) [1]

UV λ_{max}^{MeOH} nm: 238 (log ε 4.08) [1]

ESI-MS m/z: 559 $[M + Na]^+$ (100), 537 $[M + H]^+$ (36), 518 $[M\text{-}H_2O]^+$ (3), 541 $[M + Na\text{-}H_2O]^+$ (12), 501 $[M + H\text{-}2H_2O]^+$ (2), 445 (10), 385 $[M + H\text{-}H_2O\text{-}C_6O_3H_{14}]^+$ (3), 315 (12), 304 (24) [1]

HR-ESI-MS m/z: for $C_{30}H_{49}O_8$ $[M + H]^+$ calcd. 537.3414, found 537.3420 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.50 (m, Ha-1), 1.84 (m, He-1), 1.77 (m, Ha-2), 1.96 (m, He-2), 4.08 (br s, He-3), 1.61 (m, Ha-4), 2.035 (m, He-4), 5.86 (s br, H-7), 3.28 (m, H-9), 1.73 (m, Ha-11), 2.12 (td, J = 12.4, 5.7, Ha-12), 1.86 (m, He-12), 1.61 (m, Ha-15), 1.97 (m, Hb-15), 1.88 (m, Ha-16), 2.04 (m, Hb-16), 2.32 (t, J = 8.7, H-17), 0.83 (s, CH_3-18), 0.89 (s, CH_3-19), 1.18 (s, CH_3-21), 3.70 (m, H-22), 1.55 (m, Ha-23), 1.55 (m, Hb-23), 1.53 (m, Ha-24), 1.72 (m, Hb-24), 3.36 (d, J = 11.0, Ha-26), 3.37 (d, J = 11.0, Hb-26), 1.15 (s, CH_3-27), Other: 1.32 and 1.39 (s, 20,22-iPr) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

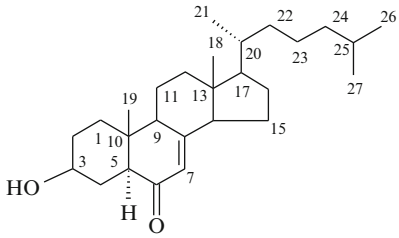
C-1	25.6	C-11	22.5	C-21	22.7
2	29.3	12	32.6	22	83.6
3	67.2	13	48.7	23	24.05
4	36.9	14	85.4	24	37.2
5	81.2	15	31.8	25	73.6
6		16	22.5	26	70.7
7	120.7	17	50.6	27	23.8
8	167.8	18	17.8	20,22-iPr	29.5
9	38.1	19	17.3		27.3
10	43.25	20	86.0		108.2

References

1. N. Toth, A. Simon, G. Toth, Z. Kele, A. Hunyadi, M. Bathori, J. Nat. Prod. **71**, 1461 (2008)

Deoxyviperidone

CAS Registry Number: 14858-06-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Wilcoxia viperina* [1]

$C_{27}H_{44}O_2$: 400.3341

Mp: 195–196°C (CH_2Cl_2–Me_2CO–EtOH) [2], 198–199°C (MeOH) [3]

IR (KBr) ν_{max} cm^{-1}: 1675, 1627 [2], 1675 [3]

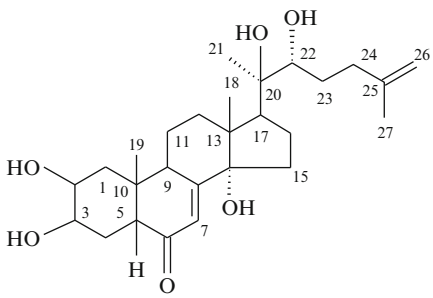
UV λ_{max}^{EtOH} nm: 244 (ε 13920) [2], 243 (ε 15800) [3]

References

1. C. Djerassi, J. C. Knight, H. Brockmann, Chem. Ber. **97**, 3118 (1964) [Chem. Abst. 62. 1712e (1965)]
2. H. Hoffmeister, C. Rufer, H.H. Keller, H. Schairer, P. Karlson, Chem. Ber. **98**, 2361 (1965)
3. M.N. Galbraith, D.H.S. Horn, E.J. Middleton, Aust. J. Chem. **27**, 1087 (1974)

25,26-Didehydroponasterone A

CAS Registry Number: 82413-55-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Klaseopsis chinensis* [1]

$C_{27}H_{42}O_6$: 462.2981

Mp: amorphous powder [1]

$[\alpha]_D^{25}$ + 45° (c 0.006, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3377, 2945, 1646, 1445, 1380, 1356, 1062, 892, 875, 685, 616 [1]

UV λ_{max}^{MeOH} nm: 240.8 [1]

ESI-MS m/z: 461 $[M-H]^-$; 521 $[M + CH_3COO]^-$, 559 $[M + HSO_4]^-$ [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.923 (m, Ha-1), 2.165 (m, He-1), 4.175 (dt, J = 10.4, Ha-2), 4.228 (br s, He-3), 3.011 (dd, J = 3.6, 12.2, H-5), 6.257 (1 H, d, J = 2.4, H-7), 3.597 (m, H-9), 2.924 (t, J = 9.0, H-17), 1.221 (s, CH_3-18), 1.075 (s, CH_3-19), 1.575 (s, CH_3-21), 3.84 (br d, J = 10.0, H-22), 2.277 (m, Ha-24), 2.568 (m, Hb-24), 4.754 (br s, Ha-26), 4.791 (br s, Ha-26), 1.676 (s, CH_3-27), 4.791 (1H, br s, OH), 5.930 (1H, s, OH), 6.032 (2H, br s, OH), 6.302 (1H, s, OH) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

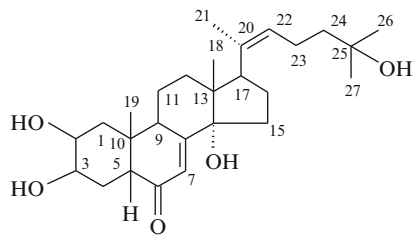
C-1	38.27	C-10	38.94	C-19	24.72
2	68.39	11	21.88	20	76.95
3	68.33	12	32.28	21	21.68
4	32.72	13	48.37	22	76.31
5	51.67	14	84.44	23	30.88
6	203.70	15	32.03	24	36.08
7	121.96	16	21.39	25	146.49
8	166.31	17	50.30	26	110.59
9	34.72	18	18.13	27	22.87

References

1. T. Ling, Zh Zhang, T. Xia, W. Ling, X. Wan, Biochem. Sys. Ecol. **37**, 49 (2009)

20,22-Didehydrotaxisterone

CAS Registry Number: 938112-71-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula wolffii* [1]

$C_{27}H_{42}O_5$: 446.3032

Mp: 231–233°C [1]

$[\alpha]_D^{28}$ + 71° (c 0.025, MeOH) [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (4.387) [1]

ESI-MS m/z: 485 $[M + K]^+$ (69), 447 $[M + H]^+$ (93), 429 $[M + H\text{-}H_2O]^+$ (100), 411 $[M + H\text{-}2H_2O]^+$(6), 393 $[M + H\text{-}3H_2O]^+$ (7), 347 (6), 320 (4) [1]

HR-ESI-MS m/z: for $C_{27}H_{43}O_5$ $[M + H]^+$ calcd. 447.3021, found 447.3025 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (m, Ha-1), 1.43 (dd, J = 12.2, 13.4, He-1), 3.84 (ddd, J = 3.3, 4.2, 12.0, Ha-2), 3.96 (m, He-3), 1.76 (m, Ha-4), 1.70 (td, J = 4.5, 14.2, He-4), 2.39 (dd, J = 4.5, 12.7, H-5), 5.81 (d, J = 2.6, H-7), 3.18 (ddd, J = 2.6, 7.2, 11.2, H-9), 1.84 (m, Ha-11), 1.63 (m, He-11), 2.09 (dt, J = 8.0, 13.0, Ha-12), 1.54 (ddd, J = 1.7, 5.3, 13.0, Hb-12), 2.02 (m, Ha-15), 1.66 (m, Hb-15), 1.83 (m, Ha-16), 1.95 (ddt, J = 2.3, 9.2, 12.0, Hb-16), 2.90 (t, J = 9.2, H-17), 0.57 (s, CH_3-18), 0.96 (s, CH_3-19), 1.69 (s, CH_3-21), 5.30 (t, J = 7.1, H-22), 2.13 (m, H-23), 1.50 (m, H-24), 1.20 (s, CH_3-26), 1.20 (s, CH_3-27) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

C-1	37.6	C-10	39.5	C-19	24.6
2	68.85	11	21.8	20	134.9
3	68.67	12	31.1	21	18.4
4	33.0	13	48.9	22	127.7
5	52.0	14	85.0	23	24.4
6	206.7	15	32.3	24	45.0
7	121.9	16	24.1	25	71.5
8	167.9	17	54.3	26	29.3
9	35.4	18	17.7	27	29.3

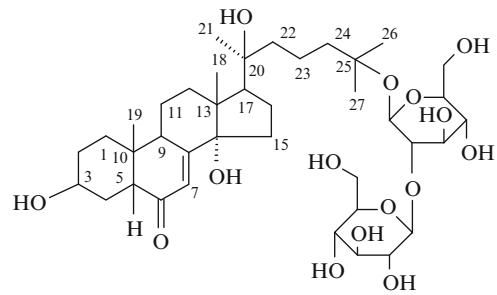
Pharm./Biol.: *Acyrthosiphon pisum* aphid larvae: inactive [1].

References

1. E. Liktor-Busa, A. Simon, G. Toth, G. Fekete, Z. Kele, M. Bathori, J. Nat. Prod. **70**, 884 (2007)

2,22-Dideoxyecdysone-25-O-β-D-Glucopyranosyl-(1 → 2)-β-D-Glucopyranoside

CAS Registry Number: 1140954-70-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Froelichia floridana* [1]

$C_{39}H_{64}O_{14}$: 756.4296

Mp: amorphous [1]

$[\alpha]_D^{21}$ + 48° (c 0.92, MeOH) [1]

UV λ_{max}^{MeOH} nm: 248 [1]

HR-ESI-MS m/z: for $C_{39}H_{64}O_{14}Li$ $[M + Li]^+$ calcd. 763.4456, found 763.4463 [1]

^{1}H NMR (600 MHz, J/Hz, DMSO-d_6): 1.26 (m, Ha-1), 1.42 (m, He-1), 1.43 (m, Ha-2), 1.56 (m, He-2), 3.78 (br s, He-3), 1.32 (m, Ha-4), 2.19 (dd, J = 12.2, 3.3, H-5), 5.59 (s, H-7), 3.07 (m, H-9), 1.37 (m, Ha-11), 1.51 (m, He-11), 1.86 (m, Ha-12), 1.53 (m, He-12), 1.42 (m, Ha-15), 1.73 (m, Hb-15), 1.86 (m, Ha-16), 1.19 (Hb-16), 1.79 (t, J = 9.0, H-17), 0.50 (s, CH_3-18), 0.78 (s, CH_3-19), 1.28 (m, H-20), 0.79 (d, J = 6.7, CH_3-21), 1.25 (m, Ha-22), 0.87 (m, Hb-22), 1.99 (m, Ha-23), 1.25 (m, Hb-23), 1.37 (m, Ha-24), 1.25 (m, Hb-24), 1.08 (s, CH_3-26), 1.08 (s, CH_3-27), Other: β-D-Glcp′: 4.38 (d, J = 7.4, H-1), 3.14 (d, J = 8.4, H-2), 3.34 (d, J = 8.3, H-3), 3.04 (m, H-4), 3.07 (m, H-5), 3.60 (d, J = 11.6, Ha-6), 3.43 (m, Hb-6), β-D-Glcp ″: 4.33 (d, J = 7.7, H-1), 2.96 (t, J = 8.4, H-2), 3.13 (m, H-3), 3.07 (m, H-4), 3.06 (m, H-5), 3.55 (d, J = 11.6, Ha-6), 3.37 (m, Hb-6) [1]

^{13}C NMR (150 MHz, DMSO-d_6) [1]:

Table 1

C-1	28.8	C-11	20.6	C-21	19.2	Glc′-4	70.4
2	27.7	12	30.9	22	36.7	5	77.3
3	62.0	13	49.1	23	20.6	6	61.3
4	32.2	14	84.0	24	42.3	Glc″-1	104.3
5	50.7	15	30.8	25	78.0	2	75.4
6	205.0	16	26.9	26	25.7	3	76.3
7	120.4	17	50.4	27	26.9	4	70.2
8	167.0	18	15.8	Glc′-1	95.9	5	76.3
9	31.7	19	24.1	2	82.1	6	61.4
10	36.5	20	35.4	3	76.7		

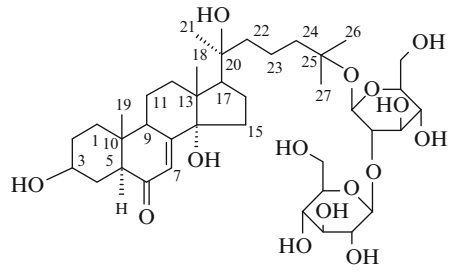
Pharm./Biol.: Human DNA Topoisomerase I test: not active [1].

References

1. P. Wang, Sh Li, S. Ownby, Zh Zhang, W. Yuan, W. Zhang, R. Scott Beasley, Phytochemistry **70**, 430 (2009)

(5α)-2,22-Dideoxyecdysone-25-O-β-D-Glucopyranosyl-(1 → 2)-β-D-Glucopyranoside

CAS Registry Number: 1140954-74-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Froelichia floridana* [1]

$C_{39}H_{64}O_{14}$: 756.4296

Mp: amorphous [1]

$[\alpha]_D^{21}$ + 32° (c 0.92, MeOH) [1]

UV λ_{max}^{MeOH} nm: 248 [1]

HR-ESI-MS m/z: for $C_{39}H_{64}O_{14}H$ $[M + H]^+$ calcd. 757.4374, found 757.4299 [1]

^{1}H NMR (600 MHz, J/Hz, DMSO-d_6): 1.39 (m, Ha-1), 1.85 (m, He-1), 1.39 (m, Ha-2), 2.10 (m, He-2), 3.61 (m, He-3), 1.78 (m, Ha-4), 2.11 (m, Hb-4), 2.36 (dd, J = 12.3, 3.5, H-5), 5.85 (d, J = 2.7, H-7), 2.75 (m, H-9), 1.58 (m, Ha-11), 1.77 (m, He-11), 2.07 (m, Ha-12), 1.73 (m, He-12), 1.58 (m, Ha-15), 1.92 (m, Hb-15), 2.03 (m, Ha-16), 1.40 (Hb-16), 1.92 (m, H-17), 0.72 (s, CH_3-18), 0.86 (s, CH_3-19), 1.47 (m, H-20), 0.97 (d, J = 6.5, CH_3-21), 1.46 (m, Ha-22), 1.10 (m, Hb-22), 1.56 (m, Ha-23), 1.32 (m, Hb-23), 1.53 (m, Ha-24), 1.42 (m, Hb-24), 1.27 (s, CH_3-26), 1.27 (s, CH_3-27), Other: β-D-Glcp′: 4.59 (d, J = 8.5, H-1), 3.41 (m, H-2), 3.53 (m, H-3), 3.54 (m, H-4), 3.27 (m, H-5), 3.84 (d, J = 11.5, Ha-6), 3.69 (m, Hb-6), β-D-Glcp″: 4.58 (d, J = 8.1, H-1), 3.22 (m, H-2), 3.38 (m, H-3), 3.31 (m, H-4), 3.24 (m, H-5), 3.81 (d, J = 11.8, Ha-6), 3.64 (m, Hb-6) [1]

^{13}C NMR (150 MHz, DMSO-d_6) [1]:

Table 1

C-1	38.0	C-11	21.8	C-21	19.8	Glc′-4	71.3
2	31.0	12	32.2	22	38.0	5	78.7
3	71.8	13	47.8	23	21.8	6	63.1
4	31.4	14	85.8	24	43.9	Glc″-1	105.5
5	54.7	15	32.0	25	79.9	2	76.5
6	203.4	16	28.0	26	26.4	3	77.7
7	123.3	17	52.0	27	27.3	4	71.6
8	166.7	18	16.5	Glc′-1	97.4	5	77.9
9	47.6	19	13.4	2	82.7	6	62.9
10	39.7	20	37.1	3	78.4		

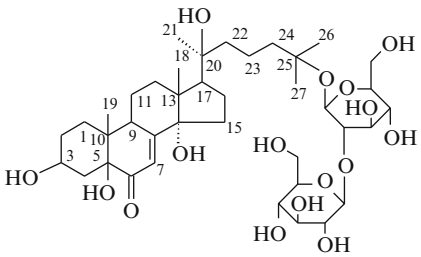
Pharm./Biol.: human DNA Topoisomerase I test: not active [1].

References

1. P. Wang, Sh Li, S. Ownby, Zh Zhang, W. Yuan, W. Zhang, R. Scott Beasley, Phytochemistry **70**, 430 (2009)

2,22-Dideoxy-5-Hydroxyecdysone-25-O-β-D-Glucopyranosyl-(1 → 2)-β-D-Glucopyranoside

CAS Registry Number: 1140954-76-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Froelichia floridana* [1]

$C_{39}H_{64}O_{15}$: 772.4245

Mp: amorphous [1]

$[\alpha]_D^{21}$ + 46° (c 0.11, MeOH) [1]

UV λ_{max}^{MeOH} nm: 248 [1]

HR-ESI-MS m/z: for $C_{39}H_{64}O_{15}H$ $[M + H]^+$ calcd. 773.4324, found 773.3975 [1]

^{1}H NMR (600 MHz, J/Hz, DMSO-d_6): 1.45 (m, Ha-1), 1.83 (m, He-1), 1.77 (m, Ha-2), 1.96 (m, He-2), 4.09 (br s, He-3), 1.61 (m, Ha-4), 2.03 (m, Hb-4), 5.86 (s, H-7), 3.38 (m, H-9), 1.55 (m, Ha-11), 1.70 (m, He-11), 2.09 (m, Ha-12), 1.76 (m, He-12), 1.58 (m, Ha-15), 1.93 (m, Hb-15), 2.01 (m, Ha-16), 1.40 (Hb-16), 1.94 (m, H-17), 0.73 (s, CH_3-18), 0.89 (s, CH_3-19), 1.48 (m, H-20), 0.97 (d, J = 6.5, CH_3-21), 1.42 (m, Ha-22), 1.05 (m, Hb-22), 1.45 (m, Ha-23), 1.30 (m, Hb-23), 1.55 (m, Ha-24), 1.44 (m, Hb-24), 1.27 (s, CH_3-26), 1.29 (s, CH_3-27), Other: β-D-Glcp′: 4.59 (d, J = 8.1, H-1), 3.42 (m, H-2), 3.55 (m, H-3), 3.63 (m, H-4), 3.27 (m, H-5), 3.85 (m, Ha-6), 3.68 (m, Hb-6), β-D-Glcp″: 4.58 (d, J = 8.1, H-1), 3.24 (m, H-2), 3.39 (m, H-3), 3.28 (m, H-4), 3.26 (m, H-5), 3.83 (m, Ha-6), 3.66 (m, Hb-6) [1]

^{13}C NMR (150 MHz, DMSO-d_6) [1]:

Table 1

C-1	25.5	C-11	22.4	C-21	19.6	Glc′-4	71.7
2	29.2	12	32.3	22	38.0	5	78.5
3	67.1	13	47.9	23	21.8	6	63.1
4	36.7	14	86.0	24	43.8	Glc″-1	105.4
5	81.0	15	32.0	25	79.8	2	76.4
6	203.0	16	27.9	26	26.4	3	77.6
7	120.4	17	52.1	27	27.2	4	71.7
8	167.0	18	16.4	Glc′-1	97.3	5	77.8
9	38.1	19	17.2	2	82.6	6	62.0
10	43.4	20	37.0	3	78.3		

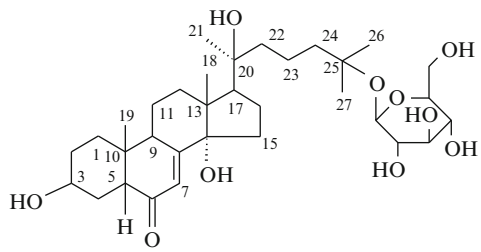
Pharm./Biol.: Human DNA Topoisomerase I test: not active [1].

References

1. P. Wang, Sh Li, S. Ownby, Zh Zhang, W. Yuan, W. Zhang, R. Scott Beasley, Phytochemistry **70**, 430 (2009)

2,22-Dideoxy-20-Hydroxyecdysone-25-Glucoside

CAS Registry Number: 1140954-68-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Froelichia floridana* [1]

$C_{33}H_{54}O_{10}$: 610.3717

Mp: amorphous [1]

$[\alpha]_D^{21}$ + 26° (c 0.07, MeOH) [1]

UV λ_{max}^{MeOH} nm: 246 [1]

HR-ESI-MS m/z: for $C_{33}H_{54}O_{10}Li$ $[M + Li]^+$ calcd. 617.3877, found 617.3881 [1]

^{1}H NMR (600 MHz, J/Hz, DMSO-d_6): 1.22 (m, Ha-1), 1.49 (m, He-1), 1.32 (m, Ha-2), 1.63 (m, He-2), 3.84 (br s, He-3), 1.37 (m, Ha-4), 2.27 (dd, J = 12.1, 3.7, H-5), 5.63 (d, J = 3.0, H-7), 3.07 (m, H-9), 1.47 (m, Ha-11), 1.59 (m, He-11), 1.99 (dd, J = 11.8, 7.8, Ha-12), 1.66 (m, He-12), 1.50 (m, Ha-15), 1.79 (m, Hb-15), 1.82 (m, Ha-16), 1.67 (m, Hb-16), 2.17 (t, J = 9.0, H-17), 0.73 (s, CH_3-18), 0.85 (s, CH_3-19), 1.13 (s, CH_3-21), 1.33 (m, Ha-22), 1.26 (m, Hb-22), 1.38 (m, Ha-23), 1.27 (m, Hb-23), 1.38 (m, Ha-24), 1.15 (s, CH_3-26), 1.15 (s, CH_3-27), Other: β-D-Glcp′: 4.26 (d, J = 7.7, H-1), 2.90 (m, H-2), 3.13 (m, H-3), 3.01 (m, H-4), 3.04 (m, H-5), 3.76 (d, J = 11.0, Ha-6), 3.63 (m, Hb-6) [1]

^{13}C NMR (150 MHz, DMSO-d_6) [1]:

Table 1

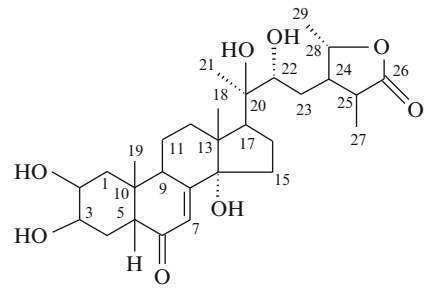
C-1	29.1	C-12	30.7	C-23	18.2
2	28.2	13	48.6	24	42.1
3	62.8	14	85.0	25	76.5
4	32.1	15	29.9	26	26.3
5	50.8	16	20.7	27	26.2
6	203.4	17	51.2	Glc′-1	97.1
7	120.3	18	17.7	2	73.3
8	165.8	19	23.8	3	77.0
9	32.1	20	73.6	4	70.3
10	36.1	21	26.6	5	76.5
11	20.1	22	44.5	6	61.2

Pharm./Biol.: Human DNA Topoisomerase I test: not active [1].

References

1. P. Wang, Sh Li, S. Ownby, Zh Zhang, W. Yuan, W. Zhang, R. Scott Beasley, Phytochemistry **70**, 430 (2009)

24,28-Diepi-Cyasterone



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Microsorum scolopendria* [1]

$C_{29}H_{44}O_8$: 520.3036

CI/D-MS m/z: 538 $[M + NH_4]^+$, 521 $[M + H]^+$, 520 $[M + NH_4–H_2O]^+$, 503 $[M + H-H_2O]^+$, 485 $[M + H–2H_2O]^+$, 411, 279, 174, 136 [1]

^{1}H NMR (J/Hz, D_2O): 1.38 (t, J = 12.8, Ha-1), 1.88 (He-1), 3.99 (Ha-2), 4.07 (He-3), 1.75 (Ha-4), 1.75 (He-4), 2.34 (t, J = 8.8, H-5), 5.97 (d, J = 2.0, H-7), 3.11 (Ha-9), 1.73 (Ha-11), 1.86 (He-11), 1.99 (Ha-12), 1.96 (He-12), 1.67 (Ha-15), 2.07 (Hb-15), 1.90 (Ha-16), 1.76 (Hb-16), 2.26 (t, J = 9.2, H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.25 (d, J = 6.8, CH_3-21), 3.54 (dd, J = 2.8, 9.9, Hb-22), 1.51 (m, Ha-23), 1.49 (Hb-23), 2.49 (m, Ha-24), 3.09 (m, H-25), 1.175 (d, J = 7.5, CH_3-27), 4.59 (dq, J = 6.2, 6.4, Ha-28), 1.446 (d, J = 6.4, CH_3-29) [1]

^{1}H NMR (J/Hz, C_5D_5N): 1.92 (Ha-1), 2.14 (He-1), 4.17 (Ha-2), 4.22 (He-3), 1.79 (Ha-4), 2.05 (He-4), 3.01 (dd, J = 3.9, 13.0, H-5), 6.27 (d, J = 2.2, H-7), 3.59 (Ha-9), 1.75 (Ha-11), 1.90 (He-11), 2.60 (Ha-12), 2.04 (He-12), 1.93 (Ha-15), 2.21 (Hb-15), 2.47 (m, Ha-16), 2.05 (Hb-16), 2.88 (t, J = 9.2, H-17), 1.224 (s, CH_3-18), 1.073 (s, CH_3-19), 1.221 (d, J = 6.8, CH_3-21), 3.86 (d, J = 9.4, Hb-22), 1.68 (Ha-23), 1.70 (Hb-23), 2.58 (Ha-24), 3.04 (q, J = 8.0, H-25), 1.215 (d, J = 8.1, CH_3-27), 4.32 (q, J = 6.4, Ha-28), 1.243 (d, J = 6.6, CH_3-29) [1]

^{13}C NMR (D_2O) [1]:

Table 1

C-1	38.3	C-11	22.4	C-21	21.9
2	69.8	12	33.5	22	76.8

(*continued*)

Table 1 (continued)

3	69.8	13	50.0	23	31.2
4	33.7	14	87.8	24	44.6
5	52.8	15	33.0	25	40.7
6	211.1	16	22.4	26	187.4
7	123.7	17	51.5	27	12.5
8		18	19.7	28	84.3
9	36.6	19	25.7	29	21.8
10	40.8	20	80.6		

^{13}C NMR (C_5D_5N) [1]:

Table 2

C-1	38.2	C-11	21.3	C-21	21.6
2	68.3	12	32.3	22	75.5
3	68.2	13	48.7	23	29.7
4	32.6	14	84.6	24	44.7
5	51.6	15	32.0	25	38.9
6	203.9	16	21.6	26	180.1
7	121.8	17	50.2	27	11.5
8	166.5	18	18.1	28	79.6
9	34.7	19	24.7	29	20.0
10	39.0	20	77.2		

References

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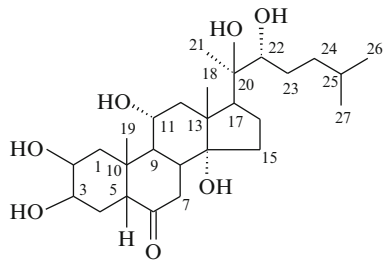
7,8-Dihydroajugasterone C

CAS Registry Number: 175413-32-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Nierembergia hippomanica* [1]

$C_{27}H_{46}O_7$: 482.3243

Mp: amorphous [1]

$[\alpha]_D^{22}$ + 43.2° (c 0.01, $CHCl_3$) [1]

IR (Nujol) ν_{max} cm^{-1}: 3350, 2870, 1695, 1445, 1375, 1265, 1230, 1215, 1200, 1095, 1010, 860 [1]

EI-MS m/z: 467 $[M\text{-}CH_3]^+$ (2), 464 $[M\text{-}H_2O]^+$ (5), 428 $[M\text{-}3H_2O]^+$ (2), 413 $[428\text{-}CH_3]^+$ (2), 381 [M-C-22 to C-27]$^+$ (4), 363 $[381\text{-}H_2O]^+$ (84), 345 $[363\text{-}H_2O]^+$ (41), 327 $[345\text{-}H_2O]^+$ (28), 309 $[327\text{-}H_2O]^+$ (16), 285 (8), 267 (10), 189 (12), 157 [C-17 to C-27]$^+$ (11), 145 [C-20 to C-27]$^+$ (41), 127 $[145\text{-}H_2O]^+$ (9), 109 $[127\text{-}H_2O]^+$ (33), 101 [C-22 to C-27]$^+$ (2), 83 $[101\text{-}H_2O]^+$ (75), 71 (36), 67 (33), 55 (100), 43 (94) [1]

FAB-MS m/z: 483 $[M + H]^+$ [1]

^{1}H NMR (200 MHz, J/Hz, C_5D_5N): 2.00 (m, Ha-1), 3.45 (dd, J = 16.0, 4.0, He-1), 4.60 (m, Ha-2), 4.30 (m, He-3), 1.80 (m, Ha-4), 2.20 (dt, J = 14.0, 4.0, He-4), 3.20 (m, H-5), 2.23 (dd, J = 14.0, 4.0, Ha-7), 1.85 (m, He-7), 2.30 (m, H-8), 3.90 (t, J = 9.0, H-9), 4.68 (m, Ha-11), 3.42 (t, J = 12.0, Ha-12), 2.70 (dd, J = 12.0, 6.0, He-12), 1.95 (m, Ha-15), 2.10 (m, Hb-15), 2.10 (Ha-16), 2.50 (Hb-16), 3.00 (t, J = 8.0, H-17), 1.23 (s, CH_3-18), 1.40 (s, CH_3-19), 1.53 (s, CH_3-21), 3.80 (dd, J = 10.0, 5.0, H-22), 1.40 (Ha-23), 1.68 (m, Hb-23), 1.50 (Ha-24), 1.71 (m, Hb-24), 1.58 (m, H-25), 0.82 (d, J = 6.0, CH_3-26), 0.82 (d, J = 6.0, CH_3-27) [1]

^{13}C NMR (50 MHz, C_5D_5N) [1]:

Table 1

C-1	43.9	C-10	41.2	C-19	16.4
2	65.2	11	67.5	20	76.7
3	67.8	12	43.5	21	21.5
4	32.3	13	60.1	22	77.0
5	55.4	14	93.8	23	31.8
6	214.5	15	37.9	24	36.4
7	40.6	16	32.9	25	28.7
8	37.7	17	53.3	26	22.6
9	51.4	18	26.9	27	22.0

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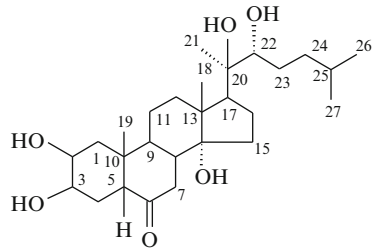
7,8β-Dihydroponasterone A

CAS Registry Number: 227780-00-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Taxus cuspidata* [1]

$C_{27}H_{46}O_6$: 466.3294

Mp: amorphous solid [1]

$[\alpha]_D^{22}$ + 76° (c 0.20, MeOH) [1]

HR-FAB-MS m/z: for $C_{27}H_{46}O_6Na$ $[M + Na]^+$ calcd. 489.3192, found 489.3193, for $C_{27}H_{46}O_6K$ $[M + K]^+$ calcd. 505.2931, found 505.2921 [1]

^{1}H NMR (500 MHz, J/Hz, $CDCl_3$): 1.38 (m, Ha-1), 1.81 (m, He-1), 3.82 (dt, J = 12.3, 3.8, Ha-2), 4.04 (ddd, J = 2.9, 2.9, 2.9, He-3), 1.99 (m, Ha-4), 1.84 (m, He-4), 2.42 (dd, J = 3.9, 13.5, H-5), 2.55 (dd, J = 12.0, 14.3, Ha-7), 2.06 (dd, J = 3.6, 14.3, Hb-7), 2.14 (m, H-8), 2.18 (m, H-9), 1.46 (m, Ha-11), 1.79 (m, He-11), 1.84 (m, Ha-12), 1.60 (m, He-12), 1.84 (m, Ha-15), 1.35 (m, Hb-15), 1.99 (m, Ha-16), 1.65 (m, Hb-16), 2.21 (t, J = 9.3, H-17), 1.00 (s, CH_3-18), 0.91 (s, CH_3-19), 1.18 (s, CH_3-21), 3.38 (br d, J = 8.6, H-22), 1.46 (m, Ha-23), 1.22 (m, Hb-23), 1.44 (m, Ha-24), 1.21 (m, Hb-24), 1.54 (m, H-25), 0.91 (d, J = 6.4, CH_3-26), 0.90 (d, J = 6.4, CH_3-27) [1]

^{13}C NMR (125 MHz, $CDCl_3$) [1]:

Table 1

C-1	37.2	C-10	40.0	C-19	22.9
2	67.1	11	20.2	20	76.9
3	67.8	12	32.2	21	20.3
4	31.9	13	47.8	22	76.6
5	53.3	14	84.7	23	29.3
6	215.1	15	32.3	24	36.3
7	37.0	16	20.4	25	27.9
8	39.1	17	49.3	26	22.9
9	32.8	18	17.4	27	22.5

(*continued*)

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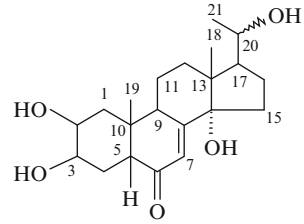
Dihydroposttsterone

CAS Registry Number: 128574-64-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene otites* [1]

$C_{21}H_{32}O_5$: 364.2249

CI-MS m/z: 382, 365, 347, 345 [1]

CD (c, $6.8x10^{-5}$, MeOH): Δε = -2.94 (290 nm), Δε = +4.30 (248 nm) [1]

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.42 (dd, J = 13.0, 12.0, Ha-1), 3.84 (m, Ha-2), 3.95 (m, He-3), 2.38 (dd, J = 12.0, 5.0, H-5), 5.82 (d, J = 2.5, H-7), 3.14 (m, Ha-9), 0.69 (s, CH_3-18), 0.96 (s, CH_3-19), 0.65 (m, 20-CH-OH), 1.22 (d, J = 6.5, CH_3-21) [1]

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 7.5x10^{-4}$ M [2].

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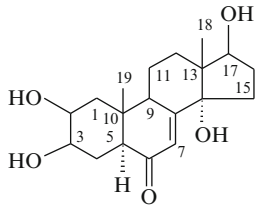
2. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **41**, 1 (1999)

5α-Dihydrorubrosterone

CAS Registry Number: 232280-44-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene otites* [1]

$C_{19}H_{28}O_5$: 336.1936

CI-MS m/z: 354 $[M + H + NH_3]^+$, 337 $[M + H]^+$, 319, 303, 301, 249, 231 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 3.96 (m, Ha-2), 3.57 (m, He-3), 2.38 (dd, H-5), 5.82 (d, J = 2.5, H-7), 2.74 (m, Ha-9), 4.29 (dd, J = 6.4, 8.8, H-17), 0.71 (s, CH_3-18), 1.03 (s, CH_3-19) [1]

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 5.6 \times 10^{-6}$ M [2].

References

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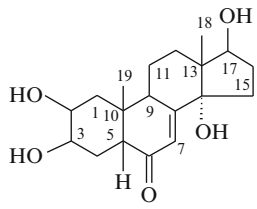
5β-Dihydrorubrosterone

CAS Registry Number: 232280-43-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1], *Lychnis flos-cuculi* [2], *Silene otites* [3]

$C_{19}H_{28}O_5$: 336.1936

Mp: 268–270°C (MeOH) [4], 256–258°C [5], 254–257°C (EtOH-benzene) [6]

$[\alpha]_D^{20}$ + 52° (c 1.0) [6]

IR (KBr) ν_{max} cm^{-1}: 3365, 1646 [1], 3340, 1648 [4], 3450, 1660, 1625 [6]

UV λ_{max}^{EtOH} nm: 241 (ε 11400) [5], (-) (ε 10800) [6]

CI-MS m/z: 354 $[M + H + NH_3]^+$, 337 $[M + H]^+$, 319, 303, 301, 249, 231 [2, 3]

FAB-MS m/z: 337 $[M + H]^+$ (11), 319 $[M + H–H_2O]^+$ (5), 301 $[M + H–2H_2O]^+$ (4) [1]

HR-MS m/z: for $C_{19}H_{29}O_5$ $[M + H]^+$ calcd. 337.2005, found 337.2015 [1]

Anal. Calcd. for $C_{19}H_{28}O_5$: C, 70.2; H, 8.6. Found: C, 70.3; H, 8.4 [6]

^{1}H NMR (500 MHz, CD_3OD): 1.44 (dd, Ha-1), 1.80 (Hb-1), 3.83 (ddd, Ha-2), 3.95 (br q, He-3), 1.73 (Ha-4), 1.68 (Hb-4), 2.39 (dd, H-5), 5.78 (d, H-7), 3.15 (ddd, Ha-9), 1.85 (Ha-11), 1.66 (He-11), 2.06 (Ha-12), 1.60 (He-12), 1.61 (Ha-15), 2.08 (Hb-15), 1.58 (Ha-16), 2.27 (Hb-16), 4.31 (dd, H-17), 0.71 (s, CH_3-18), 0.98 (s, CH_3-19) [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.44 (t, J = 13.0, Ha-1), 3.83 (m, Ha-2), 3.95 (m, He-3), 2.40 (dd, H-5), 5.78 (d, J = 2.5, H-7), 3.16 (m, Ha-9), 4.31 (dd, J = 6.4, 8.8, H-17), 0.72 (s, CH_3-18), 0.98 (s, CH_3-19) [3]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

C-1	37.40	C-8	166.90	C-15	29.05
2	68.68	9	35.46	16	29.74
3	68.48	10	39.35	17	79.24
4	32.87	11	21.34	18	15.84
5	51.88	12	31.48	19	24.45
6	206.48	13	48.27		
7	121.59	14	83.37		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: inactive [7].

References

1. K. Vokac, M. Budesinsky, J. Harmata, Coll. Czech. Chem. Comm. **67**, 124 (2002)

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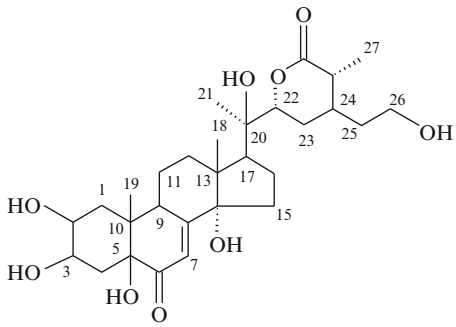
5,29-Dihydroxycapitasterone

CAS Registry Number: 179308-43-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{29}H_{44}O_9$: 536.2985

IR (KBr) ν_{max} cm^{-1}: 3405, 1714, 1671 [1]

TSP-MS m/z: 555 $[M + H + NH_4]^+$ (17), 554 $[M + NH_4]^+$ (42), 537 $[M + H]^+$ (100), 536 $[M]^+$ (82), 519 $[M + H–H_2O]^+$ (54), 501 $[(M + H–2H_2O]^+$ (11) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 2.24 (Ha-1), 2.08 (He-1), 4.24 (m, Ha-2), 4.18 (m, He-3), 2.04 (Ha-4), 1.95 (He-4), 6.26 (d, J = 2.7, H-7), 3.62 (m, H-9), 1.87 (Ha-11), 1.75 (He-11), 2.58 (Ha-12), 1.90 (He-12), 2.20 (Ha-15), 1.85 (Hb-15), 2.35 (m, Ha-16), 2.07 (Hb-16), 2.90 (t, J = 8.8, H-17), 1.11 (s, CH_3-18), 1.16 (s, CH_3-19), 1.44 (s, CH_3-21), 4.78 (dd, J = 11.5, 4.5, H-22), 2.22 (Ha-23), 1.85 (Hb-23), 2.22 (H-24), 2.62 (H-25), 1.25 (d, J = 7.2, CH_3-27), 1.83 (m, Ha-28), 1.55 (m, He-28), 3.86 (m, Ha-29), 3.86 (m, He-29) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	34.8	C-11	22.0	C-21	20.7
2	67.9	12	32.0	22	83.5
3	69.9	13	47.9	23	28.6
4	36.0	14	83.9	24	33.5
5	79.9	15	31.6	25	41.0
6	200.9	16	21.1	26	174.5
7	120.0	17	49.7	27	13.7
8	166.6	18	18.0	28	31.1
9	38.2	19	17.1	29	60.2
10	44.8	20	76.3		

References

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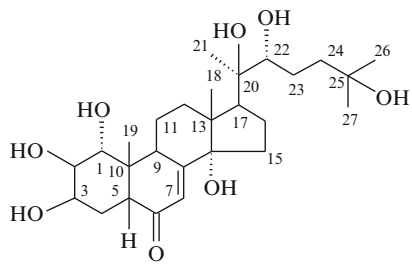
1α,20R-Dihydroxyecdysone (1-epi-Integristerone A)

CAS Registry Number: 82373-20-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Axyris amaranthoides* [1]

$C_{27}H_{44}O_8$: 496.3036

Mp: amorphous [1]

UV λ_{max}^{EtOH} nm (log ε): 240.6 (4.00) [1]
LSI-MS m/z: 495 $[M\text{-}H]^-$ (negative ion mode) [1]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.31 (bs, H-1), 4.29 (m, Ha-2), 4.30 (m, He-3), 1.85 (Ha-4), 2.10 (He-4), 3.30 (H-5), 6.30 (d, J = 2.5, H-7), 3.60 (m, H-9), 1.76 (Ha-11), 1.89 (He-11), 2.60 (dd, J = 5.0, 13.0, Ha-12), 2.00 (He-12), 2.20 (Ha-15), 1.90 (Hb-15), 2.46 (Ha-16), 2.10 (Hb-16), 3.01 (t, J = 8.0, H-17), 1.25 (s, CH_3-18), 1.44 (s, CH_3-19), 1.59 (s, CH_3-21), 3.87 (m, H-22), 1.84 (Ha-23), 2.14 (Hb-23), 2.30 (Ha-24), 1.85 (Hb-24), 1.38 (s, CH_3-26), 1.38 (s, CH_3-27) [1]
^{1}H NMR (400 MHz, J/Hz, CD_3OD): 3.82 (bs, H-1), 3.87 (bt, Ha-2), 4.03 (m, He-3), 1.70 (Ha-4), 1.80 (He-4), 2.60 (dd, J = 4.0, 13.0, H-5), 5.82 (d, J = 2.3, H-7), 3.07 (m, H-9), 1.70 (Ha-11), 1.80 (He-11), 2.14 (dd, J = 5.0, 13.0, Ha-12), 1.82 (He-12), 2.01 (Ha-15), 1.57 (Hb-15), 1.95 (Ha-16), 1.76 (Hb-16), 2.38 (t, J = 8.0, H-17), 0.90 (s, CH_3-18), 1.08 (s, CH_3-19), 1.19 (s, CH_3-21), 3.33 (H-22), 1.32 (Ha-23), 1.65 (Hb-23), 1.75 (Ha-24), 1.43 (Hb-24), 1.20 (s, CH_3-26), 1.20 (s, CH_3-27) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	76.2	C-10	42.0	C-19	20.3
2	68.1	11	21.4	20	76.8
3	70.5	12	32.0	21	21.6
4	33.0	13	47.0	22	77.5
5	46.4	14	84.2	23	27.5
6		15	31.5	24	42.6
7	121.6	16	21.5	25	69.5
8		17	50.1	26	30.0
9	35.0	18	17.8	27	30.1

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 2.5 \times 10^{-7}$ M [1–3].

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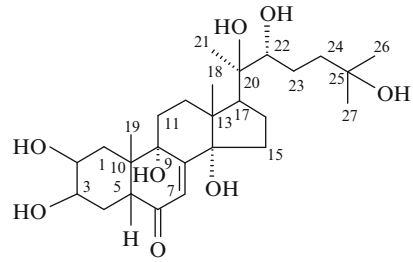
9α,20-Dihydroxyecdysone

CAS Registry Number: 157977-59-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Silene italica* ssp. *nemoralis* [1, 2]
$C_{27}H_{44}O_8$: 496.3036
Mp: 269–271°C [1]
$[\alpha]_D^{24}$ −10° (c 0.05, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3460, 3380, 1660 [1]
UV λ_{max}^{MeOH} nm (log ε): 228 (3.7) [1]
EI-MS m/z: 460 (2), 442 (2), 424 (2), 410 (4), 392 (4), 379 (1), 374 (6), 361 (59), 343 (43), 325 (19), 316 (1), 301 (94), 283 (96), 250 (54), 232 (28), 211 (40), 161 (22), 143 (46), 125 (40), 99 (62), 81 (100), 69 (63) [1]
ESI-MS m/z: 503 $[M + Li]^+$, 485 $[M + Li–H_2O]^+$ [1]
HR-EI-MS m/z: for $C_{27}H_{40}O_6$ $[M\text{-}2H_2O]^+$, calcd. 460.5962, found 460.5998 [1]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.38 (t, Ha-1), 2.06 (d, He-1), 4.45 (dt, J = 3.9, 10.4, Ha-2), 3.96 (q, J = 2.6, He-3), 2.44 (dt, J = 2.3, 13.3, Ha-4), 1.74 (d, He-4), 2.56 (dd, J = 3.9, 13.3, H-5), 5.85 (s, H-7), 2.04 (Ha-11), 1.95 (He-11), 2.19 (td, J = 4.6, 13.1, Ha-12), 1.83 (d, He-12), 1.98 (Ha-15), 1.67 (Hb-15), 1.71 (Ha-16), 2.01 (Hb-16), 2.45 (H-17), 0.89 (s, CH_3-18), 1.01 (s, CH_3-19), 1.22 (s, CH_3-21), 3.32 (dd, H-22), 1.31 (q, Ha-23), 1.66 (t, Hb-23), 1.44 (td, J = 4.2, 11.6, Ha-24), 1.81 (t, Hb-24), 1.19 (s, CH_3-26), 1.205 (s, CH_3-27) [1]
^{13}C NMR (125 MHz, CD_3OD) [1, 2]:

Table 1

C-1	37.6	C-10	43.0	C-19	29.6
2	69.7	11	30.9	20	78.0
3	69.8	12	29.6	21	21.2

(*continued*)

Table 1 (continued)

4	36.3	13	49.1	22	78.6
5	51.4	14	87.2	23	27.5
6	206.7	15	31.6	24	42.5
7	123.8	16	21.4	25	71.4
8	162.6	17	50.4	26	29.1
9	76.6	18	18.5	27	29.9

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.6 \times 10^{-5}$ M [3, 4].

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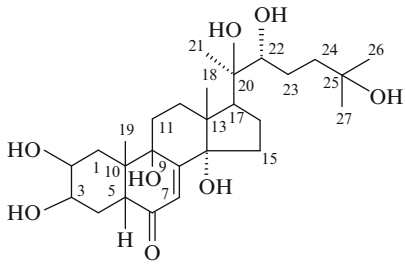
4. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

9β,20-Dihydroxyecdysone

CAS Registry Number: 790701-24-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene italica* ssp. *nemoralis* [1]

$C_{27}H_{44}O_8$: 496.3036

$[\alpha]_D^{24}$ + 14° (c 0.1, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3450, 3400, 1660 [1]

UV λ_{max}^{MeOH} nm (log ε): 206 (1.80), 243 (3.8) [1]

ESI-MS m/z: 497 $[M + H]^+$ (14), 479 (10), 461 (11), 446 (10), 441 (10), 436 (20), 423 (17), 361 (12), 339 (32), 324 (34), 317 (30), 301 (100) [1]

HR-EI-MS m/z: for $C_{27}H_{45}O_8$ $[M + H]^+$, calcd. 497.3114, found 497.3119 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.67 (Ha-1), 1.86 (He-1), 3.88 (q, J = 3.1, Ha-2), 3.195 (dt, J = 3.5, 12.1, He-3), 2.34 (dt, J = 3.9, 13.6, Ha-4), 2.01 (He-4), 2.72 (dt, J = 2.3, 4.5, H-5), 5.82 (s, H-7), 1.69 (Ha-11), 2.37 (dt, J = 9.8, 14.0, He-11), 2.04 (Ha-12), 1.83 (He-12), 1.73 (Ha-15), 1.97 (Hb-15), 1.73 (Ha-16), 1.99 (Hb-16), 2.46 (t, J = 8.8, H-17), 1.235 (s, CH_3-18), 1.37 (s, CH_3-19), 1.21 (s, CH_3-21), 3.32 (H-22), 1.315 (Ha-23), 1.71 (Hb-23), 1.44 (ddd, J = 4.0, 11.7, 13.0, Ha-24), 1.81 (Hb-24), 1.19 (s, CH_3-26), 1.205 (s, CH_3-27) [1]

^{1}H NMR (500 MHz, J/Hz, DMSO-d_5): 1.43 (dt, J = 2.3, 14.8, Ha-1), 1.74 (He-1), 3.67 (q, J = 2.2, Ha-2), 2.96 (dt, J = 3.5, 12.0, He-3), 2.11 (dt, J = 3.5, 12.6, Ha-4), 1.79 (dt, J = 4.9, 12.2, He-4), 2.52 (H-5), 5.61 (s, H-7), 1.52 (dd, J = 8.7, 13.7, Ha-11), 2.21 (dt, J = 9.6, 13.4, He-11), 1.86 (dd, J = 9.6, 13.6, Ha-12), 1.67 (dt, J = 8.8, 13.8, He-12), 1.65 (Ha-15), 1.75 (Hb-15), 1.55 (Ha-16), 1.89 (qd, J = 1.9, 12.0, Hb-16), 2.34 (t, J = 9.1, H-17), 1.13 (s, CH_3-18), 1.24 (s, CH_3-19), 1.07 (s, CH_3-21), 3.115 (d, J = 10.6, H-22), 1.15 (Ha-23), 1.50 (Hb-23), 1.26 (Ha-24), 1.66 (Hb-24), 1.06 (s, CH_3-26), 1.09 (s, CH_3-27), Other: 4.56 (s, OH-9), 4.45 (s, OH-14) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]: **^{13}C NMR** (125 MHz, DMSO-d_5) [1]:

Table 1

C-1	37.2	C-15	32.3	C-1	35.7	C-15	30.6
2	70.6	16	21.8	2	68.5	16	20.4
3	69.9	17	52.4	3	67.7	17	50.3
4	26.2	18	23.4	4	25.3	18	22.5
5	50.3	19	21.6	5	48.4	19	20.9
6	204.4	20	78.1	6	201.2	20	75.6
7	124.3	21	20.8	7	122.0	21	20.5
8	166.4	22	78.7	8	164.5	22	76.3
9	75.3	23	27.6	9	72.8	23	26.1
10	44.2	24	42.6	10	42.3	24	41.4
11	27.0	25	71.5	11	25.3	25	68.7
12	32.9	26	29.1	12	31.4	26	29.0
13	46.2	27	29.8	13	44.4	27	30.0
14	85.9			14	83.4		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.6 \times 10^{-5}$ M [2, 3].

References

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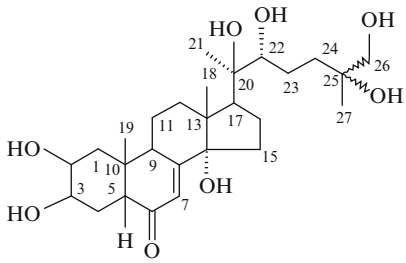
20,26-Dihydroxyecdysone (Podecdysone C)

CAS Registry Number: 19458-46-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Chenopodium pallidicaule* [1], *Coronaria flos-cuculi* [2], *Cyanotis arachnoidea* [3], *Klaseopsis chinensis* [4], *Ourisia caespitosa, O. macrocarpa, O. macrophylla* [5], *Palisota schweinfurthii* [6], *Podocarpus elatus* [7], *Silene fridvaldszkyana* [8], *S. nutans* [9], *S. viridiflora* [10], *Vitex canascens, V. glabrata, V. pinnata* [11]

$C_{27}H_{44}O_8$: 496.3036

Mp: amorphous [11], 149–153°C [12]

IR (KBr) ν_{max} cm^{-1}(C-25 epimer-1): 3400, 2924, 1649, 1443, 1383, 1315, 1120, 1055, 880, (C-25 epimer-2): 3400, 2928, 1648, 1382, 1185, 1105, 1052, 875 [12]

IR (KBr) ν_{max} cm^{-1}: 3430, 1655 [12], 3486, 1652 [13]

UV λ_{max}^{EtOH} nm (ε): 242 (11000) [7], 245 (10400) [12]

EI-MS m/z: 496 $[M]^+$, 460 $[M\text{-}2H_2O]^+$, 442 $[M\text{-}3H_2O]^+$, 427 $[M\text{-}3H_2O\text{-}Me]^+$, 409, 391, 363 $[M\text{-}C_{22}\text{-}C_{27}]^+$, 345 $[M\text{-}C_{22}\text{-}C_{27}\text{-}H_2O]^+$, 133 $[C_{22}\text{-}C_{27}]^+$, 115 [7, 12]

HR-MS m/z: for $C_{27}H_{43}O_8$ $[M\text{-}H]^-$ calcd. 495.2957, found (for C-25 epimer-1): 495.2962, found (for C-25 epimer-2): 495.2945 [11]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 1.22 (s, CH_3-18), 1.08 (s, CH_3-19), 1.58 (s, CH_3-21), 1.48 (s, CH_3-27) [12]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N) (for C-25 epimer-1): 4.19 (m, Ha-2), 4.23 (br s, He-3), 3.01 (H-5), 6.25 (d, J = 2.4, H-7), 3.58 (m, H-9), 3.03 (H-17), 1.204 (s, CH_3-18), 1.06 (s, CH_3-19), 1.58 (s, CH_3-21), 3.92 (br d, J = 10.3, H-22), 3.87 and 3.88 (H-26), 6.29 (s, OH-26), 1.47 (s, CH_3-27); (for C-25 epimer-2): 4.18 (m, Ha-2), 4.23 (br s, He-3), 3.01 (H-5), 6.25 (d, J = 2.4, H-7), 3.58 (m, H-9), 3.08 (H-17), 1.208 (s, CH_3-18), 1.06 (s, CH_3-19), 1.57 (s, CH_3-21), 3.90 (dd, J = 1.8, 10.6, H-22), 3.86 (H-26), 6.31 (s, OH-26), 1.46 (s, CH_3-27) [11]

^{13}C NMR (125 MHz, C_5D_5N) **^{13}C NMR** (125 MHz, C_5D_5N) (for C-25 epimer-1) [11]: (for C-25 epimer-2) [11]:

Table 1

C-1	37.95	C-15	31.96	C-1	37.95	C-15	31.98
2	68.05	16	21.66	2	68.05	16	21.70
3	68.12	17	50.07	3	68.14	17	50.09
4	31.68	18	17.35	4	31.70	18	17.86
5	51.37	19	24.52	5	51.39	19	24.76
6	203.48	20	76.87	6	203.50	20	76.87
7	121.62	21	21.09	7	121.62	21	21.09
8	166.10	22	77.65	8	166.12	22	77.68
9	34.40	23	26.76	9	34.45	23	26.70
10	38.62	24	37.55	10	38.64	24	37.52
11	21.40	25	72.66	11	21.45	25	72.60
12	32.41	26	70.79	12	32.44	26	70.62
13	48.08	27	24.41	13	48.08	27	24.43
14	84.18			14	84.18		

Pharm./Biol.: *Calliphora* bioassay: about 1/10 that of 20-hydroxyecdysone [7], *Musca* bioassay: 0.05-0.075 µg or 1/15 the biological activity of α-ecdysone [12], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 7.3 \times 10^{-6}$ M [13].

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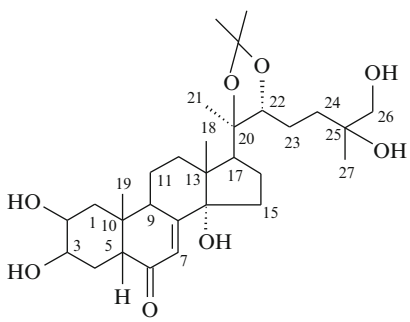
20,26-Dihydroxyecdysone-20,22-Acetonide

CAS Registry Number: 245323-26-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *S. viridiflora* [1]

$C_{30}H_{48}O_8$: 536.3349

$[\alpha]_D^{25}$ + 145° (c 0.005, MeOH) [1]

UV λ_{max}^{MeOH} nm: 242 (log ε 4.01) [1]

ESI-MS m/z: 575 $[M + K]^+$ (14), 560 $[M + H + Na]^+$ (6), 559 $[M + Na]^+$ (5), 542 (100), 521 $[M\text{-}CH_3]^+$ (23), 519 $[M + H\text{–}H_2O]^+$ (2), 503 $[M\text{-}H_2O\text{–}CH_3]^+$ (7), 501 $[M + H\text{–}2H_2O]^+$ (23), 478 [M-acetone]$^+$ (4), 445 (14), 413 (6), 314 (10), 304 (55) [1]

HR-ESI-MS m/z: for $C_{30}H_{49}O_8$ $[M + H]^+$ calcd. 537.3414, found 537.3418 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 2.42 (dd, J = 12.6, 4.0, H-5), 5.86 (d, J = 2.6, H-7), 2.33 (dd, J = 9.2, 8.6, H-17), 0.83 (s, CH_3-18), 0.96 (s, CH_3-19), 1.18 (s, CH_3-21), 3.70 (m, H-22), 3.36 (d, J = 11.0, Ha-26), 3.38 (d, J = 10.9, Hb-26), 1.15 (s, CH_3-27), Other: 1.32 and 1.39 (s, 20,22-iPr) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

C-1		C-11		C-21	22.7
2		12	32.55	22	83.6
3		13	49.3	23	
4		14	85.5	24	37.1
5		15		25	73.2
6		16		26	70.7
7	121.8	17	50.5	27	23.7
8		18	17.8	20,22-iPr	27.3
9		19	24.4		29.4
10		20	85.9		

References

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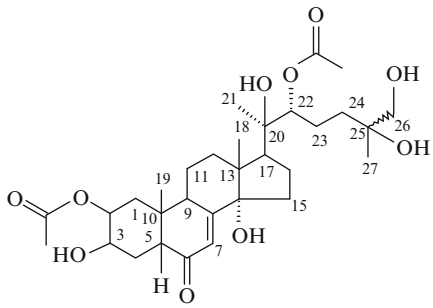
20,26-Dihydroxyecdysone-2,22-Diacetate

CAS Registry Number: 809239-25-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene viridiflora* [1]

$C_{31}H_{48}O_{10}$: 580.3247

FAB-MS m/z: 603.3 $[M + Na]^+$, 581.3 $[M + H]^+$, 563.3 $[M + H–H_2O]^+$ [1]

CI-MS m/z: 682, 664, 640, 622, 598, 580, 562, 556, 538, 520, 502, 496, 478, 461, 443, 422, 404, 236, 218, 192, 174, 136, 132, 77 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.53 (Ha-1), 1.96 (He-1), 5.08 (m, Ha-2), 4.22 (m, He-3), 1.80 (Ha-4), 1.83 (He-4), 2.41 (dd, J = 13.0, 5.0, H-5), 5.99 (d, J = 2.5, H-7), 3.18 (m, H-9), 1.73 (Ha-11), 1.86 (He-11), 1.76 (Ha-12), 1.96 (He-12), 1.67 (Ha-15), 2.06 (Hb-15), 1.88 (Ha-16), 1.80 (Hb-16), 2.31 (t, J = 9.5, H-17), 0.86 (s, CH_3-18), 1.02 (s, CH_3-19), 1.34 (s, CH_3-21), 4.85 (dd, J = 10.5, 2.0, H-22), 1.56 (Ha-23), 1.76 (Hb-23), 1.75 (Ha-24), 1.46 (Hb-24), 3.42 (s, CH_2OH-26), 1.15 (s, CH_3-27), Other: 2.127 (s, CH_3COO-2), 2.167 (s, CH_3COO-22) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

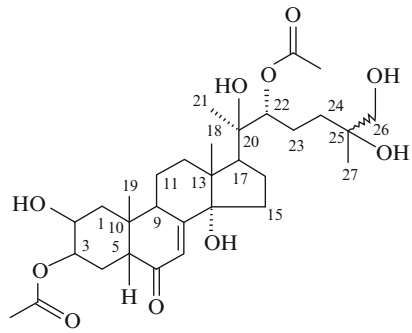
C-1	39.2	C-11	n.d.	C-21	23.0
2	74.5	12	33.8	22	82.9
3	67.8	13	50.2	23	n.d.
4	n.d.	14	88.1	24	37.4
5	53.0	15	33.1	25	76.0
6	n.d.	16	22.9	26	71.3
7	123.8	17	52.1	27	24.6
8	n.d.	18	19.7	2-$\underline{CH_3}$COO	23.6
				2-$CH_3\underline{COO}$	176.5
9	36.6	19	25.6	22-$\underline{CH_3}$COO	23.4
10	41.0	20	79.9	22-$CH_3\underline{COO}$	177.6

References

1. N.Z. Mamadalieva, L.N. Zibareva, N. Edvard-Todeschi, J.P. Girault, A. Maria, N.Sh. Ramazanov, Z. Saatov, R. Lafont, Coll. Czech. Chem. Comm. **69**, 1675 (2004)

20,26-Dihydroxyecdysone-3,22-Diacetate

CAS Registry Number: 50907-59-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene viridiflora* [1]

$C_{31}H_{48}O_{10}$: 580.3247

FAB-MS m/z: 603.3 $[M + Na]^+$, 581.3 $[M + H]^+$, 563.3 $[M + H-H_2O]^+$ [1]

CI-MS m/z: 682, 664, 640, 622, 598, 580, 562, 556, 538, 520, 502, 496, 478, 461, 443, 422, 404, 236, 218, 192, 174, 136, 132, 77 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.48 (Ha-1), 1.99 (He-1), 4.13 (m, Ha-2), 5.17 (m, He-3), 1.78 (Ha-4), 1.85 (He-4), 2.35 (dd, J = 13.5, 4.2, H-5), 5.98 (d, J = 2.5, H-7), 3.11 (m, H-9), 1.74 (Ha-11), 1.86 (He-11), 1.76 (Ha-12), 1.96 (He-12), 1.67 (Ha-15), 2.06 (Hb-15), 1.88 (Ha-16), 1.80 (Hb-16), 2.31 (t, J = 9.5, H-17), 0.86 (s, CH_3-18), 1.02 (s, CH_3-19), 1.34 (s, CH_3-21), 4.85 (dd, J = 10.5, 2.0, H-22), 1.56 (Ha-23), 1.76 (Hb-23), 1.75 (Ha-24), 1.46 (Hb-24), 3.42 (s, CH_2OH-26), 1.15 (s, CH_3-27), Other: 2.176 (s, CH_3COO-2), 2.165 (s, CH_3COO-22) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

C-1	39.0	C-11	n.d.	C-21	22.8
2	68.5	12	33.5	22	84.2

(*continued*)

Table 1 (continued)

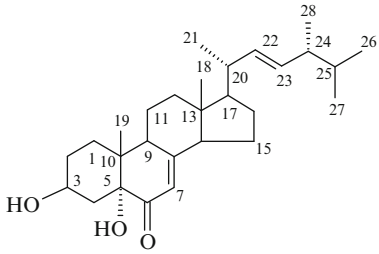
3	73.9	13	50.0	23	n.d.
4	n.d.	14	87.8	24	37.4
5	53.4	15	32.8	25	75.9
6	n.d.	16	22.2	26	71.4
7	123.9	17	52.1	27	24.7
8	n.d.	18	19.6	3-CH_3COO	23.2
				3-CH_3COO	176.6
9	36.5	19	25.7	22-CH_3COO	23.2
10	40.6	20	79.9	22-CH_3COO	177.5

References

1. N.Z. Mamadalieva, L.N. Zibareva, N. Edvard-Todeschi, J.P. Girault, A. Maria, N.Sh. Ramazanov, Z. Saatov, R. Lafont, Coll. Czech. Chem. Comm. **69**, 1675 (2004)

3β,5α-Dihydroxy-(22E,24R)-Ergosta-7,22-dien-6-one

CAS Registry Number: 14858-07-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Agaricus blazei* [1], *Grifola frondosa* [2], *Pleurotus ostreatus* [3]

$C_{28}H_{44}O_3$: 428.3290

Mp: amorphous [2]

$[\alpha]_D^{25}$ + 9.1° (c 0.1, $CHCl_3$) [2]

IR ($CHCl_3$) ν_{max} cm^{-1}: 3457, 1667 [2]

UV λ_{max}^{MeOH} nm (log ε): 248 (3.9) [2]

HR-MS m/z: for $C_{28}H_{44}O_3$ $[M]^+$ calcd. 428.3290, found 428.3307 [2]

^{1}H NMR (270 MHz, J/Hz, $CHCl_3$): 4.04 (m, He-3), 5.66 (br s, H-7), 0.61 (s, CH_3-18), 0.96 (s, CH_3-19), 1.04 (d, J = 6.6, CH_3-21), 5.15 (dd, J = 7.6, 15.2, H-22), 5.25 (dd, J = 7.1, 15.2, H-23), 0.82 (d, J = 6.8, CH_3-26), 0.84 (d, J = 6.8, CH_3-27), 0.92 (d, J = 6.8, CH_3-28) [2]

Pharm./Biol.: Showed growth inhibition of *HeLa* cells in concentration 32 μg/ml [1].

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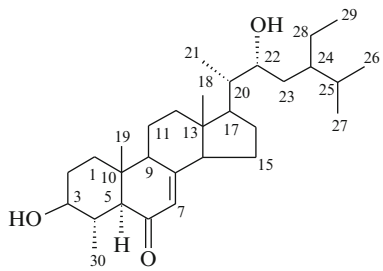
3β,22-Dihydroxy-4α-Methyl-24-Ethyl-5α-Cholest-7-en-6-one

CAS Registry Number: 55487-84-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Solanum xanthocarpum* [1]

$C_{30}H_{50}O_3$: 458.3760

Mp: 188–190°C (acetone) [1]

$[\alpha]_D^{20}$ + 14.3° [1]

IR ($CHCl_3$) ν_{max} cm^{-1}: 3600, 3510, 1668, 1625 [1]

EI-MS m/z: 458 $[M]^+$ (22.2), 440 (51.1), 330 (100), 297 (27.8), 275 (95.6), 257 (52.2) [1]

^{1}H NMR (J/Hz, $CDCl_3$): 3.18 (m, H-3), 5.68 (br s, H-7), 0.61 (s, CH_3-18), 0.86 (s, CH_3-19), 3.74 (d, J = 12.0, H-22), 1.16 (d, J = 6.0, CH_3-30) [1].

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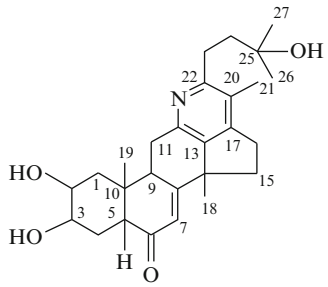
1. G. Kusano, T. Takemoto, J.A. Beisler, Y. Sato, Phytochemistry **14**, 529 (1975)

Diploclidine

CAS Registry Number: 645406-01-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Diploclisia glaucescens* [1]

$C_{27}H_{37}O_4N$: 439.2723

$[\alpha]_D^{24}$ + 78.9° (c 0.8, MeOH) [1]

UV λ_{max}^{MeOH} nm: 215, 240, 275 [1]

FAB-HR-MS m/z: for $C_{27}H_{38}O_4N$ $[M + H]^+$ calcd. 440.2801, found 440.2837 [1]

^{1}H NMR (500 MHz, J/Hz, $CDCl_3$): 1.66 (dd, J = 12.0, 13.7, Ha-1), 1.94 (dd, J = 3.8, 13.7, He-1), 3.73 (ddd, J = 2.5, 3.8, 12.0, Ha-2), 4.04 (ddd, J = 2.5, He-3), 1.59 (ddd, J = 2.5, 13.4, 14.2, Ha-4), 1.89 (dt, J = 2.5, 4.5, 14.2, He-4), 2.48 (dd, J = 4.5, 13.4, H-5), 6.04 (d, J = 2.7, H-7), 2.67 (m, H-9), 2.42 (dd, J = 13.0, 14.4, Ha-11), 3.24 (dd, J = 4.0, 14.4, He-11), 2.12 (ddd, J = 8.6, 11.0, 12.4, Ha-15), 2.40 (dd, J = 7.0, 12.4, Hb-15), 2.86 (dd, J = 8.6, 16.5, Ha-16), 3.20 (ddd, J = 7.0, 11.0 16.5, Hb-16), 1.31 (s, CH_3-18), 1.07 (s, CH_3-19), 2.57 (s, CH_3-21), 2.72 (td, J = 5.9, 12.5, Ha-23), 2.92 (ddd, J = 2.8, 12.5, 13.0, Hb-23), 1.35 (m, Ha-24), 1.77 (td, J = 5.9, 13.0, Hb-24), 1.37 (s, CH_3-26), 1.33 (s, CH_3-27) [1]

^{13}C NMR (125 MHz, $CDCl_3$) [1]:

Table 1

C-1	36.9	C-10	40.3	C-19	22.6
2	67.6	11	21.4	20	130.2
3	67.4	12	158.6	21	22.1
4	31.1	13	136.6	22	155.2
5	49.3	14	47.1	23	22.9
6	202.0	15	40.1	24	44.4
7	123.5	16	31.9	25	70.9
8	171.7	17	142.0	26	27.6
9	40.8	18	26.3	27	30.4

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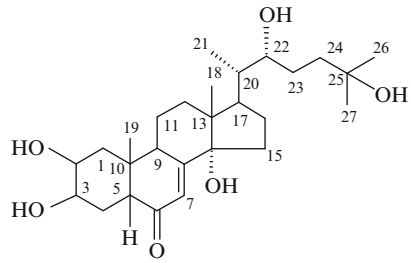
α-Ecdysone

CAS Registry Number: 3604-87-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Achyranthes bidentata* [1], *Acrostichum speciosum* [2], *Athyrium yokoscence* [3], *Ajuga austarlis* [4], *A. turkestanica* [5], *Bassia quinquecuspus* [2], *Blandfordia punicea* [6], *Blechnum minus, B. penna-marina* [7–9], *Blechnum spicant* [10], *B. vulcanicum* [7–9], *Briza maxima* [11], *Cheilantes seiberi* [2],

Cheilantes tenuifolia [12], *Centaurea moschata* [13], *Coronaria flos-cuculi* [14], *Ipomoea calonyction* [15], *Lemmaphyllum macrophyllum* [16], *Leuzea carthamoides* [17], *Limnanthes alba* [18], *Lychnis chalcedonica* [19, 20], *L. fulgends* [19, 21], *L. wilfordii* [19], *Microsorum membranifolium* [22], *Microsorum commutatum, M. punctatum* [23], *M. scolopendria* [24], *Neocheiropteris ensata* [25], *Osmunda asiatica, O. japonica* [26], *Paris verticillata* [27], *Phymatodes novaezelandiae, P. virginianum* [28], *Plenasium banksiifolium* [29], *Polypodium virginianum* [30], *P. vulgare* [31], *Pteridium aquilinum* [32], *Rhaponticum carthamoides* [33], *Serratula coronata* [34, 35], *S. wolffii* [36], *Sida acuta* [37], *S. rhombifolia* [37, 38], *Silene disticha, S. echinata, S. italica* [39], *S. italica* ssp. *nemoralis* [40], *S. linicola* [41], *S. otites* [42], *S. portensis* [39], *S. praemixta* [43], *Spinacia oleracea* [44], *Tectaria* sp. [2], *Thelypteris japonica* [45], *Trianthema galericulata* [2]

$C_{27}H_{44}O_6$: 464.3137

Mp: 241–243°C [7], 240–241°C (MeOH–Me_2CO) [15], 236–238°C (MeOH–H_2O) [20, 41], 232–235°C [32], 234–236°C (MeOH–EtOAc) [19, 34], 242–243°C [35], 235–237°C [46], 237–239.5°C [47]

$[\alpha]_D^{20}$ + 67.8° (c 1.0, MeOH) [15], $[\alpha]_D^{20}$ + 63.0 ± 2° (c 0.65, MeOH) [19, 20], $[\alpha]_D^{20}$ + 60.9 ± 2° (c 0.82, MeOH) [34], $[\alpha]_D^{15}$ + 64.7° (c 0.80, MeOH) [35], $[\alpha]_D^{22}$ + 63.6° (c 0.83, MeOH) [41], $[\alpha]_D^{20}$ + 58.5 ± 2° (c, EtOH) [46], $[\alpha]_D$ + 58.5 ± 2° (c 0.1, EtOH) [47]

IR (KBr) ν_{max} cm^{-1}: 1658, 1652 [32], 3200–3400 [34], 3400–3460, 1665 [41]

IR (Nujol) ν_{max} cm^{-1}: 3600–3200, 1650, 1615 [15]

UV λ_{max}^{MeOH} nm (ε): 244 (11800) [15], 244 (11600) [32]

UV λ_{max}^{EtOH} nm: 245 (ε 4.01) [34], 244 [46], 241 (ε 12300) [47], 242 (ε 11900) [48]

EI-MS m/z: 464 $[M]^+$, 446, 431, 428, 413, 410, 395, 377, 348, 330, 315, 300, 126, 117, 109, 99, 81 [20], 446 $[M\text{-}H_2O]^+$ (0.2), 431 (0.7), 428 (1.6), 418 (2), 413 (3), 348 (8), 315 (8), 301 (4), 300 (3), 279 (52), 250 (50), 99 (100), 81 (99) [41], 446 $[M\text{-}H_2O]^+$ (3), 428 (29), 418 (2), 413 (2), 410 (3), 372 (3), 359 (4), 348 (8), 330 (15), 315 (18), 300 (23), 279 (17), 267 (5), 255 (8), 250 (13), 249 (10), 99 (100), 81 (61) [49]

CI/D-MS m/z: 482 $[M + H + NH_3]^+$ (44), 465 $[M + H]^+$ (48), 447 $[M + H\text{-}H_2O]^+$ (100), 429 $[M + H\text{-}2H_2O]^+$ (38), 411 $[M + H\text{–}3H_2O]^+$ (1) [43]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 3.82 (m, H-2), 4.06 (m, H-3), 6.02 (br s, H-7), 3.36 (m, H-9), 0.59 (s, CH_3-18), 0.94 (s, CH_3-19), 1.14 (d, J = 6.0, CH_3-21), 3.82 (m, H-22), 1.24 (s, CH_3-26), 1.24 (s, CH_3-27) [20]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.10 (m, H-2), 4.22 (m, H-3), 6.18 (br s, H-7), 3.52 (m, H-9), 0.74 (s, CH_3-18), 1.07 (s, CH_3-19), 1.24 (d, J = 6.0, CH_3-21), 1.37 (s, CH_3-26), 1.37 (s, CH_3-27) [41]

^{1}H NMR (J/Hz, C_5D_5N): 4.10 (m, Ha-2), 4.22 (br s, He-3), 2.99 (q, J = 4.0, 13.0, H-5), 6.18 (br s, H-7), 3.52 (m, H-9), 0.74 (s, CH_3-18), 1.07 (s, CH_3-19), 1.24 (d, CH_3-21), 4.10 (m, H-22), 1.37 (s, CH_3-26), 1.37 (s, CH_3-27) [49]

^{1}H NMR (250 MHz, J/Hz, C_5D_5N): 1.90 (Ha-1), 2.10 (He-1), 4.15 (m, Ha-2), 4.21 (m, He-3), 1.80 (Ha-4), 2.03 (He-4), 3.01 (dd, J = 4.0, 13.0, H-5), 6.25 (d, J = 2.5, H-7), 3.54 (m, H-9), 1.60 (Ha-11), 1.80 (He-11), 2.53 (Ha-12), 1.83 (He-12), 1.85 (Ha-15), 1.75 (Hb-15), 2.19 (Ha-16), 1.59 (Hb-16), 2.51 (H-17), 0.70 (s, CH_3-18), 1.06 (s, CH_3-19), 2.12 (H-20), 1.28 (d, J = 7.0, CH_3-21), 4.05 (H-22), 1.80 (Ha-23), 1.94 (Hb-23), 2.26 (Ha-24), 1.79 (Hb-24), 1.37 (s, CH_3-26), 1.37 (s, CH_3-27) [50]

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.43 (Ha-1), 1.78 (He-1), 3.83 (ddd, J = 3.0, 3.0, 12.0, Ha-2), 3.94 (ddd, J = 3.0, 3.0, 3.0, He-3), 1.65 (Ha-4), 1.75 (He-4), 2.38 (dd, J = 5.0, 12.0, H-5), 5.81 (d, J = 2.5, H-7), 3.14 (m, H-9), 1.65 (Ha-11), 1.78 (He-11), 2.10 (ddd, J = 5.0, 13.0, 13.0, Ha-12), 1.70-1.80 (He-12), 2.00 (Ha-15), 1.53 (Hb-15), 1.98 (Ha-16), 1.48 (Hb-16), 2.01 (H-17), 0.73 (s, CH_3-18), 0.97 (s, CH_3-19), 1.72 (H-20), 0.95 (d, J = 7.5, CH_3-21), 3.59 (m, H-22), 1.30 (Ha-23), 1.60 (Hb-23), 1.75 (Ha-24), 1.45 (Hb-24), 1.19 (s, CH_3-26), 1.20 (s, CH_3-27) [50]

^{1}H NMR (250 MHz, J/Hz, D_2O): 1.35 (Ha-1), 1.85 (He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.34 (t, H-5), 5.98 (d, J = 2.5, H-7), 3.10 (m, H-9), 1.65 (Ha-11), 1.80 (He-11), 0.74 (s, CH_3-18), 1.00 (s, CH_3-19), 1.70 (H-20), 0.94 (d, J = 7.0, CH_3-21), 3.70 (m, H-22), 1.35 (Ha-23), 1.65 (Hb-23), 1.23 (s, CH_3-26), 1.23 (s, CH_3-27) [50]

^{1}H NMR (250 MHz, J/Hz, $CDCl_3$): 3.90 (m, Ha-2), 4.03 (He-3), 2.42 (dd, J = 4.0, 13.0, H-5), 5.84 (H-7), 2.97 (m, H-9), 0.67 (s, CH_3-18), 0.98 (s, CH_3-

19), 0.94 (d, J = 6.6, CH_3-21), 3.65 (m, H-22), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27) [50]

^{13}C NMR (75 MHz, C_5D_5N) [31, 50]: **^{13}C NMR** (75 MHz, C_5D_5N) [49]:

Table 1

C-1	38.08	C-15	32.03	C-1	38.3	C-15	32.2
2	68.10	16	26.74	2	68.3	16	26.9
3	68.10	17	48.28	3	68.3	17	48.6
4	32.45	18	15.89	4	32.5	18	16.1
5	51.41	19	24.55	5	51.5	19	24.7
6	203.36	20	43.04	6	203.7	20	43.2
7	121.61	21	13.74	7	121.9	21	13.9
8	165.53	22	74.07	8	165.8	22	74.4
9	34.63	23	25.69	9	34.9	23	25.9
10	38.76	24	42.55	10	38.9	24	42.5
11	21.20	25	69.80	11	21.4	25	70.2
12	31.49	26	30.09	12	31.0	26	30.5
13	47.70	27	30.01	13	47.9	27	30.2
14	83.97			14	84.2		

^{13}C NMR (62.9 MHz, CD_3OD) [50]: **^{13}C NMR** (25 MHz, C_5D_5N) [51]:

Table 2

C-1	37.48	C-15	32.08	C-1	37.6	C-15	31.3
2	68.70	16	26.98	2	67.9	16	26.5
3	68.50	17	48.82	3	67.9	17	48.1
4	32.82	18	16.20	4	32.2	18	15.6
5	51.76	19	24.45	5	51.2	19	24.3
6	203.36	20	43.88	6	203.6	20	42.3
7	121.98	21	13.35	7	121.4	21	13.4
8	167.48	22	75.27	8	165.5	22	73.8
9	35.33	23	25.52	9	34.4	23	25.4
10	39.25	24	42.23	10	38.5	24	42.7
11	21.62	25	71.36	11	21.0	25	69.6
12	32.08	26	29.28	12	31.7	26	29.8
13	48.18	27	29.51	13	47.3	27	29.8
14	85.06			14	83.6		

Pharm./Biol.: Antimicrobial tests: inactive >20 μg/ml; antimalarial test: inactive >4.76 μg/ml; antiprotozoal test: in active >40 μg/ml [38], *Calliphora* bioassay: high active [48, 52, 53], *Musca domestica* bioassay: high active [52, 53], *Galleria mellonella* bioassay: ED_{50} = 7.8 μg/g, *Sarcophaga bullata* bioassay: ED_{50} = 4.2 μg/g, *Dermestes vulpinus* bioassay: ED_{50} = 42.0 μg/g [54], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.1 \times 10^{-6}$ M [55–58], $EC_{50} = 2.0 \times 10^{-7}$ M [59], Ecdysone enhanced the rate of protein synthesis in mammalian tissue [60], showed activity on 0.5–100 μg in 15 ml medium on growth of the *HeLa* cells in culture [61], and had no consistent effect on growth of the vertebrate cells in culture [62] and had antitumor activity [63–69].

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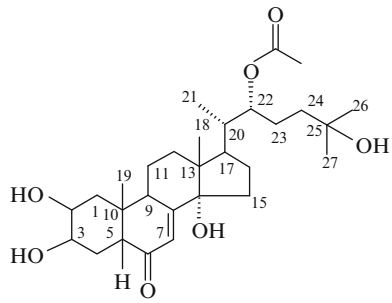
Ecdysone-22-Acetate

CAS Registry Number: 100495-91-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula coronata* [1]

$C_{29}H_{46}O_7$: 506.3243

CI-MS m/z: 524 $[M + H + NH_3]^+$, 507 $[M + H]^+$, 506 $[M]^+$, 489, 462, 458, 448, 428, 414, 391, 370, 326, 279, 260, 244, 191, 148, 141 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.38 (t, J = 13.4, Ha-1), 1.88 (m, He-1), 3.99 (m, Ha-2), 4.07 (m, He-3),

1.75 (t, Ha-4), 1.75 (t, He-4), 2.35 (t, H-5), 5.97 (d, J = 2.5, H-7), 3.11 (m, H-9), 1.73 (Ha-11), 1.86 (He-11), 1.93 (Ha-12), 1.86 (He-12), 1.65 (Ha-15), 2.05 (Hb-15), 1.74 (Ha-16), 1.88 (Hb-16), 1.94 (m, H-17), 0.72 (s, CH_3-18), 1.00 (s, CH_3-19), 1.94 (m, H-20), 0.995 (d, J = 6.0, CH_3-21), 4.86 (dd, J = 10.5, 2.0, H-22), 1.56 (Ha-23), 1.76 (Hb-23), 1.56 (Ha-24), 1.46 (Hb-24), 1.23 (s, CH_3-26), 1.23 (s, CH_3-27) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

C-1	36.4 (t)	C-11	21.0 (d)	C-21	14.0 (q)
2	68.3 (d)	12	31.4 (t)	22	80.3 (d)
3	68.2 (d)	13	48.3 (s)	23	26.4 (t)
4	32.3 (t)	14	86.4 (s)	24	40.6 (t)
5	51.4 (d)	15	31.6 (t)	25	72.8 (s)
6		16	21.0 (t)	26	28.9 (q)
7	122.1 (d)	17	48.4 (d)	27	28.9 (q)
8		18	16.3 (q)	$COCH_3$	21.9 (q)
9	34.9 (d)	19	24.2 (q)	$COCH_3$	175.8 (s)
10	39.1 (s)	20	39.8 (d)		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.10 \times 10^{-6}$ M [1].

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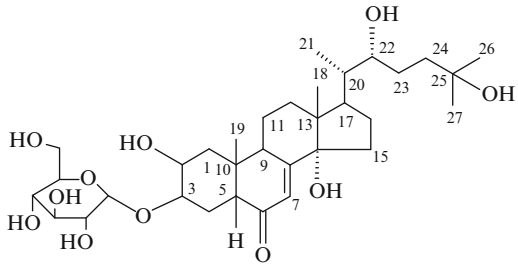
Ecdysone-3-Glucoside

CAS Registry Number: 130690-19-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Sida rhombifolia* [1]

$C_{33}H_{54}O_{11}$: 626.3666

Mp: 275–277°C (dec.) [1]

$[\alpha]_D^{20}$ + 36.6° (c 3.27; Pyridine) [1]

IR (NaCl) ν_{max} cm^{-1}: 3359, 1651, 1448, 1364, 1074, 1040 [1]

UV λ_{max}^{MeOH} nm (ε): 245 (1647) [1]

HR-ESI-MS m/z: for $C_{33}H_{54}NaO_{11}$ $[M + Na]^+$ calcd. 649.3564, found 649.3604 [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.77-1.80 (Ha-1), 2.06-2.09 (He-1), 4.10-4.14 (Ha-2), 4.30 (br s, He-3), 1.68-1.71 (Ha-4), 2.20-2.23 (He-4), 2.93 (br d, J = 10.4, H-5), 6.18 (s, H-7), 3.50 (br s, Ha-9), 1.72-1.75 (H-11), 1.80-1.82 (Ha-12), 2.50-2.52 (He-12), 2.06 (br s, H-15), 1.91 (br s, H-16), 2.50-2.52 (H-17), 0.70 (s, CH_3-18), 0.90 (s, CH_3-19), 2.09-2.13 (H-20), 1.28 (d, J = 6.4, CH_3-21), 4.12-4.15 (H-22), 1.57 (br s, H-23), 1.79-1.82 (Ha-24), 2.19 (br s, Hb-24), 1.39 (s, CH_3-26), 1.39 (s, CH_3-27), Other: β-D-Glcp′: 4.93 (d, J = 7.2, H-1), 4.05 (br s, H-2), 3.92 (br s,H-3), 4.21 (m, H-4), 4.21 (m, H-5), 4.34 (m, Ha-6), 4.53 (d, J = 10.4, Hb-6) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.9	C-12	31.6	C-23	26.9
2	67.6	13	47.7	24	42.8
3	77.7	14	84.0	25	70.0
4	30.7	15	32.2	26	30.3
5	51.6	16	21.3	27	30.5
6	203.5	17	48.6	Glc′-1	104.3
7	121.8	18	16.0	2	74.9
8	166.3	19	24.3	3	78.9
9	34.5	20	43.3	4	71.8
10	39.2	21	13.9	5	78.7
11	21.3	22	74.2	6	62.7

Pharm./Biol.: Antimicrobial tests: inactive > 20 μg/ml; antimalarial test: inactive >4.76 μg/ml; antiprotozoal test: in active >40 μg/ml [1].

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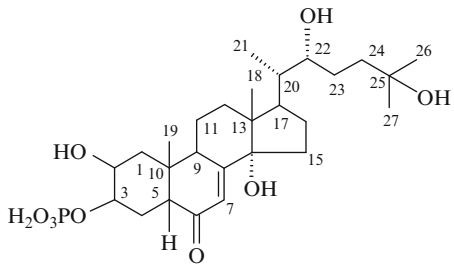
Ecdysone-3-Phosphate

CAS Registry Number: 130690-29-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Spinacia oleracea* [1]

$C_{27}H_{45}O_9P$: 544.2801

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.05 (m, Ha-2), 4.20 (m, He-3), 6.25 (d, J = 2.0, H-7), 075 (s, CH_3-18), 0.89 (s, CH_3-19), 1.28 (d, J = 7.0, CH_3-21), 3.60 (m, H-22), 1.38 (s, CH_3-26), 1.38 (s, CH_3-27) [1]

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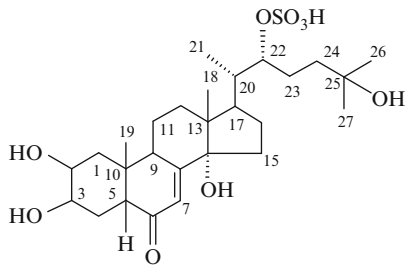
Ecdysone-22-Sulfate

CAS Registry Number: 93552-65-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1]

$C_{27}H_{44}O_9S$: 544.2706

Mp: 224–226°C [1]

$[\alpha]_D^{20}$ + 63.3 ± 2° (c 0.91, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3445–3210, 1652, 1235 [1]

UV λ_{max}^{EtOH} nm (log ε): 245 (4.15) [1]

EI-MS m/z: 428 (4), 410 (57), 392 (57), 380 (18), 377 (16), 359 (7), 349 (6), 336 (8), 322 (8), 312 (20), 297 (8), 295 (9), 282 (38), 267 (21), 265 (14), 255 (14), 225 (20), 211 (13), 126 (20), 109 (19), 99 (100), 81 (43), 69 (19) [1]

CD (c, 0.10, MeOH): Δε = −4.19 (250 nm), Δε = +1.92 (330 nm) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.15 (dt, J = 12.3, 4.4, 3.5, Ha-2), 4.23 (br s, He-3), 3.00 (q, J = 13.2, 4.4, H-5), 6.20 (d, J = 2.4, H-7), 3.54 (m, Ha-9), 0.79 (s, CH_3-18), 1.01 (s, CH_3-19), 3.09 (m, J = 21.4, H-20), 1.27 (d, J = 7, CH_3-21), 5.21 (m, J = 15.1, H-22), 1.31 (s, CH_3-26), 1.32 (s, CH_3-27) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

C-1	37.8	C-10	38.6	C-19	24.4
2	68.1	11	21.1	20	39.7
3	68.1	12	31.4	21	13.8
4	32.0	13	47.6	22	82.9
5	51.2	14	83.9	23	24.0
6	203.3	15	32.0	24	41.1
7	121.5	16	26.5	25	69.8
8	165.6	17	48.2	26	30.3
9	34.5	18	15.9	27	29.5

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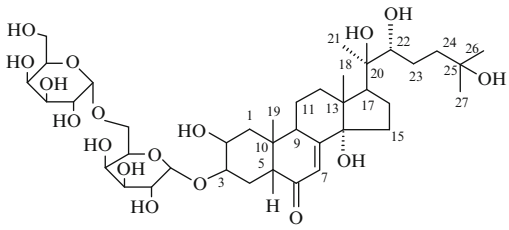
Ecdysteroside

CAS Registry Number: 209850-88-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene tatarica* [1]

$C_{39}H_{64}O_{17}$: 804.4143

Mp: 228–230°C (EtOAc-MeOH) [1]

$[\alpha]_D^{20}$ + 100.4° (c 2.59, MeOH) [1]

EI-MS m/z: 588 (3), 573 (3), 570 (6), 555 (2.1), 552 (2.4), 534 (2.1), 516 (1.5), 501, 462, 455, 444 (30), 426 (36), 411 (15), 408 (15), 393 (10), 375, 357, 345 (12), 327, 300 (100), 99 (30), 81 (27) [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.04 (Ha-2), 4.08 (He-3), 6.19 (H-7), 3.45 (m, H-9), 1.19 (s, CH_3-18), 0.98 (s, CH_3-19), 1.57 (s, CH_3-21), 3.84 (dd, H-22), 1.35 (s, CH_3-26), 1.35 (s, CH_3-27), Other: α-D-Gal′: 5.56 (d, J = 4.0, H-1), α-D-Gal″: 5.16 (d, J = 4.0, H-1) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

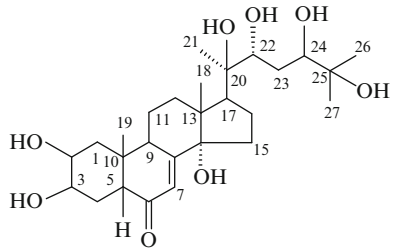
C-1	38.53	C-11	21.04	C-21	21.67	Gal′-4	71.02
2	68.08	12	31.68	22	77.57	5	73.46
3	79.15	13	48.06	23	22.45	6	62.62
4	31.41	14	84.12	24	42.60	Gal″-1	101.75
5	52.43	15	31.68	25	69.57	2	70.95
6	202.97	16	21.46	26	29.99	3	71.66
7	121.51	17	50.10	27	30.06	4	70.56
8	166.51	18	17.84	Gal′-1	103.71	5	72.59
9	34.25	19	24.27	2	71.02	6	62.62
10	39.39	20	76.87	3	71.78		

References

1. U.A. Baltaev, Phytochemistry **47**, 1233 (1998)

24-epi-Abutasterone

CAS Registry Number: 194673-68-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Vitex canascens* [1], *V. scabra* [2]

$C_{27}H_{44}O_8$: 496.3036

Mp: 257–259°C (MeOH–EtOAc) [3]

IR (KBr) ν_{max} cm^{-1}: 3408, 2962, 1651, 1444, 1383, 1303, 1057, 950, 877 [1]

FAB-MS m/z: 497.3118 $[M + H]^+$ [3]

HR-MS m/z: 497.3123 $[M + H]^+$, calcd. for $C_{27}H_{45}O_8$: 497.3114 [1, 3]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.18 (m, Ha-2), 4.23 (br s, He-3), 2.99 (dd, J = 12.9, 3.5, H-5), 6.22 (d, J = 2.1, H-7), 3.57 (m, H-9), 3.08 (t, J = 9.1, H-17), 1.22 (s, CH_3-18), 1.06 (s, CH_3-19), 1.63 (s, CH_3-21), 4.51 (dd, J = 9.6, 2.3, H-22), 4.37 (dd, J = 9.0, 2.7, H-24), 1.46 (s, CH_3-26), 1.47 (s, CH_3-27) [1, 3]

^{13}C NMR (125.65 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-10	38.6	C-19	24.4
2	68.1	11	21.1	20	76.8
3	68.0	12	31.7	21	21.7

(*continued*)

Table 1 (continued)

4	32.3	13	48.1	22	73.7
5	51.3	14	84.2	23	35.2
6	203.4	15	31.9	24	75.9
7	121.6	16	21.3	25	72.6
8	166.1	17	50.0	26	26.1
9	34.4	18	17.9	27	26.0

Pharm./Biol.: *Musca* bioassay: very less active than 20-hydroxyecdysone [3].

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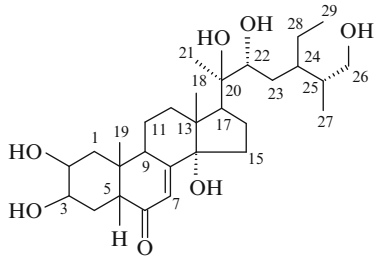
25-epi-Amarasterone A



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Microsorum scolopendria* [1]

$C_{29}H_{48}O_7$: 508.3400

CI/D-MS m/z: 526 $[M + NH_4]^+$, 509 $[M + H]^+$, 491 $[M + H–H_2O]^+$, 473 $[M + H–2H_2O]^+$, 455 $[M + H–3H_2O]^+$, 364 $[M + NH_4–H_2O\text{-}C_{22}\text{-}C_{29}]^+$, 347 $[M + H–H_2O\text{-}C_{22}\text{-}C_{29}]^+$, 329 $[M + H–2H_2O\text{-}C_{22}\text{-}C_{29}]^+$, 171, 127, 124 [1]

^{1}H NMR (J/Hz, D_2O): 1.38 (Ha-1), 1.88 (He-1), 3.99 (Ha-2), 4.07 (He-3), 1.75 (Ha-4), 1.75 (He-4), 2.34 (t, H-5), 5.97 (d, J = 2.0, H-7), 3.11 (Ha-9), 1.73 (Ha-11), 1.86 (He-11), 1.99 (Ha-12), 1.96 (He-12), 1.64 (Ha-15), 2.05 (Hb-15), 1.89 (Ha-16), 1.80 (Hb-16), 2.30 (m, H-17), 0.867 (s, CH_3-18), 1.00 (s, CH_3-19), 1.22 (s, CH_3-21), 3.56 (d, J = 10.0, Hb-22), 1.29 (Ha-23), 1.24 (Hb-23), 1.56 (Ha-24), 1.88 (H-25), 3.46 (dd, J = 7.2, 10.8, Ha-26), 3.55 (m, Ha-26), 0.809 (d, J = 6.8, CH_3-27), 1.30 (Ha-28), 1.52 (Hb-28), 0.896 (t, J = 7.4, CH_3-29) [1]

^{13}C NMR (D_2O) [1]:

Table 1

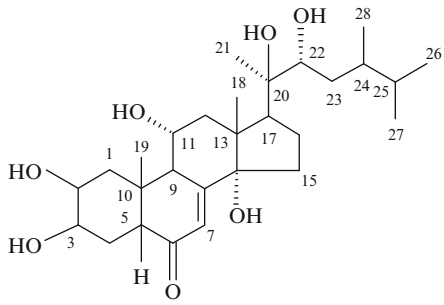
C-1	38.3	C-11	22.8	C-21	22.3
2	70.2	12	33.8	22	76.8
3	70.1	13	50.0	23	33.2
4	34.0	14	87.4	24	39.0
5	53.1	15	33.0	25	38.3
6		16	22.4	26	68.4
7	123.7	17	52.0	27	13.7
8		18	19.8	28	25.5
9	36.4	19	25.8	29	14.0
10	40.8	20	80.6		

References

1. E. Snogan, I.L. Lechat, R. Ho, G. Bertho, J.P. Girault, S. Ortiga, A. Maria, R. Lafont, Phytochem. Anal. **18**, 441 (2007)

24-epi-Atrotosterone A

CAS Registry Number: 1236073-70-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotus longifolia* [1]

$C_{28}H_{46}O_7$: 494.3243

CI-MS m/z: 512 $[M + NH_4]^+$, 495 $[M + H]^+$, 477 $[M + H–H_2O]^+$, 459 $[M + H–2H_2O]^+$ [1]

^{1}H NMR (J/Hz, D_2O): 1.40 (t, J = 3.3, Ha-1), 2.48 (dd, J = 13.3, 3.8, He-1), 4.11 (m, Ha-2), 4.10 (m, He-3), 1.78 (Ha-4), 1.78 (He-4), 2.32 (t, H-5), 5.99 (d, J = 2.4, H-7), 3.14 (dd, J = 8.7, 2.5, H-9), 4.23 (ddd, J = 11.4, 9.9, 5.9, Ha-11), 2.06 (Ha-12), 2.28 (He-12), 2.06 (Ha-15), 1.66 (Hb-15), 1.88 (Ha-16), 1.81 (Hb-16), 2.33 (t, J = 10.5, H-17), 0.87 (s, CH_3-18), 1.10 (s, CH_3-19), 1.25 (s, CH_3-21), 3.56 (d, J = 10.0, H-22), 1.30 (Ha-23), 1.35 (Hb-23), 1.55 (Ha-24), 1.55 (H-25), 0.86 (d, J = 6.9, CH_3-26), 0.89 (d, J = 6.9, CH_3-27), 0.87 (d, J = 6.7, CH_3-28) [1]

^{13}C NMR (D_2O) [1]:

Table 1

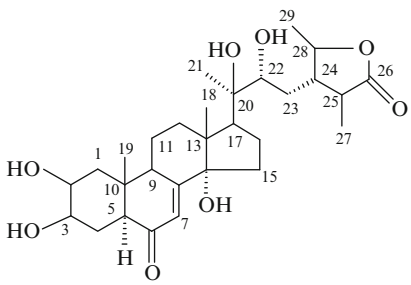
C-1	39.1	C-11	70.3	C-21	21.5
2	69.3	12	44.0	22	76.4
3	69.3	13	49.1	23	37.0
4	33.7	14	86.9	24	36.2
5	53.2	15	n.d.	25	35.7
6	n.d.	16	n.d.	26	20.0
7	123.7	17	50.4	27	21.9
8	n.d.	18	19.8	28	16.4
9	43.5	19	25.3		
10	40.0	20	80.3		

References

1. S. Crouzet, A. Maria, L. Dinan, R. Lafont, J.P. Girault, Arch. Insect Biochem. Physiol. **72**, 194 (2009)

5-epi-Cyasterone

CAS Registry Number: 31581-82-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyathula capitata* [1]

$C_{29}H_{44}O_8$: 520.3036

Mp: 274–275°C [1]

$[\alpha]_D^{20}$ + 116° (c, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 1750, 1658 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 [1]

EI-MS m/z: 520 $[M]^+$, 363, 345, 327, 201, 183, 157, 113 [1]

CD (c, dioxane): $[\theta]_{333}$ +8.35 x 10^3 [1]

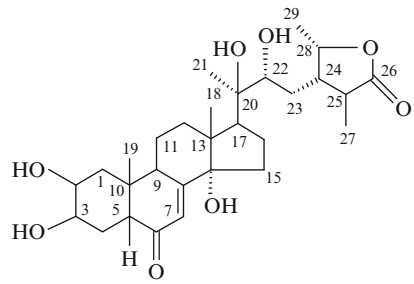
^{1}H NMR (100 MHz, C_5D_5N): 6.26 (d, H-7), 1.23 (s, CH_3-18), 1.41 (s, CH_3-19), 1.57 (s, CH_3-21), 1.35 (d, CH_3-27), 1.89 (d, CH_3-29) [1]

References

1. H. Hikino, K. Nomoto, T. Takemoto, Chem. Pharm. Bull. **19**, 433 (1971)

28-epi-Cyasterone

CAS Registry Number: 849206-13-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyathula capitata* [1], *Eriophyton wallchii* [2]

$C_{29}H_{44}O_8$: 520.3036

Mp: 248–250°C (MeOH) [1], 161–165°C [2]

IR (KBr) ν_{max} cm^{-1}: 3340, 2939, 2877, 1755, 1665, 1652, 1446, 1385, 1319, 1262, 1228, 1191, 1148, 1053, 953, 927, 878 [2]
UV λ_{max}^{MeOH} nm: 242 (log ε 4.11) [1], 241 [2]
FAB-MS m/z: 521 $[M + H]^+$, 503 $[M + H–H_2O]^+$, 485 $[M + H–H_2O]^+$, 449, 431, 363, 347, 345, 303, 285, 249, 201, 183, 157, 121 [2]
FAB-HR-MS m/z: for $C_{29}H_{45}O_8$ $[M + H]^+$, calcd. 521.3114, found 521.3152 [1]
HRAPCI-MS m/z: for $C_{29}H_{44}O_8Na$ $[M + Na]^+$, calcd. 543.2933, found 543.2968, [2]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.92 (Ha-1), 2.13 (dd, J = 4.6, 13.3, He-1), 4.16 (dt, J = 3.6, 11.0, Ha-2), 4.22 (br s, He-3), 1.81 (Ha-4), 2.03 (He-4), 3.00 (dd, J = 3.7, 13.2, H-5), 6.25 (d, J = 2.3, H-7), 3.59 (br t, J = 8.6, H-9), 1.75 (Ha-11), 1.90 (He-11), 2.60 (td, J = 4.7, 13.0, Ha-12), 2.03 (He-12), 1.92 (Ha-15), 2.22 (Hb-15), 2.47 (Ha-16), 2.03 (Hb-16), 2.86 (t, J = 9.2, H-17), 1.21 (s, CH_3-18), 1.05 (s, CH_3-19), 1.58 (s, CH_3-21), 3.89 (dd, J = 2.1, 11.0, H-22), 1.64 (Ha-23), 1.80 (Hb-23), 2.47 (H-24), 2.34 (dq, J = 7.0, 11.5, H-25), 1.18 (d, J = 7.0, CH_3-27), 4.98 (dq, J = 6.6, 6.8, H-28), 1.29 (d, J = 6.6, CH_3-29) [1]
^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-11	21.1	C-21	21.3
2	68.1	12	32.0	22	76.4
3	68.0	13	48.2	23	30.8
4	32.7	14	84.1	24	45.9
5	51.4	15	31.7	25	38.7
6	203.6	16	21.2	26	179.2
7	121.8	17	50.2	27	16.3
8	166.0	18	17.9	28	78.8
9	34.4	19	24.4	29	14.4
10	38.6	20	76.8		

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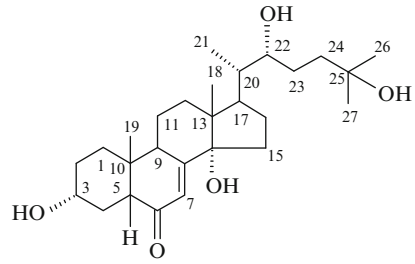
1. K. Okuzumi, N. Hara, H. Uekusa, Y. Fujimoto, Org. Biomol. Chem. **3**, 1227 (2005)
2. J. Yi, Y. Luo, B. Li, G. Zhang, Steroids **69**, 809 (2004)

3-epi-2-Deoxyecdysone

CAS Registry Number: 77732-73-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Blechnum vulcanicum* [1]
$C_{27}H_{44}O_5$: 448.3188
Mp: 264–265°C [1]
$[\alpha]_D^{20}$ + 98° ($CHCl_3$) [1]
IR (KBr) ν_{max} cm^{-1}: 3450, 1650 [1]
UV λ_{max}^{EtOH} nm (log ε): 243 (4.061) [1]
EI-MS m/z: 448 $[M]^+$ (0.2), 430 (2), 412 (5), 397 (5), 396 (3), 379 (3), 361 (1), 332 (8), 314 (11), 299 (5), 284 (9), 283 (6), 263 (8), 251 (5), 99 (100), 81 (54) [1], 430 $[M-H_2O]^+$ (4), 394 $[M-3H_2O]^+$ (4), 343 $[M-5H_2O-Me]^+$ (5), 332 $[M-(C_{22}-C_{27})]^+$ (8), 284 $[M-(C_{22}-C_{27})-H_2O]^+$ (18), 99 $[(C_{22}-C_{27})-H_2O]^+$ (100), 81 $[99-H_2O]^+$ (68) [2]
CI-MS m/z: 449 $[M + H]^+$ (1) [2]
^{1}H NMR (60 MHz, J/Hz, C_5D_5N): 6.20 (m, H-7), 0.73 (s, CH_3-18), 0.99 (s, CH_3-19), 1.23 (d, J = 6.0, CH_3-21), 1.38 (s, CH_3-26), 1.38 (s, CH_3-27) [1]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 0.759 (s, CH_3-18), 1.01 (s, CH_3-19), 1.32 (d, J = 6.0, CH_3-21), 1.41 (s, CH_3-26), 1.41 (s, CH_3-27) [2]
^{13}C NMR (20 MHz, C_5D_5N) [1]:

Table 1

C-1	35.6 (t)	C-10	36.8 (s)	C-19	23.9 (q)
2	31.4 (t)	11	20.8 (t)	20	43.0 (d)
3	69.1 (d)	12	31.6 (t)	21	15.7 (q)
4	34.3 (t)	13	47.6 (s)	22	74.0 (d)

(*continued*)

Table 1 (continued)

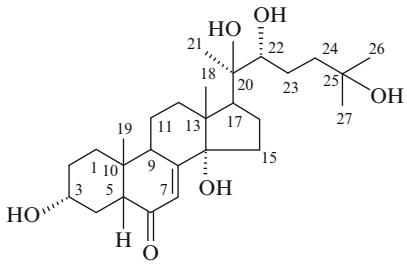
5	57.2 (d)	14	83.8 (s)	23	25.6 (t)
6	201.9 (s)	15	31.9 (t)	24	42.5 (t)
7	121.3 (d)	16	26.7 (t)	25	69.7 (s)
8	165.8 (s)	17	48.3 (d)	26	30.0 (q)
9	34.0 (d)	18	15.8 (q)	27	30.3 (q)

References

1. G.B. Russel, D.R. Greenwood, G.A. Lane, J.W. Blunt, M.H. G. Munro, Phytochemistry **20**, 2407 (1981)
2. R.E. Isaac, H.H. Rees, T.W. Goodwin, Chem. Comm. **418** (1981)

3-epi-2-Deoxy-20-Hydroxyecdysone

CAS Registry Number: 22785-88-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Tinospora capillipes* [1]

$C_{27}H_{44}O_6$: 464.3137

Mp: 234–237°C (EtOAc–EtOH) (Kofler block), 230–231°C (evac. cap) [2]

$[\alpha]_D^{28}$ + 60.6° (c 0.201, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 1640 [2], 3340, 2960, 1640, 1558, 1408, 1381, 1299, 1054, 963, 926, 874, 654 [3]

UV λ_{max}^{EtOH} nm (ε): 243 (12300) [2]

EI-MS m/z: 464 $[M]^+$, 446, 428, 410, 395, 392, 377, 347, 329, 311, 297, 294, 284, 269, 251, 215, 212, 201, 199, 175, 147, 121, 113, 99, 95, 81, 69, 55 [2]

FAB-MS m/z: $C_{27}H_{45}O_6$ $[M + H]^+$ calc. 465.3216 [3]

^{1}H NMR (J/Hz, C_5D_5N): 3.83 (br m, Ha-3), 2.29 (dd, J = 3.6, 13.4, H-5), 6.23 (d, J = 2.4, H-7), 3.70 (m, H-9), 3.02 (t, J = 9.0, H-17), 1.22 (s, CH_3-18), 0.98 (s, CH_3-19), 1.59 (s, CH_3-21), 3.88 (br d, J = 10.0, 1.0, H-22), 1.37 (s, CH_3-26), 1.37 (s, CH_3-27) [3]

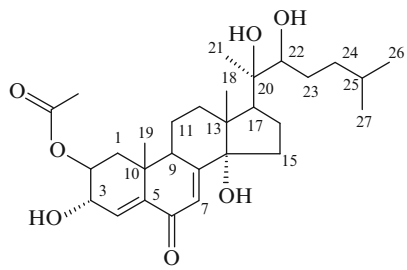
Pharm./Biol.: *Calliphora* assay: 1/3 of 20-hydroxyecdysone activity [3].

References

1. C. Song, R. Xu, Chin. Chem. Lett. **2**, 13 (1991)
2. M.N. Galbraith, D.H.S. Horn, E.J. Middleton, R.J. Hackney, Aust. J. Chem. **22**, 1059 (1969)
3. A. Suksamrarn, B.E. Yingyongnarongkul, Tetrahedron **53**, 3145 (1997)

22-epi-14α-Hydroxy-2-Acetylpinnasterol

CAS Registry Number: 104418-60-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Laurencia pinnata* [1]

$C_{29}H_{44}O_7$: 504.3087

Mp: 144–145°C (Me_2CO-hexane) [1]

$[\alpha]_D$ + 65° (c 0.23, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3490, 1730, 1675, 1638, 1250 [1]

UV λ_{max}^{EtOH} nm (log ε): 253 (3.93) [1]

FD-MS m/z: 504 $[M]^+$, 486, 403, 359 [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 5.26 (ddd, J = 10.0, 7.0, 3.5, Ha-2), 4.68 (dd, J = 7.0, 2.5, He-3), 6.86 (d, J = 2.5, H-4), 6.49 (d, J = 2.5, H-7), 3.45 (ddd, J = 12.0, 7.0, 2.5, Ha-9), 2.26 (dt, J = 13.0, 5.0, Ha-12), 2.70 (t, J = 9.3, H-17), 1.25 (s, CH_3-18), 1.30 (s, CH_3-19), 1.52 (s, CH_3-21), 3.75 (d, J = 10.0, Ha-22), 0.86 (d, J = 6.5, CH_3-26), 0.88 (d, J = 6.5, CH_3-27), 2.01 (s, CH_3COO) [1]

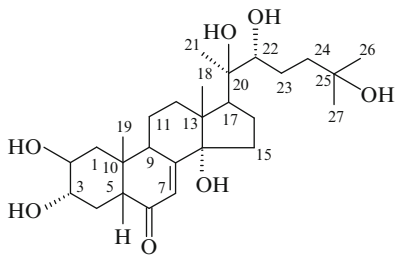
Pharm./Biol.: *Sarcophaga* test: ED_{50} = 2 µg [1].

References

1. A. Fukuzawa, M. Miyamoto, Y. Kumagai, T. Masamune, Phytochemistry **25**, 1305 (1986)

3-epi-20-Hydroxyecdysone

CAS Registry Number: 54053-93-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1], *Serratula coronata* [2]

$C_{27}H_{44}O_7$: 480.3087

Mp: 215–216°C [2], 225–229°C [3]

$[\alpha]_D^{15}$ + 61.5° (c 0.88, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3410, 1653 [1]

UV λ_{max}^{EtOH} nm (ε): 241.2 (12400) [2]

EI-MS m/z: 445 $[M\text{-}H_2O\text{-}OH]^+$ (2.3), 444 $[M\text{-}2H_2O]^+$ (2.6), 428 (13.6), 426 $[M\text{-}3H_2O]^+$ (10.6), 411 $[M\text{-}3H_2O\text{-}CH_3]^+$ (8.9), 408 $[M\text{-}4H_2O]^+$ (4.9), 393 $[M\text{-}4H_2O\text{-}CH_3]^+$ (3.2), 363 $[M\text{-}117]^+$ (18.0), 347 $[M\text{-}117\text{-}O]^+$ (100), 346 (80.5), 345 $[M\text{-}117\text{-}H_2O]^+$ (89.9), 344 (21.6), 329 $[M\text{-}117\text{-}O\text{-}H_2O]^+$ (47.3), 328 (35.9), 327 $[M\text{-}117\text{-}2H_2O]^+$ (46.0), 311 $[M\text{-}117\text{-}O\text{-}2H_2O]^+$ (22.1), 309 $[M\text{-}117\text{-}3H_2O]^+$ (20.7), 301 (19.0), 300 (20.7), 285 (27.2), 269 (25.3), 173 (26.4), 161 (14.8), 159 (15.7), 157 (14.7), 143 (23.4), 125 (13.7), 121 (16.9), 119 (15.0), 117 (11.4), 109 (12.7), 107 (15.1), 105 (21.4), 99 (50.4), 81 (34.4), 59 (22.3), 43 (36.4) [2]

CI-MS m/z: 497 $[M + NH_3]^+$ (7.3), 480 $[M]^+$ (7.8), 463 $[M\text{-}OH]^+$ (77.34), 445 $[M\text{-}OH\text{-}H_2O]^+$ (100), 427 $[M\text{-}OH\text{-}2H_2O]^+$ (60.2), 409 $[M\text{-}OH\text{-}3H_2O]^+$ (3.1), 362 (2.3), 345 (10.2), 320 (3.9), 303 (13.3), 291 (8.6), 285 (6.3), 279 (5.5), 172 (7.8), 160 (3.9), 141 (21.9), 124 (59.4), 116 (32.0) [2]

FAB-MS m/z: 503 $[M + Na]^+$ (85), 481 $[M + H]^+$ (21), 463 (34), 445 (100), 427 (98), 409 (36) [1]

HR-MS m/z: for $C_{27}H_{43}O_7$ $[M\text{-}H]^-$ calcd. 479.3009, found 479.2971 [1]

^{1}H NMR (500.13 MHz, CD_3OD): 1.09 (dd, Ha-1), 2.10 (dd, He-1), 3.64 (ddd, Ha-2), 3.35 (ddd, Ha-3), 1.57 (Ha-4), 1.75 (He-4), 2.40 (dd, H-5), 5.82 (d, H-7), 3.18 (ddd, H-9), 1.82 (Ha-11), 1.70 (He-11), 2.14 (Ha-12), 1.88 (He-12), 1.96 (Ha-15), 1.61 (Hb-15), 1.74 (Ha-16), 1.99 (Hb-16), 2.40 (H-17), 0.89 (s, CH_3-18), 0.96 (s, CH_3-19), 1.21 (s, CH_3-21), 3.33 (dd, H-22), 1.66 (Ha-23), 1.29 (Hb-23), 1.80 (Ha-24), 1.43 (Hb-24), 1.20 (s, CH_3-26), 1.19 (s, CH_3-27) [1]

^{1}H NMR (500.13 MHz, J/Hz, C_5D_5N): 1.47 (dd, J = 12.9, 11.0, Ha-1), 2.45 (dd, J = 12.9, 4.3, He-1), 4.24 (ddd, J = 11.0, 8.8, 4.3, Ha-2), 3.86 (m, Ha-3), 1.95 (m, Ha-4), 2.17 (m, He-4), 2.47 (m, H-5), 6.24 (d, J = 2.1, H-7), 3.71 (ddd, J = 8.8, 4.7, 2.1, H-9), 1.84 (m, Ha-11), 1.76 (He-11), 2.02 (m, Ha-12), 2.54 (ddd, J = 12.9, 12.8, 4.9, He-12), 1.88 (m, Ha-15), 2.17 (m, Hb-15), 2.09 (m, Ha-16), 2.45 (m, Hb-16), 3.00 (m, H-17), 1.23 (s, CH_3-18), 1.06 (s, CH_3-19), 1.59 (s, CH_3-21), 3.88 (m, H-22), 1.83 (m, Ha-23), 2.15 (m, Hb-23), 2.28 (m, Ha-24), 1.74 (m, Hb-24), 1.39 (s, CH_3-26), 1.39 (s, CH_3-27) [2]

^{13}C NMR (125.7 MHz, CD_3OD) [1]: **^{13} C NMR** (125.76 MHz, C_5D_5N) [2]:

Table 1

C-1	43.03	C-15	31.74	C-1	42.91	C-15	31.41
2	72.11	16	21.50	2	71.62	16	21.19
3	75.36	17	50.55	3	74.95	17	49.79
4	33.65	18	18.03	4	33.48	18	17.58
5	57.47	19	23.88	5	56.87	19	23.65
6	204.65	20	77.93	6	201.44	20	76.54

(*continued*)

Table 1 (continued)

7	121.99	21	21.04	7	121.15	21	21.40
8	168.12	22	78.44	8	165.84	22	77.26
9	35.97	23	27.35	9	35.08	23	27.21
10	39.61	24	42.40	10	38.67	24	42.36
11	21.50	25	71.31	11	20.78	25	69.24
12	32.48	26	29.69	12	31.67	26	29.74
13	49.00	27	28.96	13	47.81	27	29.80
14	85.10			14	83.80		

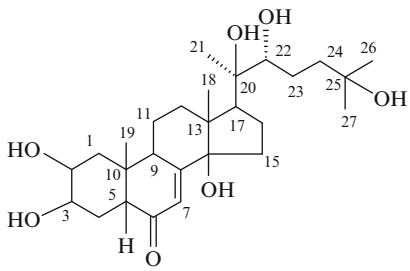
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.6 \times 10^{-7}$ M [2].

References

1. K. Vokac, M. Budesinsky, J. Harmatha, Coll. Czech. Chem. Comm. **67**, 124 (2002)
2. V.N. Odinokov, I.V. Galyautdinov, D.V. Nedopekin, L.M. Khalilov, A.S. Shashkov, V.V. Kachala, L. Dinan, R. Lafont, Insect Biochem. Mol. Biol. **32**, 161 (2002)
3. M.J. Thompson, J.N. Kaplanis, W.E. Robbins, S.R. Dutky, H.N. Nigg, Steroids **24**, 359 (1974)

14-epi-20-Hydroxyecdysone

CAS Registry Number: 405509-12-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula wolffii* [1]

$C_{27}H_{44}O_7$: 480.3087

IR (KBr) ν_{max} cm^{-1}: 3380, 1653, 1063 [1]

FAB-MS m/z: 503 $[M + Na]^+$ (34), 481 $[M + H]^+$ (41), 463 $[M + H–H_2O]^+$ (25), 445 $[M + H–2H_2O]^+$ (65), 427 $[M + H–3H_2O]^+$ (37), 363 (41), 303 (71), 279 (80), 211 (100) [1]

HR-ESI-MS m/z: for $C_{27}H_{45}O_7$ $[M + H]^+$ calcd. 481.3165, found 481.3158 [1]

^{1}H NMR (CD_3OD): 1.43 (Ha-1), 1.80 (He-1), 3.86 (Ha-2), 3.94 (He-3), 1.59 (Ha-4), 1.73 (He-4), 2.36 (H-5), 6.29 (H-7), 2.85 (H-9), 1.68 (Ha-11), 1.79 (He-11), 1.77 (Ha-12), 1.67 (He-12), 2.28 (Ha-15), 1.43 (He-15), 2.08 (Ha-16), 1.89 (Hb-16), 1.98 (H-17), 1.26 (s, CH_3-18), 0.94 (s, CH_3-19), 1.29 (s, CH_3-21), 3.50 (H-22), 1.58 (Ha-23), 1.29 (Hb-23), 1.80 (Ha-24), 1.43 (Hb-24), 1.19 (s, CH_3-26), 1.21 (s, CH_3-27) [1]

^{13}C NMR (CD_3OD) [1]:

Table 1

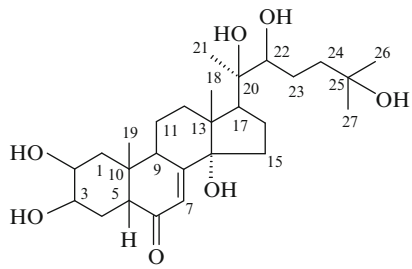
C-1	37.23	C-10	39.27	C-19	24.64
2	68.66	11	22.25	20	77.64
3	68.41	12	41.67	21	20.45
4	33.34	13	52.64	22	78.44
5	51.01	14	85.68	23	27.41
6	206.12	15	40.75	24	42.20
7	123.12	16	24.64	25	71.24
8	167.68	17	56.61	26	28.84
9	37.41	18	19.24	27	29.88

References

1. A. Hunyadi, A. Gergely, A. Simon, G. Toth, G. Veress, M. Bathori, J. Chrom. Sci. **45**, 76 (2007)

22-epi-20-Hydroxyecdysone

CAS Registry Number: 123238-67-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Serratula tinctoria* [1]
$C_{27}H_{44}O_7$: 480.3087
Mp: 259–260°C [2], 258–260°C (MeOH) [3]
IR (KBr) ν_{max} cm^{-1}: 1650 [3]
UV λ_{max}^{EtOH} nm (ε): 242 (11700) [2]
CI-MS m/z: 498 $[M + H + NH_3]^+$, 481, 463, 455, 427, 409, 380 $[M + H + NH_3 - C_6H_{13}O_2]^+$, 363 $[M-C_6H_{13}O_2]^+$, 345 [1]
FAB-MS m/z: 481 $[M + H]^+$ (30), 463 (78), 445 (100), 427.6 (36), 411.5 (23), 393 (20), 371 (42), 347 (40), 331 (57), 329 (72), 303 (70), 301 (93) [3]
^{1}H NMR (500 MHz, J/Hz, D_2O): 1.40 (t, J = 13.0, Ha-1), 1.85 (Hb-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.34 (t, H-5), 5.98 (d, J = 2.5, H-7), 3.10 (m, Ha-9), 1.75 (Ha-11), 1.85 (He-11), 1.75 (Ha-12), 1.95 (He-12), 2.05 (m, Ha-15), 1.65 (Hb-15), 1.85 (Ha-16), 1.90 (Hb-16), 2.55 (t, H-17), 0.85 (s, CH_3-18), 1.00 (s, CH_3-19), 1.27 (s, CH_3-21), 3.35 (d, J = 10.0, H-22), 1.38 (Ha-23), 1.88 (Hb-23), 1.76 (Ha-24), 1.48 (Hb-24), 1.238 (s, CH_3-26), 1.243 (s, CH_3-27) [1]
^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

C-1	36.3	C-10	39.1	C-19	24.2
2	68.3	11		20	78.6
3	68.2	12	32.1	21	21.3
4	32.4	13	48.0	22	78.6
5	51.4	14	86.3	23	
6		15		24	41.7
7	122.1	16		25	73.0
8		17	50.2	26	28.3
9	35.1	18	18.1	27	29.3

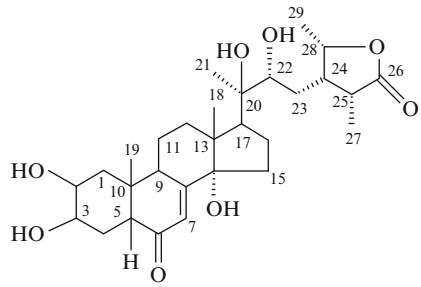
Pharm./Biol.: *Calliphora* assay: 0.5 mg – inactive [2].

References

1. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, R. Lafont, J. Nat. Prod. **61**, 415 (1998)
2. U. Kerb, R. Wiechert, A. Furlenmeier, A. Furst, Tetrah. Lett. **4277** (1968)
3. U. Hedtman, R. Klintz, K. Hobert, J. Frelek, J. Vlanov, P. Welzel, Tetrahedron **47**, 3753 (1991)

28-epi-Isocyasterone

CAS Registry Number: 851727-39-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Cyathula officinalis* [1]
$C_{29}H_{44}O_8$: 520.3036
Mp: amorphous [1]
UV λ_{max}^{MeOH} nm (log ε): 241.2 (4.11) [1]
HR-MS m/z: for $C_{29}H_{45}O_8$ $[M + H]^+$ calcd. 521.3114, found 521.3109 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.94 (Ha-1), 2.15 (dd, J = 4.7, 13.1, He-1), 4.19 (br d, J = 11.5, Ha-2), 4.23 (br s, He-3), 1.81 (Ha-4), 2.03 (He-4), 3.02 (dd, J = 3.7, 13.2, H-5), 6.27 (d, J = 2.1, H-7), 3.59 (br t, J = 9.9, H-9), 1.74 (Ha-11), 1.89 (He-11), 2.57 (td, J = 4.2, 13.0, Ha-12), 1.98 (He-12), 1.89 (Ha-15), 2.18 (Hb-15), 2.49 (m, Ha-16), 2.05 (Hb-16), 2.89 (t, J = 8.1, H-17), 1.22 (s, CH_3-18), 1.08 (s, CH_3-19), 1.59 (s, CH_3-21), 3.82 (br d, J = 11.5, H-22), 1.69 (Ha-23), 1.85 (Hb-23), 3.14 (H-24), 2.89 (m, H-25), 1.28 (d, J = 7.5, CH_3-27), 4.65 (qui, J = 6.7, H-28), 1.29 (d, J = 6.6, CH_3-29) [1]
^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-11	21.0	C-21	21.3
2	68.1	12	31.9	22	74.9
3	68.0	13	48.0	23	26.6

(*continued*)

Table 1 (continued)

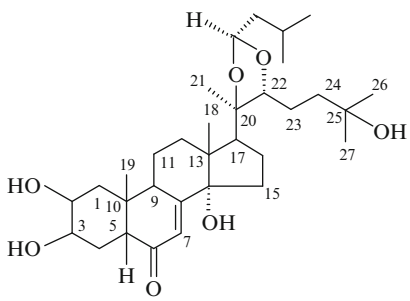
4	32.4	14	84.0	24	39.8
5	51.3	15	31.7	25	39.5
6	203.4	16	21.6	26	180.0
7	121.6	17	49.9	27	17.4
8	165.8	18	17.7	28	78.6
9	34.4	19	24.4	29	12.8
10	38.6	20	76.6		

References

1. K. Okuzumi, N. Hara, H. Uekusa, Y. Fujimoto, Org. Biomol. Chem. **3**, 1227 (2005)

20,22-epi-Isovaleriate-5β-Cholest-7-en-2β,3β,14α,20R,22R,25-Hexahydroxy-6-on

CAS Registry Number: 404589-60-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene claviformis* [1]

$C_{32}H_{52}O_7$: 548.3713

CI-MS m/z: 566 $[M + H + NH_3]^+$, 549 $[M + H]^+$, 531 $[M + H–H_2O]^+$, 464, 462, 447, 445, 429, 427 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.38 (Ha-1), 1.88 (He-1), 3.99 (m, Ha-2), 4.08 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.36 (t-like, H-5), 5.98 (d, J = 2.0, H-7), 3.11 (m, H-9), 1.73 (Ha-11), 1.86 (He-11), 1.96 (Ha-12), 1.96 (He-12), 2.05 (Ha-15), 1.68 (Hb-15), 1.95 (Ha-16), 1.95 (Hb-16), 2.32 (t, J = 8.1, H-17), 0.85 (s, CH_3-18), 1.00 (s, CH_3-19), 1.27 (s, CH_3-21), 3.82 (m, H-22), 1.55 (Ha-23), 1.73 (Hb-23), 1.55 (Ha-24), 1.55 (Hb-24), 1.237 (s, CH_3-26), 1.241 (s, CH_3-27), Other: 5.07 (t, J = 5.4, H), 1.54 (H), 1.75 (H), 0.943 (d, J = 6.5, CH_3), 0.948 (d, J = 6.5, CH_3) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

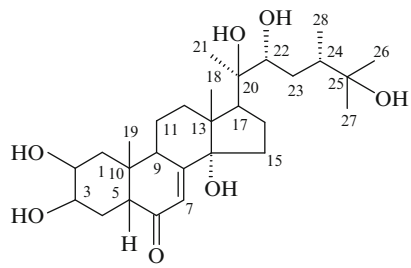
C-1	36.4	C-12	31.9	C-23	
2		13	47.9	24	41.4
3	68.2	14		25	72.7
4	32.3	15		26	28.7
5	51.3	16		27	28.7
6		17	50.7	Other: a	102.7
7		18	17.8	b	24.1
8		19	24.2	c	44.0
9	34.9	20	86.4	d-CH_3	23.3
10	34.9	21	20.1	d'-CH_3	23.3
11		22	83.2		

References

1. Z. Sadikov, Z. Saatov, M. Garcia, J.P. Girault, R. Lafont, Chem. Nat. Comp. **37**, 262 (2001)

24-epi-Makisterone A

CAS Registry Number: 96790-37-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Diploclisia glaucescens* [1], *Leuzea carthamoides* [2], *Vitex canescens* [3], *V. leptobotrys* [4], *V. scabra* [5]

$C_{28}H_{46}O_7$: 494.3243

CI-MS m/z: 495 $[M + H]^+$ [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.18 (m, Ha-2), 4.23 (br s, He-3), 3.01 (dd, J = 13.1, 3.6, H-5), 6.26 (d, J = 2.7, H-7), 3.59 (m, H-9), 3.00 (t, J = 9.4, H-17), 1.21 (s, CH_3-18), 1.06 (s, CH_3-19), 1.58 (s, CH_3-21), 4.07 (br d, J = 9.4H-22), 1.33 (s, CH_3-26), 1.38 (s, CH_3-27) [3]

^{13}C NMR (22.63 MHz, C_5D_5N) [1]:

Table 1

C-1	38.1 (t)	C-11	21.2 (t)	C-21	21.4 (q)
2	68.1 (d)	12	31.8 (t)	22	76.2 (d)
3	68.1 (d)	13	48.2 (s)	23	35.3 (t)
4	32.5 (t)	14	84.2 (s)	24	43.5 (d)
5	51.4 (d)	15	32.1 (t)	25	72.3 (s)
6	203.3 (s)	16	21.6 (t)	26	27.0 (q)
7	121.6 (d)	17	50.1 (d)	27	29.0 (q)
8	166.1 (s)	18	17.9 (q)	28	16.8 (q)
9	34.6 (d)	19	24.5 (q)		
10	38.7 (s)	20	77.1 (s)		

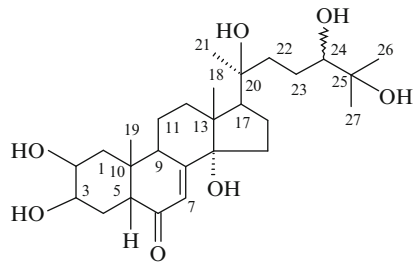
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 2.2 \times 10^{-7}$ M [6–8].

References

1. R.W. Miller, J. Clardy, J. Kozlowski, L. Mikolajczak, R.D. Plattner, R.G. Powell, C.R. Smith, D. Weisleder, Q.T. Zheng, Planta Med. **47**, 40 (1985)
2. M. Budesinsky, K. Vokas, J. Harmatha, J. Cvacka, Steroids **73**, 502 (2008)
3. A. Suksamrarn, N. Promrangsan, B. Chitkul, S. Homvisasevongsa, A. Sirikate, Phytochemistry **45**, 1149 (1997)
4. T.T. Thuy, A. Porzel, H. Ripperger, T.V. Sing, G. Adam, Phytochemistry **49**, 2603 (1998)
5. A. Suksamrarn, S. Kumpun, B. Yingyongnarongkul, J. Nat. Prod. **65**, 1690 (2002)
6. J. Harmatha, L. Dinan, Arch. Insect Biochem. Physiol. **35**, 219 (1997)
7. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
8. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

24-epi-Pinnatasterone (24α-Hydroxy-22-Deoxy-20-Hydroxyecdysone)

CAS Registry Number: 474524-74-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Lychnis miqueliana* [1, 2], *Vitex scabra* [3]

$C_{27}H_{44}O_7$: 480.3087

IR (KBr) ν_{max} cm^{-1}: 3422, 2929, 1648, 1384, 1057 [3]

FAB-HR-MS m/z: 479.3001 $[M-H]^-$ calc. for $C_{27}H_{43}O_7$ 479.3008 [3]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.15 (m, Ha-2), 4.23 (br s, He-3), 2.96 (dd, J = 13.1, 3.6, H-5), 6.19 (d, J = 2.1, H-7), 3.56 (m, H-9), 2.90 (t, J = 9.3, H-17), 1.08 (s, CH_3-18), 1.00 (s, CH_3-19), 1.55 (s, CH_3-21), 3.76 (br d, J = 8.8 H-24), 1.42 (s, CH_3-26), 1.46 (s, CH_3-27) [3]

^{13}C NMR (100 MHz, C_5D_5N) [3]:

Table 1

C-1	37.7	C-10	38.5	C-19	24.2
2	68.0	11	20.9	20	74.4
3	67.9	12	31.7	21	26.8
4	32.3	13	47.4	22	42.6
5	51.3	14	84.3	23	26.8
6	203.6	15	31.4	24	79.9
7	121.6	16	21.8	25	72.7
8	166.3	17	53.5	26	25.9
9	34.2	18	17.8	27	25.7

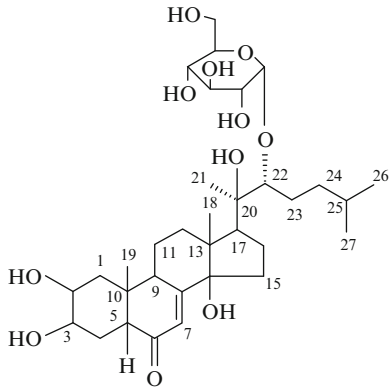
Pharm./Biol.: *Musca* bioassay: $EC_{50} = 5.2 \times 10^{-4}$ M very low activity [3].

References

1. M. Kozuka, M. Takasaki, T. Konoshima, T. Shingu, M. Saitoh, Y. Asaka, G. de Boer, I. Kubo, *16th International Symposium on the Chemistry of Natural Products*. (IUPAC), Kyoto, 1988
2. S. Imai, T. Toyosato, M. Sakai, Y. Sato, S. Fujioka, E. Murata, M. Goto, Chem. Pharm. Bull. **17**, 340 (1969)
3. A. Suksamrarn, S. Kumpun, B. Yingyongnarongkul, J. Nat. Prod. **65**, 1690 (2002)

14-epi-Ponasterone A-22-Glucoside

CAS Registry Number:1026800-44-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{33}H_{54}O_{11}$: 626.3666

$[\alpha]_D^{20}$ + 59.2° (c 0.03, EtOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3413, 1652, 1099, 1071, 1056, 1030 [1]

ESI-MS m/z: 627 $[M + H]^+$, 609 $[M + H–H_2O]^+$, 591 $[M + H–2H_2O]^+$, 573 $[M + H–3H_2O]^+$, 465 $[M + H–C_6H_{10}O_5]^+$, 447 $[M + H–C_6H_{10}O_5–H_2O]^+$, 429 $[M + H–C_6H_{10}O_5–2H_2O]^+$, 411 $[M + H–C_6H_{10}O_5–3H_2O]^+$, 347, 303, 279, 145 [1]

HR-ESI-MS m/z: for $C_{33}H_{55}O_{11}$ $[M + H]^+$ calcd. 627.3758, found 627.3758 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.80 (dd, J = 4.2, 13.3, Ha-1), 1.43 (dd, J = 12.0, 13.2, He-1), 3.86 (ddd, J = 3.0, 4.2, 12.0, Ha-2), 3.94 (q, J = 3.0, He-3), 1.73 (Ha-4), 1.60 (He-4), 2.36 (dd, J = 4.0, 13.2, H-5), 6.32 (dd, J = 0.8, 2.4, H-7), 2.85 (m, Ha-9), 1.79 (Ha-11), 1.66 (He-11), 1.75 (Ha-12), 1.69 (He-12), 2.28 (m, Ha-15), 1.43 (He-15), 1.86 (Ha-16), 2.08 (Hb-16), 1.91 (H-17), 1.26 (s, CH_3-18), 0.94 (s, CH_3-19), 1.32 (s, CH_3-21), 3.58 (dd, J = 1.5, 10.0, H-22), 1.57 (Ha-23), 1.48 (Hb-23), 1.74 (Ha-24), 1.24 (Hb-24), 1.56 (H-25), 0.93 (d, J = 6.8, CH_3-26), 0.93 (d, J = 6.8, CH_3-27), Other: β-D-Glcp′: 4.34 (d, J = 7.8, H-1), 3.26 (dd, J = 7.8, 8.8, H-2), 3.36 (m, H-3), 3.36 (m, H-4), 3.36 (m, H-5), 3.69 (dd, J = 5.5, 11.8, Ha-6), 3.87 (dd, J = 1.8, 11.8, Hb-6) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

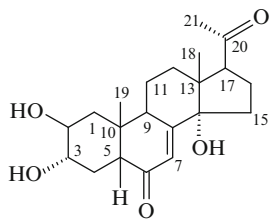
C-1	37.22	C-12	41.90	C-23	31.00
2	68.67	13	52.77	24	36.44
3	68.39	14	85.47	25	29.36
4	32.90	15	41.14	26	22.84
5	50.98	16	24.43	27	23.25
6	206.22	17	57.30	Glc′-1	105.95
7	123.14	18	19.37	2	75.27
8	167.38	19	24.67	3	77.94
9	37.25	20	77.07	4	77.90
10	39.21	21	21.83	5	71.41
11	22.20	22	90.44	6	62.31

References

1. M. Budesinsky, K. Vokas, J. Harmatha, J. Cvacka, Steroids **73**, 502 (2008)

3-epi-Poststerone

CAS Registry Number: 144405-75-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula tinctoria* [1]
$C_{21}H_{30}O_5$: 362.2093
^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.10 (dd, J = 12.0, 14.0, Ha-1), 2.10 (Hb-1), 3.65 (m, Ha-2), 3.40 (m, Ha-3), 1.60 (Ha-4), 1.80 (He-4), 2.15 (H-5), 5.83 (d, J = 2.8, H-7), 3.23 (ddd, J = 2.8, 7.0, 11.0, Ha-9), 1.73 (Ha-11), 1.90 (He-11), 2.10 (Ha-12), 1.65 (He-12), 2.00 (Ha-15), 1.65 (Hb-15), 2.25 (Ha-16), 1.90 (Hb-16), 3.35 (m, H-17), 0.63 (s, CH_3-18), 0.96 (s, CH_3-19), 2.16 (s, CH_3 and CO) [1]

References

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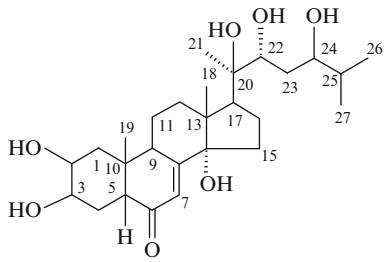
24-epi-Pterosterone

CAS Registry Number: 173655-42-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Athyrium yokoscense* [1]
$C_{27}H_{44}O_7$: 480.3087
Mp: 151–152°C (MeOH–H_2O) [1], 164–165°C (MeOH–$CHCl_3$) [2]
$[\alpha]_D^{25}$ + 66° (c 0.63, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3400, 1660 [1], 3382, 2964, 1656, 1469, 1383, 1334, 1052 [2]
UV λ_{max}^{EtOH} nm (ε): 243 (10600), 336 (100) [1]
CI-MS m/z: 481 $[M + H]^+$, 463 $[M + H–H_2O]^+$, 445 $[M + H–2H_2O]^+$, 427$[M + H–3H_2O]^+$ [1]
CD (9.1 × 10^{-5} M, dioxane): $[\theta]_{337}$ +4.17 × 10^3, $[\theta]_{246}$ −12.4 × 10^3, $[\theta]_{220}$ +11.0 × 10^3 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.97 (m, Ha-1), 2.17 (m, He-1), 4.19 (br d, J = 11.9, Ha-2), 4.24 (br s, He-3), 1.80 (m, Ha-4), 2.02 (m, He-4), 3.03 (m, H-5), 6.25 (d, J = 4.8, H-7), 3.60 (m, Ha-9), 1.80 (m, Ha-11), 1.90 (m, He-11), 2.10 (m, Ha-12), 2.66 (m, He-12), 1.89 (m, Ha-15), 1.89 (m, Hb-15), 2.36 (m, Ha-16), 2.50 (m, Hb-16), 3.08 (m, H-17), 1.25 (s, CH_3-18), 1.09 (s, CH_3-19), 1.66 (s, CH_3-21), 4.13 (br s, H-22), 1.87 (m, Ha-23), 2.03 (m, Hb-23), 4.50 (br d, J = 10.1, H-24), 1.85 (m, H-25), 1.01 (d, J = 6.4, CH_3-26), 1.10 (d, J = 6.4, CH_3-27) [1]
^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

C-1	38.0	C-10	38.7	C-19	24.4
2	68.1	11	21.1	20	76.8
3	68.1	12	32.0	21	21.3
4	32.4	13	48.1	22	73.4
5	51.4	14	84.2	23	37.5
6	203.4	15	31.8	24	73.5
7	121.7	16	21.7	25	35.0
8	166.1	17	50.0	26	19.5
9	34.4	18	17.9	27	18.6

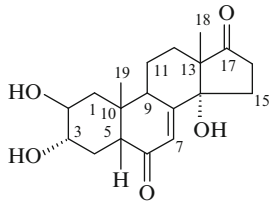
Pharm./Biol.: *Musca* bioassay: 7-fold less active than pterosterone [2].

References

1. S. Ohta, J.R. Guo, Y. Hiraga, T. Suga, Phytochemistry **41**, 745 (1996)
2. A. Suksamrarn, B.E. Yingyongnarongkul, S. Charoensuk, Tetrahedron **55**, 255 (1999)

3-epi-Rubrosterone

CAS Registry Number: 144405-76-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula tinctoria* [1]

$C_{19}H_{26}O_5$: 334.1780

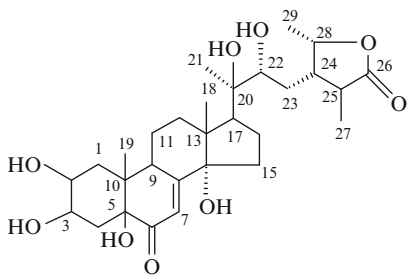
^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.12 (dd, J = 12.0, 13.0, Ha-1), 2.10 (He-1), 3.64 (m, Ha-2), 3.35 (m, Ha-3), 2.14 (H-5), 5.92 (d, J = 2.5, H-7), 3.20 (ddd, J = 2.5, 7.0, 11.0, Ha-9), 0.88 (s, CH_3-18), 0.98 (s, CH_3-19) [1]

References

1. D. Rudel, M. Bathori, J. Gharbi, J.P. Girault, I. Racz, K. Melis, K. Szendrei, R. Lafont, Planta Med. **58**, 358 (1992)

28-epi-Sengosterone

CAS Registry Number: 179308-42-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{29}H_{44}O_9$: 536.2985

IR (KBr) ν_{max} cm^{-1}: 3416, 1749, 1670 [1]

TSP-MS m/z: 554 $[M + NH_4]^+$ (25), 537 $[M + H]^+$ (100), 536 $[M]^+$ (82), 519 $[M + H–H_2O]^+$ (34), 501 $[M + H–2H_2O]^+$ (21) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.27 (m, Ha-2), 4.18 (m, He-3), 6.27 (d, J = 2.1, H-7), 3.66 (m, H-9), 2.62 (Ha-12), 2.08 (He-12), 2.88 (t, J = 8.4, H-17), 1.24 (s, CH_3-18), 1.18 (s, CH_3-19), 1.61 (s, CH_3-21), 3.90 (m, H-22), 1.81 (Ha-23), 1.69 (Hb-23), 2.48 (H-24), 2.33 (dq, J = 11.4, 6.9, H-25), 1.17 (d, J = 7.0, CH_3-27), 5.01 (H-28), 1.31 (d, J = 6.0, CH_3-29), 5.56 (H-2, OH), 5.88 (H-3, OH), 6.11 (H-22, OH) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

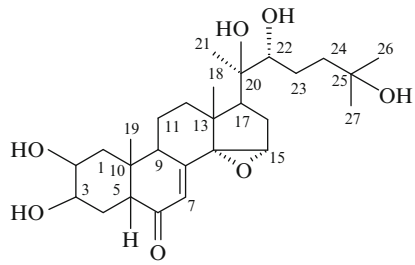
C-1	34.8	C-11	22.0	C-21	21.1
2	67.9	12	32.1	22	76.4
3	69.8	13	48.2	23	30.8
4	35.9	14	83.9	24	46.0
5	79.8	15	31.6	25	38.7
6	200.9	16	21.3	26	179.1
7	120.0	17	50.0	27	16.3
8	166.6	18	17.9	28	78.7
9	38.2	19	17.1	29	14.3
10	44.8	20	76.7		

References

1. M.P. Calcagno, F. Camps, J. Coll, E. Male, F.S. Baeza, Tetrahedron **52**, 10137 (1996)

14α,15α-Epoxy-14,15-Dihydrostachysterone B

CAS Registry Number: 1009011-97-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula wolffii* [1]

$C_{27}H_{42}O_7$: 478.2930

$[\alpha]_D^{28}$ −5° (c 0.1, MeOH) [1]

UV λ_{max}^{MeOH} nm (log ε): 240 (3.8) [1]

ESI-MS m/z: 501 $[M + Na]^+$ (13), 479 $[M + H]^+$ (100), 461 $[M + H–H_2O]^+$ (24), 443 $[M + H–2H_2O]^+$ (27.5), 425 $[M + H + 3H_2O]^+$ (2.6), 393 (3), 330 (53) [1]

HR-ESI-MS m/z: for $C_{27}H_{42}O_7$ $[M]^+$ calcd. 478.2919, found 474.2924 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.46 (t, J = 12.8, Ha-1), 1.82 (dd, J = 4.3, 13.5, He-1), 3.84 (ddd, J = 3.3, 4.2, 12.1, Ha-2), 3.95 (q, J = 3.0, He-3), 1.66 (J = 3.0, 7.8, Ha-4), 1.66 (He-4), 2.41 (dd,

J = 8.4, 9.0, H-5), 5.89 (d, J = 2.8, H-7), 2.84 (ddd, J = 2.8, 6.9, 10.2, H-9), 1.81 (Ha-11), 1.93 (He-11), 2.20 (dd, J = 2.8, 9.0, Ha-12), 1.81 (He-12), 3.97 (s, Ha-15), 1.92 (Ha-16), 1.94 (Hb-16), 1.71 (dd, J = 7.0, 10.6, H-17), 1.02 (s, CH_3-18), 1.01 (s, CH_3-19), 1.19 (s, CH_3-21), 3.29 (dd, J = 1.8, 10.5, H-22), 1.28 (dt, J = 4.4, 11.8, Ha-23), 1.55 (ddt, J = 1.8, 4.4, 11.8, Hb-23), 1.79 (dt, J = 4.6, 12.6, Ha-24), 1.44 (dt, J = 4.2, 12.4, Hb-24), 1.19 (s, CH_3-26), 1.20 (s, CH_3-27) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

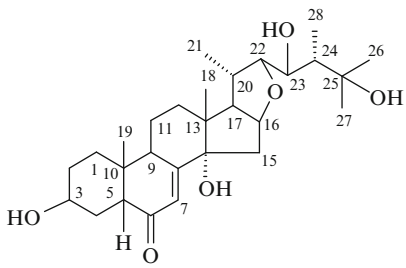
C-1	37.1	C-10	39.7	C-19	24.5
2	68.7	11	21.7	20	77.0
3	68.5	12	35.6	21	20.8
4	32.8	13	42.4	22	78.4
5	52.0	14	73.3	23	27.4
6	205.9	15	61.3	24	42.3
7	124.0	16	27.9	25	71.4
8	159.8	17	48.4	26	29.0
9	39.1	18	16.5	27	30.0

References

1. A. Simon, G. Toth, E. Luktor-Busa, Z. Kele, M. Takacs, A. Gergely, M. Bathori, Steroids **72**, 751 (2007)

16,22-Epoxy-3β,14α,23β,25-Tetrahydroxyergost-7-en-6-one

CAS Registry Number: 1021913-46-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polyporus umbellatus* [1]

$C_{28}H_{44}O_6$: 476.3138

Mp: amorphous (MeOH) [1]

$[\alpha]_D^{20}$ + 65.7° (c 0.39, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3350, 1650 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (4.01) [1]

EI-MS m/z: 458 $[M\text{-}H_2O]^+$ (8), 440 (10), 425 (4), 359 $[M\text{-}C_6H_{13}O_2]^+$ (39), 342 (63), 341 $[M\text{-}C_6H_{13}O_2\text{–}H_2O]^+$ (100), 300 (12), 285 (71), 286 (66), 263 (20), 95 (66), 79 (25) [1]

HR-FAB-MS m/z: for $C_{28}H_{44}O_6Na$ $[M + Na]^+$ calcd. 499.3030, found 499.3030 [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.13 (br s, He-3), 2.97 (m, H-5), 6.18 (br s, H-7), 3.54 (br s, H-9), 5.29 (m, H-16), 2.85 (d, J = 8.0, H-17), 0.97 (s, CH_3-18), 1.04 (s, CH_3-19), 2.70 (m, H-20), 1.39 (d, J = 7.1, CH_3-21), 4.44 (dd, J = 5.6, 9.2, H-22), 4.69 (br d, J = 9.1, H-23), 2.21 (m, H-24), 1.47 (s, CH_3-26), 1.56 (s, CH_3-27), 1.45 (d, J = 7.0, CH_3-28) [1]

^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

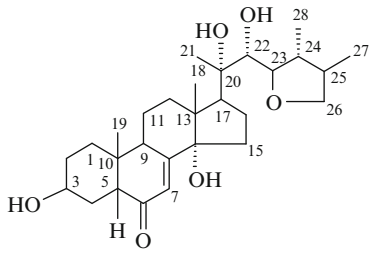
C-1	36.5	C-11	22.0	C-21	17.0
2	29.6	12	32.9	22	84.1
3	63.8	13	49.1	23	69.8
4	34.2	14	84.9	24	43.1
5	51.6	15	41.0	25	73.3
6	202.9	16	82.8	26	29.5
7	120.9	17	61.4	27	28.9
8	165.1	18	17.8	28	7.8
9	35.2	19	24.0		
10	37.0	20	37.0		

References

1. W.W. Zhou, W.H. Lin, S.X. Guo, Chem. Pharm. Bull. **55**, 1148 (2007)

23,26-Epoxy-3β,14α,21α,22α-Tetrahydroxyergost-7-en-6-one

CAS Registry Number: 1021913-47-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polyporus umbellatus* [1]

$C_{28}H_{44}O_6$: 476.3138

Mp: amorphous (MeOH) [1]

$[\alpha]_D^{20}$ + 58.9° (c 0.41, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3350, 1650 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (3.98) [1]

EI-MS m/z: 476 $[M]^+$ (2), 458 (11), 440 (8), 422 (3), 407 (1), 347 (57), 329 (71), 311 (34), 295 (6), 287 (18), 269 (21), 99 (100), 81 (12) [1]

FAB-HR-MS m/z: for $C_{28}H_{44}O_6Na$ $[M + Na]^+$ calcd. 499.3030, found 499.3033 [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.12 (br s, He-3), 2.98 (m, H-5), 6.26 (br s, H-7), 3.56 (br s, H-9), 2.47 (m, Ha-16), 2.30 (m, Hb-16), 3.46 (d, J = 9.1, H-17), 1.23 (s, CH_3-18), 1.05 (s, CH_3-19), 1.70 (s, CH_3-21), 3.89 (m, H-22), 3.89 (m, H-23), 1.94 (m, H-24), 1.70 (m, H-25), 3.89 (m, Ha-26), 3.38 (t, J = 8.4, Hb-26), 0.87 (d, J = 6.6, CH_3-27), 1.27 (d, J = 6.5, CH_3-28) [1]

^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

C-1	36.8	C-11	21.5	C-21	22.9
2	29.2	12	32.1	22	79.3
3	64.0	13	48.0	23	86.9
4	34.2	14	84.1	24	46.9
5	51.6	15	31.5	25	42.5
6	203.9	16	21.8	26	74.3
7	121.1	17	49.8	27	15.3
8	166.6	18	18.0	28	18.0
9	33.5	19	24.2		
10	37.2	20	76.7		

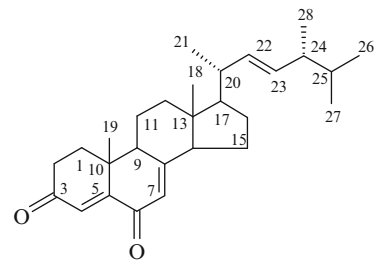
(*continued*)

References

1. W.W. Zhou, W.H. Lin, S.X. Guo, Chem. Pharm. Bull. **55**, 1148 (2007)

Ergosta-4,7,22-Triene-3,6-Dione

CAS Registry Number: 19698-66-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ganoderma lucidum* [1]

$C_{28}H_{40}O_2$: 408.3028

Mp: 156–159°C (decomp.) [1], 144–155°C (decomp.) (hexane-EtOAc) [2]

IR (KBr) ν_{max} cm^{-1}:2950, 2870, 1665, 1640, 1620, 1600 [1], 1685, 1660, 1625, 1605 [2]

UV λ_{max}^{EtOH} nm: 275 (log ε 3.8) [1], 227 (ε 8500) [2]

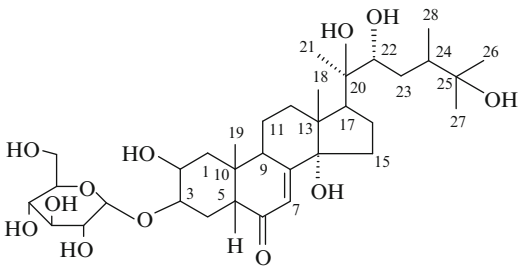
EI-MS m/z: 408 $[M]^+$ (80), 283 [M-side-chain]$^+$ (100), 229 $[M\text{-}C_{13}H_{23}]^+$ (33), 125 (13) [1]
HR-MS m/z: for $C_{28}H_{40}O_2$ calcd. 408.3028, found 408.3034 [1]
^{1}H NMR (300 MHz, J/Hz, $CDCl_3$): 0.68 (s, CH_3), 0.82 (d, J = 6.6, CH_3), 0.84 (d, J = 6.6, CH_3), 0.92 (d, J = 6.6, CH_3), 1.04 (d, J = 6.6, CH_3), 1.30 (s, CH_3), 5.14 (dd, J = 15.0, 6.7, H), 5.24 (dd, J = 15.0, 7.5, H), 5.98 (t, J = 1.8, H), 6.47 (s, H) [1]
^{1}H NMR (200 MHz, J/Hz, $CDCl_3$): 6.48 (s, H-4), 5.99 (t, J = 2.0, H-7), 0.70 (s, CH_3-18), 1.32 (s, CH_3-19), 1.06 (d, J = 6.5, CH_3-21), 5.08-5.28 (m, H-22), 5.08-5.28 (m, H-23), 0.84 (d, J = 6.5, CH_3-26), 0.86 (d, J = 6.5, CH_3-27), 0.93 (d, J = 6.5, CH_3-28) [2]

References

1. M. Hirotani, I. Asaka, C. Ino, T. Furuya, M. Shiro, Phytochemistry **26**, 2797 (1987)
2. N.V. Kovganko, S.N. Sokolov, Chem. Nat. Comp. **35**, 320 (1999)

Fibraurecdyside A

CAS Registry Number: 960506-35-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Fibraurea tinctoria* [1]
$C_{34}H_{56}O_{12}$: 656.3772
Mp: >300°C [1]
$[\alpha]_D^{25}$ + 128.8° (c 0.07; MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3380, 2962, 2882, 1648, 1442 [1]
UV λ_{max}^{MeOH} nm (log ε): 243 (3.32) [1]
FAB-MS m/z: 657 $[M + H]^+$ [1]
HR-FAB-MS m/z: for $C_{34}H_{57}O_{12}$ $[M + H]^+$ calcd. 657.3850, found 657.3853 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 2.04 (dd, J = 3.7, 12.9, Ha-1), 1.71 (dd, J = 12.8, 12.9, He-1), 4.07 (dd, J = 3.7, 12.8, Ha-2), 4.26 (s, He-3), 2.16 (m, Ha-4), 1.68 (m, He-4), 2.90 (m, H-5), 6.18 (s, H-7), 3.53 (m, Ha-9), 1.78 (m, Ha-11), 1.64 (m, He-11), 2.50 (ddd, J = 4.6, 12.6, 12.7, Ha-12), 2.13 (m, He-12), 1.93 (s, H-15), 2.41 (dd, J = 9.2, 9.4, Ha-16), 2.09 (m, Hb-16), 2.89 (m, H-17), 1.16 (s, CH_3-18), 0.85 (s, CH_3-19), 1.54 (s, CH_3-21), 3.94 (d, J = 10.8, Hb-22), 1.55 (m, H-23), 2.25 (m, H-24), 1.28 (s, CH_3-26), 1.31 (s, CH_3-27), 1.05 (d, J = 6.8, CH_3-28), Other: 6.29 (br s, OH), β-D-Glcp′: 4.85 (d, J = 7.8, H-1), 3.99 (dd, J = 7.8, 8.3, H-2), 4.16 (dd, J = 8.3, 9.1, H-3), 4.12 (dd, J = 9.1, 9.1, H-4), 3.86 (dd, J = 5.4, 9.1, H-5), 4.48 (dd, J = 1.8, 11.8, Ha-6), 4.24 (dd, J = 5.4, 11.6, Hb-6) [1]
^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	39.0	C-13	48.1	C-25	72.1
2	67.5	14	84.2	26	26.5
3	77.7	15	31.9	27	28.2
4	30.6	16	21.4	28	15.5
5	51.4	17	50.0	Glc′-1	104.2
6	203.0	18	18.0	2	74.7
7	121.6	19	24.1	3	78.6
8	166.3	20	77.0	4	71.6
9	34.2	21	21.6	5	78.5
10	38.7	22	74.7	6	62.6
11	21.1	23	34.6		
12	32.0	24	41.9		

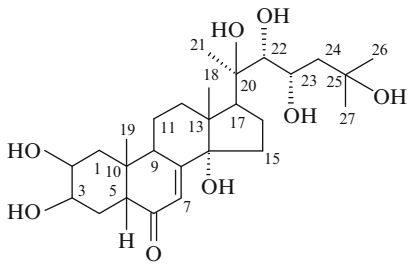
Pharm./Biol.: Inhibition of Human CYP3A4- Catalyzed Nifedipine oxidation activity: IC50 > 100 μM (inactive) [1].

References

1. C.R. Su, Y.F. Ueng, N.X. Dung, M.V. Bhaskar Reddy, T.S. Wu, J. Nat. Prod. **70**, 1930 (2007)

Gerardiasterone

CAS Registry Number: 102712-89-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula tinctoria* [1]

$C_{27}H_{44}O_8$: 496.3036

Mp: 143–146°C [2]

$[\alpha]_D^{22}$ + 52.3° (c 0.35, MeOH) [2]

UV λ_{max}^{MeOH} nm (ε): 243 (12500) [2]

DEI-MS m/z: 496 $[M]^+$, 393 (0.4), 363 (17), 133 (5), 103 (4) [2]

FAB-MS m/z: 497 $[M + H]^+$ 479, 461, 443, 425 [2]

HR-MS m/z: for $C_{27}H_{38}O_5$ calcd. 442.2719, found 442.2735 ± 0.005, for $C_{22}H_{30}O_4$ calcd. 358.2144, found 358.2091 ± 0.01, for $C_{21}H_{27}O_3$ calcd. 327.1960, found 327.1919 ± 0.05 [2]

CD (c, MeOH): $\Delta\varepsilon$ = +2.4 (330 nm), $\Delta\varepsilon$ = −6.4 (250 nm) [2]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.93 (Ha-1), 2.12 (He-1), 4.18 (m, Ha-2), 4.24 (m, He-3), 1.80 (Ha-4), 2.04 (He-4), 3.02 (dd, J = 4.0, 13.0, H-5), 6.27 (d, J = 2.1, H-7), 3.60 (m, H-9), 1.82 (Ha-11), 1.69 (He-11), 2.68 (ddd, J = 4.5, 12.0, 12.0, Ha-12), 2.04 (He-12), 2.18 (Ha-15), 2.18 (Hb-15), 2.45 (Ha-16), 2.22 (Hb-16), 3.33 (dd, J = 8.5, 8.5, H-17), 1.14 (s, CH_3-18), 1.09 (s, CH_3-19), 1.77 (s, CH_3-21), 3.75 (br s, H-22), 4.80 (br d, J = 9.7, H-23), 1.82 (Ha-24), 2.45 (Hb-24), 1.44 (s, CH_3-26), 1.47 (s, CH_3-27) [2]

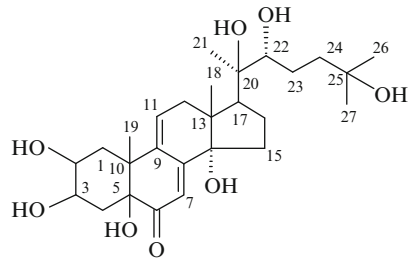
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.0 \times 10^{-7}$ M [3, 4].

References

1. M. Bathori, I. Mathe, J.P. Girault, H. Kalasz, R. Lafont, J. Nat. Prod. **61**, 415 (1998)
2. A. Guerriero, P. Traldi, F. Pietra, J. Chem. Soc. Chem. Comm. **1**, 40 (1986)
3. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
4. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

Herkesterone

CAS Registry Number: 730981-24-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Dioscorea dumetorum* [1], *Serratula wolffii* [2]

$C_{27}H_{42}O_8$: 494.2879

Mp: 218°C (dec.) [2]

$[\alpha]_D^{28}$ + 59° (c 0.1, DMSO) [2]

IR (KBr) ν_{max} cm^{-1}: 3560–3200, 1650, 1602 [2]

UV λ_{max}^{MeOH} nm (log ε): 296 (4.02) [2]

FAB-MS m/z: 495 $[M + H]^+$ (9), 477 $[M + H–H_2O]^+$ (10), 459 $[M + H–2H_2O]^+$ (23), 443 (26), 440 (11), 422 (8), 407 (49), 394 (17), 378 (9), 361 (26), 359 (10), 323 (18), 300 (100), 199 (11) [2]

HR-ESI-MS m/z: for $C_{27}H_{42}O_8$ $[M]^+$ calcd. 494.2880, found 494.2885 [2]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 2.05 (Ha-1), 2.05 (He-1), 3.83 (ddd, J = 3.2, 5.4, 10.7, Ha-2), 3.88 (q, J = 3.0, He-3), 1.92 (dd, J = 2.8, 14.5, Ha-4), 1.77 (dd, J = ?, 3.4, He-4), 5.83 (t, J = 1.2, H-7), 6.34 (dt, J = 2.0, 6.7, H-11), 2.726 (dd, J = 1.8, 18.0, Ha-12), 2.436 (dd, J = 6.7, 18.2, He-12), 1.80 (Ha-15), 1.98 (Hb-15), 1.79 (Ha-16), 1.99 (Hb-16), 2.49 (t, J = 9.0, H-17), 0.90 (s, CH_3-18), 1.05 (s, CH_3-19), 1.208 (s, CH_3-21), 3.35 (dd, J = 1.8, 10.3,

H-22), 1.30 (Ha-23), 1.68 (Hb-23), 1.44 (ddd, J = 4.2, 11.6, 13.3, Ha-24), 1.81 (Hb-24), 1.19 (s, CH_3-26), 1.206 (s, CH_3-27) [2]

^{1}H NMR (500 MHz, J/Hz, DMSO-d_6): 5.65 (s, H-7), 6.18 (br s, He-11), 2.59 (d, J = 17.8, Ha-12), 2.29 (dd, J = 6.6, 17.8, He-12), 1.60 (Ha-16), 1.89 (Hb-16), 2.36 (t, J = 9.3, H-17), 0.77 (s, CH_3-18), 0.96 (s, CH_3-19), 1.075 (s, CH_3-21), 3.13 (d, J = 10.2, H-22), 4.42 (OH-22), 1.13 (Ha-23), 1.49 (Hb-23), 1.27 (td, J = 4.3, 12.0, Ha-24), 1.65 (Hb-24), 1.06 (s, CH_3-26), 1.09 (s, CH_3-27) [2]

^{13}C NMR (125 MHz, CD_3OD) [2]:**^{13}C NMR** (125 MHz, DMSO-d_6) [2]:

Table 1

C-1	34.5	C-15	31.5	C-1		C-15	20.4
2	68.6	16	21.8	2		16	48.7
3	70.3	17	50.7	3		17	17.3
4	39.2	18	18.2	4		18	25.8
5	80.5	19	26.5	5	78.4	19	75.5
6	203.1	20	77.8	6		20	20.7
7	117.9	21	20.9	7	116.5	21	76.3
8	156.5	22	78.6	8		22	26.1
9	137.9	23	27.5	9	136.3	23	41.4
10	46.4	24	42.5	10		24	68.7
11	134.3	25	71.4	11	131.7	25	29.0
12	39.2	26	29.1	12	37.5	26	30.0
13	48.0	27	29.9	13	46.3	27	
14	84.5			14	82.0		

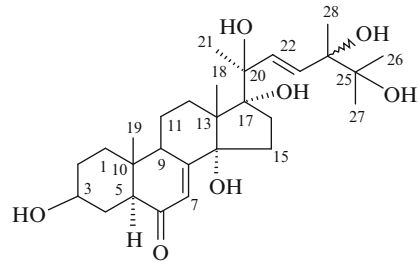
Pharm./Biol.: *Candida* tests: Not active (MIC > 200 μg/ml) [1].

References

1. M. Santour, F. Canon, T. Miyamoto, A. Dongmo, M.-A. Lacaille-Dubois, Biochem. Sys. Ecol. **36**, 559 (2008)
2. A. Hunyadi, C. Toth, A. Simon, M. Mak, Z. Kele, I. Mathe, M. Bathori, J. Nat. Prod. **67**, 1070 (2004)

3β,14α,17α,20,24,25-Hexahydroxy-5α-Ergosta-7,22-dien-6-one

CAS Registry Number: 141912-42-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Lasiosphaera nipponica* [1]

$C_{28}H_{44}O_7$: 492.3087

Mp: 254–256°C [1]

$[\alpha]_D^{23}$ + 171° (c 0.41, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3436, 1640, 1456, 1372, 1159, 1058, 1000, 800 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (4.28) [1]

EI-MS m/z: 456 $[M\text{-}2H_2O]^+$ (4.7), 420 $[M\text{-}4H_2O]^+$ (8.3), 402 $[M\text{-}5H_2O]^+$ (6.0), 301 (10.0), 239 (11.7), 161 (17.3), 139 (24.9), 123 (100), 95 (58.2) [1]

FAB-MS m/z: 515 $[M + Na]^+$, 493 $[M + H]^+$ [1]

HR-FAB-MS m/z: for $C_{28}H_{44}O_7Na$ $[M + Na]^+$ calcd. 515.2985, found 515.2971 [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.10 (td, J = 3.4, 14.7, H-1), 1.85 (m, Ha-2), 2.02 (m, He-2), 3.86 (tt, J = 6.0, 11.8, He-3), 1.82 (m, Ha-4), 2.12 (m, He-4), 2.31 (dd, J = 3.4, 13.2, H-5), 6.18 (d, J = 2.4, H-7), 3.64 (ddd, J = 2.4, 5.0, 11.0, H-9), 1.64 (m, Ha-11), 1.79 (m, He-11), 2.50 (m, Ha-12), 2.90 (m, He-12), 2.93 (m, Ha-15), 2.13 (m, Hb-15), 2.11

(m, Ha-16), 2.11 (m, Hb-16), 1.22 (s, CH_3-18), 0.97 (s, CH_3-19), 1.81 (s, CH_3-21), 6.86 (d, J = 16.1, H-22), 6.63 (d, J = 16.1, H-23), 1.55 (s, CH_3-26), 1.60 (s, CH_3-27), 1.72 (s, CH_3-28) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

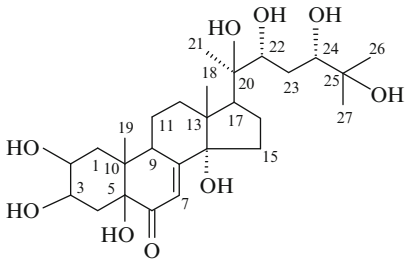
C-1	34.2	C-11	20.4	C-21	26.4
2	31.5	12	26.7	22	136.2
3	69.1	13	51.4	23	131.8
4	35.6	14	86.3	24	77.4
5	57.2	15	33.6	25	74.4
6	202.2	16	31.9	26	25.9
7	121.6	17	89.0	27	25.8
8	164.9	18	20.5	28	23.5
9	33.8	19	23.7		
10	36.7	20	78.0		

References

1. Y. Takashi, R. Adachi, Y. Murakami, T. Ohashi, K. Nakano, T. Tomimatsu, Phytochemistry **31**, 243 (1992)

5-Hydroxyabutasterone

CAS Registry Number: 156498-50-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polypodium vulgare* [1]

$C_{27}H_{44}O_9$: 512.2985

TSP-MS m/z: 530 $[M + H + NH_3]^+$, 513 $[M + H]^+$, 495 $[M + H–H_2O]^+$, 477 $[M + H–2H_2O]^+$, 459 $[M + H–3H_2O]^+$ [1]

^{1}H NMR (J/Hz, C_5D_5N): 4.26 (Ha-2), 4.17 (He-3), 6.26 (d, J = 2.4, H-7), 3.61 (d, J = 9.6, Ha-9), 2.98 (t, J = 8.4, H-17), 1.19 (s, CH_3-18), 1.15 (s, CH_3-19), 1.61 (s, CH_3-21), 4.25 (d, J = 10.5, H-22), 4.09 (d, J = 9.3, H-24), 1.47 (s, CH_3-26), 1.52 (s, CH_3-27) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

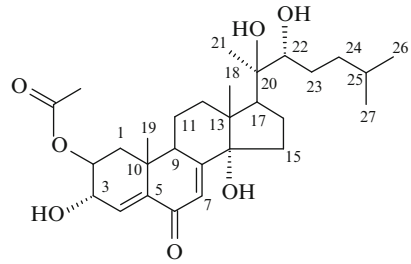
C-1	34.85	C-10	44.77	C-19	17.23
2	67.99	11	22.01	20	76.74
3	69.90	12	32.02	21	21.79
4	35.99	13	48.12	22	78.33
5	79.93	14	83.96	23	32.95
6	201.01	15	31.65	24	80.37
7	119.92	16	21.44	25	72.27
8	166.85	17	49.92	26	27.00
9	38.29	18	17.91	27	25.27

References

1. J. Coll, N. Reixach, F. Sanches-Baeza, J. Casas, F. Camps, Tetrahedron **50**, 7247 (1994)

14-Hydroxyacetylpinnasterol

CAS Registry Number: 104387-07-7



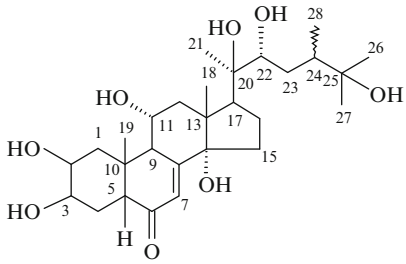
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Laurencia pinnata* [1]
$C_{29}H_{44}O_7$: 504.3087
Mp: 174–176°C ($CHCl_3$–Et_2O) [1]
$[\alpha]_D^{20}$ + 91° (c 0.55, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3480, 1730, 1675, 1645, 1260 [1]
UV λ_{max}^{EtOH} nm (log ε): 257 (3.99) [1]
FD-MS m/z: 504 $[M]^+$, 486, 444, 403, 359, 342, 145 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 2.44 (dd, J = 14.0, 3.5, Ha-1), 1.64 (dd, J = 14.0, 10.3, Hb-1), 5.31 (ddd, J = 10.3, 7.0, 3.5, Ha-2), 4.69 (dd, J = 7.0, 2.5, Hb-3), 6.72 (d, J = 2.5, H-4), 6.28 (d, J = 2.5, H-7), 3.57 (ddd, J = 12.0, 7.0, 2.5, Ha-9), 2.56 (dt, J = 13.0, 5.0, Ha-12), 2.92 (t, J = 9.1, Ha-17), 1.21 (s, CH_3-18), 1.25 (s, CH_3-19), 1.58 (s, CH_3-21), 3.83 (d, J = 10.0, Hb-22), 0.88 (d, J = 6.0, CH_3-26), 0.89 (d, J = 6.0, CH_3-27), Other: 2.00 (s, CH_3COO) [1]
Pharm./Biol.: *Sarcophaga* test: ED_{50} = 6 µg [1].

References

1. A. Fukuzawa, M. Miyamoto, Y. Kumagai, T. Masamune, Phytochemistry **25**, 1305 (1986)

25-Hydroxyatrotosterone A

CAS Registry Number: 190513-08-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Paxillis atrotomentosus* [1]
$C_{28}H_{46}O_8$: 510.3192
IR (KBr) ν_{max} cm^{-1}: 3404, 1657, 1072, 1054 [1]
FAB-MS m/z: 533 $[M + Na]^+$ (4), 511 $[M + H]^+$ (2), 493 (12), 475 (13), 457 (11), 439 (3), 387 (2), 379 (2), 373 (2), 362 (4), 345 (5), 317 (6), 299 (9), 281 (5), 249 (7), 225 (8), 213 (10), 197 (12), 181 (23), 157 (25), 113 (75), 93 (100), 83 (71), 69 (70), 57 (95) [1]
HR-MS m/z: for $C_{28}H_{46}O_8$ $[M + Na]^+$ calcd. 533.3090, found 533.3198 [1]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 2.59 (dd, J = 13.0, 4.2, Ha-1), 1.38 (dd, J = 13.0, 12.0, He-1), 4.01 (ddd, J = 12.0, 4.2, 3.5, Ha-2), 3.96 (q, J = 2.8, He-3), 1.78 (dt, J = 13.5, 13.5, 2.5, Ha-4), 1.68 (dt, J = 14.3, 3.2, 3.2, He-4), 2.34 (dd, J = 13.2, 4.0, H-5), 5.80 (dd, J = 2.7, 0.8, H-7), 3.14 (dd, 8.8, 2.7, H-9), 4.10 (ddd, 10.5, 8.8, 6.0, Ha-11), 2.21 (dd, 11.8, 10.7, Ha-12), 2.15 (dd, J = 12.2, 6.0, He-12), 1.95 (Ha-15), 1.57 (Hb-15), 2.00 (Ha-16), 1.79 (Hb-16), 2.42 (dd, J = 9.6, 8.6, H-17), 0.874 (s, CH_3-18), 1.056 (s, CH_3-19), 1.195 (s, CH_3-21), 3.47 (dd, J = 9.4, 2.0, H-22), 1.86 (ddd, J = 14.4, 4.2, 2.0, Ha-23), 1.05 (Hb-23), 1.65 (dp, J = 4.2, 7.0, 7.0, 7.0, 7.0, H-24), 1.142 (s, CH_3-26), 1.211 (s, CH_3-27), 1.034 (d, J = 7.0, CH_3-28) [1]
^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

C-1	39.07	C-11	69.50	C-21	20.66
2	68.94	12	43.75	22	77.88
3	68.56	13		23	35.12
4	33.28	14	84.95	24	44.42
5	52.78	15	31.83	25	74.07
6	206.72	16	21.61	26	28.19
7	122.78	17	50.20	27	25.86
8	165.70	18	18.85	28	16.89
9	42.93	19	24.60		
10	39.90	20	77.96		

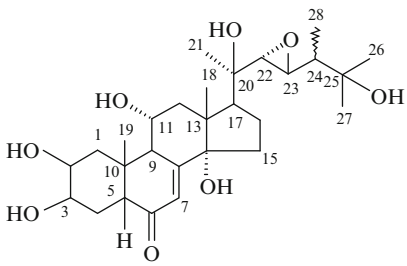
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.0 \times 10^{-5}$ M [2].

References

1. K. Vokas, M. Budesinsky, J. Harmatha, J. Pis, Tetrahedron **54**, 1657 (1998)
2. J. Harmatha, L. Dinan, Arch. Insect Biochem. Physiol. **35**, 219 (1997)

25-Hydroxyatrotosterone B

CAS Registry Number: 190513-09-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Paxillis atrotomentosus* [1]

$C_{28}H_{44}O_8$: 508.30361

IR (KBr) ν_{max} cm^{-1}: 3386, 1652, 1589 [1]

FAB-MS m/z: 531 $[M + Na]^+$ (4), 509 $[M + H]^+$ (10), 491 (14), 473 (3), 455 (2), 397 (3), 373 (3), 345 (4), 291 (22), 249 (14), 213 (11), 189 (11), 161 (19), 145 (19), 109 (30), 91 (44), 81 (50), 69 (44), 59 (100) [1]

HR-MS m/z: for $C_{28}H_{45}O_8$ $[M + H]^+$ calcd. 509.3114, found 509.3104 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 2.59 (dd, J = 12.8, 4.2, Ha-1), 1.37 (t, J = 12.8, 11.8, He-1), 4.01 (dt, J = 11.8, 3.6, 3.6, Ha-2), 3.96 (q, J = 2.8, He-3), 1.78 (dt, J = 13.6, 13.6, 2.4, Ha-4), 1.69 (dt, J = 14.0, 3.7, 3.7, He-4), 2.34 (dd, J = 13.2, 4.0, H-5), 5.81 (d, J = 2.5, H-7), 3.16 (dd, J = 9.0, 2.6, H-9), 4.10 (ddd, J = 10.5, 9.0, 6.0, Ha-11), 2.25 (t, J = 12.0, 11.0, Ha-12), 2.14 (dd, J = 12.2, 5.8, He-12), 1.96 (Ha-15), 1.61 (Hb-15), 1.96 (Ha-16), 1.96 (Hb-16), 2.50 (dd, J = 9.5, 8.8, H-17), 0.844 (s, CH_3-18), 1.055 (s, CH_3-19), 1.319 (s, CH_3-21), 2.92 (dd, J = 7.6, 2.3, H-22), 2.88 (dd, J = 7.6, 2.3, Ha-23), 1.24 (dq, J = 7.6, 7.0, 7.0, 7.0, H-24), 1.233 (s, CH_3-26), 1.230 (s, CH_3-27), 1.019 (s, CH_3-28) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

C-1	39.06	C-11	69.46	C-21	23.99
2	68.93	12	43.52	22	66.97
3	68.56	13	48.49	23	54.47
4	33.30	14	84.72	24	47.56
5	52.76	15	31.84	25	72.93
6	206.66	16	21.88	26	28.03
7	122.71	17	54.29	27	27.04
8	165.67	18	18.78	28	12.42
9	42.95	19	24.61		
10	39.89	20	72.77		

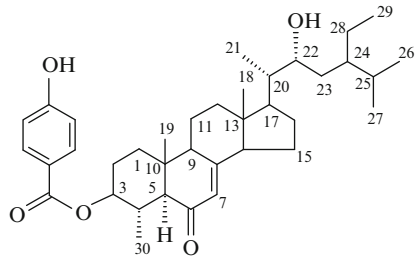
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 5.0 \times 10^{-5}$ M [2].

References

1. K. Vokas, M. Budesinsky, J. Harmatha, J. Pis, Tetrahedron **54**, 1657 (1998)
2. J. Harmatha, L. Dinan, Arch. Insect Biochem. Physiol. **35**, 219 (1997)

3β (p-Hydroxy)-Benzoxy-22-Hydroxy-4α-Methyl-24-Ethyl-5α-Cholest-7-en-6-one

CAS Registry Number: 55487-86-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Solanum xanthocarpum* [1]

$C_{37}H_{54}O_5$: 578.3971

Mp: 294–296°C (EtOAc) [1]

$[\alpha]_D^{20}$ + 71.9° [1]

IR ($CHCl_3$) ν_{max} cm^{-1}:3600, 1671, 1625 [1]

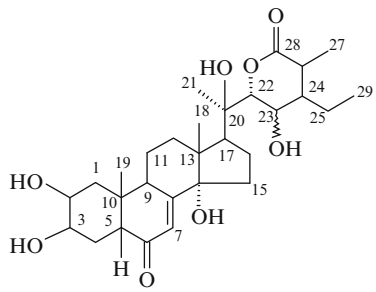
IR (Nujol) ν_{max} cm^{-1}: 3480, 3250, 1671, 1625 [1]

EI-MS m/z: 578 $[M]^+$ (17.9), 450 (7.1), 440 (67.0), 312 (66.1), 297 (35.7), 283 (22.3), 257 (100.0) [1]

References

1. G. Kusano, T. Takemoto, J.A. Beisler, Y. Sato, Phytochemistry **14**, 529 (1975)

23-Hydroxycapitasterone



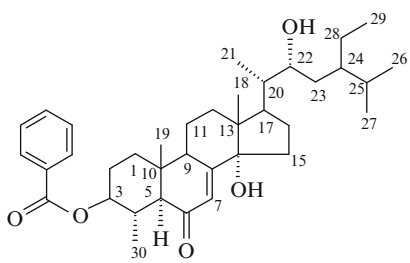
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Ajuga reptans* var. *reptans* [1]
$C_{29}H_{44}O_8$: 520.3036

References

1. M. Bathori, A. Hunyadi, A. Simon, G. Toth, L. Polgar, I. Mathe, *55th Annual Meeting and International Congress of the Society for Medicinal Plant Research*, Graz, p. 378, 942 (2007)

14α-Hydroxycarpesterol

CAS Registry Number: 55528-55-7



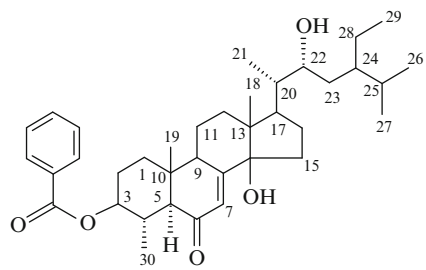
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Solanum xanthocarpum* [1]
$C_{37}H_{54}O_5$: 578.3971
Mp: 268–270°C (EtOAc) [1]
$[\alpha]_D^{20}$ + 100.7° [1]
IR ($CHCl_3$) ν_{max} cm^{-1}:3600, 3450, 1712, 1680, 1631 [1]
EI-MS m/z: 578 $[M]^+$ (1), 438 (49), 402 (100), 280 (28) [1]
^{1}H NMR (J/Hz, $CDCl_3$): 4.70 (m, H-3), 5.91 (d, J = 3.0, H-7), 0.71 (s, CH_3-18), 0.93 (s, CH_3-19), 3.74 (d, J = 12.0, H-22), 1.16 (d, J = 6.0, CH_3-30), Ar: 8.06 (q, J = 1.5, 7.0, 2H), 7.56 (q, J = 1.5, 7.0, 1H), 7.41 (t, J = 7.0, 2H) [1]

References

1. G. Kusano, T. Takemoto, J.A. Beisler, Y. Sato, Phytochemistry **14**, 529 (1975)

14β-Hydroxycarpesterol

CAS Registry Number: 55487-85-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Solanum xanthocarpum* [1]
$C_{37}H_{54}O_5$: 578.3971
Mp: 277–278°C (EtOAc) [1]
$[\alpha]_D^{20}$ + 82.2° [1]
IR ($CHCl_3$) ν_{max} cm^{-1}:3600, 3500, 1710, 1670, 1625 [1]

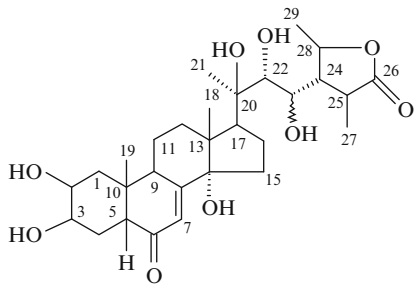
EI-MS m/z: 578 $[M]^+$ (0.5), 560 $[M\text{-}H_2O]^+$ (0.5), 542 (66.7), 438 (30.0), 420 (100) [1]

^{1}H NMR (J/Hz, $CDCl_3$): 4.70 (m, H-3), 5.91 (d, J = 3.0, H-7), 0.77 (s, CH_3-18), 0.93 (s, CH_3-19), 3.75 (d, J = 12.0, H-22), 1.16 (d, J = 6.0, CH_3-30), Ar: 8.06 (q, J = 1.5, 7.0, 2H), 7.56 (q, J = 1.5, 7.0, 1H), 7.41 (t, J = 7.0, 2H) [1]

References

1. G. Kusano, T. Takemoto, J.A. Beisler, Y. Sato, Phytochemistry **14**, 529 (1975)

23-Hydroxycyasterone



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga iva* [1]

$C_{29}H_{44}O_9$: 536.2985

Mp: 235–236°C [1]

IR (KBr) ν_{max} cm^{-1}: 3500, 1755–1785, 1715–1725, 1655, 1465, 1400, 1335–1345, 1130, 1068, 1030 [1]

UV λ_{max}^{MeOH} nm: 243 [1]

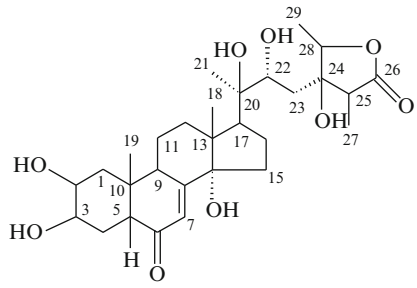
EI-MS m/z: 518 $[M\text{-}H_2O]^+$(0.8), 500 (8), 482 (3), 467 (1.5), 464 (0.5), 457 (5), 439 (1.5), 428 (0.5), 363 (33), 345 (80), 327 (55), 300 (50), 217 (5), 201 (20), 200 (83), 199 (20), 173 (42), 172 (27), 171 (100), 157 (45), 129 (31), 128 (100) [1]

References

1. N. Sabri, A. Asaad, S.M. Knafagy, Planta Med. **42**, 293 (1981)

24-Hydroxycyasterone

CAS Registry Number: 627511-34-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga iva* [1], *Cyathula officinalis* [2]

$C_{29}H_{44}O_9$: 536.2985

Mp: 181–183°C [2]

$[\alpha]_D^{25}$ + 36.3° (c 0.16, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3436, 1755, 1646 [2]

UV λ_{max}^{MeOH} nm (log ε): 243 (3.99) [2]

EI-MS m/z: 500 $[M\text{-}2H_2O]^+$, 482 $[M\text{-}3H_2O]^+$, 363 (3), 345 (8), 327 (12), 301 (7), 105 (9), 91 (12), 83 (9), 81 (10), 79 (8), 55 (23), 43 (100), 40 (61), 29 (49) [2]

ESI-MS m/z: 535 $[M\text{-}H]^-$, 1071 $[2M\text{-}H]^-$; 559 $[M + Na]^+$, 1095 $[2M + Na]^+$ [2]

HR-ESI-MS m/z: for $C_{29}H_{44}O_9Na$ $[M + Na]^+$ calcd. 559.2883, found 559.2884 [2]

^{1}H NMR (J/Hz, C_5D_5N): 4.20 (m, Ha-2), 4.26 (br s, He-3), 3.04 (dd, J = 3.6, 13.2, H-5), 6.30 (d, J = 2.4, H-7), 3.60 (br s, H-9), 2.63 (dt, J = 4.2, 12.6, He-12), 2.54 (q, J = 10.2, Ha-16), 2.90 (t, J = 9.0, H-17), 1.25 (s, CH_3-18), 1.08 (s, CH_3-19), 1.61 (s, CH_3-21), 4.28 (d, J = 10.8, H-22), 3.14 (q, J = 7.2, H-25), 1.57 (d, J = 7.2, CH_3-27), 4.59 (q, J = 6.6, H-28), 1.58 (d, J = 6.6, CH_3-29) [2]

^{13}C NMR (C_5D_5N) [2]:

Table 1

C-1	38.4 (t)	C-11	20.8 (t)	C-21	20.7 (q)
2	67.8 (d)	12	31.8 (t)	22	73.3 (d)
3	67.8 (d)	13	48.0 (s)	23	37.8 (t)
4	32.1 (t)	14	83.9 (s)	24	78.9 (s)

(*continued*)

Table 1 (continued)

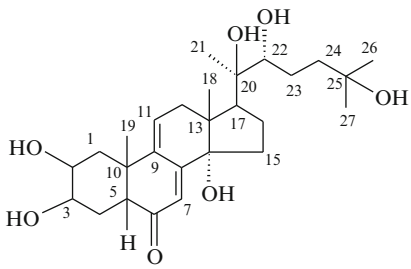
5	51.5 (d)	15	31.6 (t)	25	45.6 (d)
6	203.2 (s)	16	21.2 (t)	26	178.3 (s)
7	121.6 (d)	17	49.7 (d)	27	8.9 (q)
8	165.5 (s)	18	17.6 (q)	28	82.1 (d)
9	34.4 (d)	19	24.2 (q)	29	12.8 (q)
10	37.2 (s)	20	76.4 (s)		

References

1. J. Coll, Afinidad **64**, 242 (2007)
2. R. Zhou, B.G. Li, G.L. Zhang, J. Asian Nat. Prod. Res. **7**, 245 (2005)

25-Hydroxydacryhainansterone

CAS Registry Number: 58347-77-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Asparagus filicinus* [1], *Serratula wolffii* [2]

$C_{27}H_{42}O_7$: 478.2930

$[\alpha]_D^{29}$ + 17.0° (0.5; MeOH) [2]

UV λ_{max}^{MeOH} nm (log ε): 299 (3.33) [2]

ESI-MS m/z: 479 $[M + H]^+$, 461.6 $[M + H–H_2O]^+$, 443 $[M + H–2H_2O]^+$, 427 $[M + H–3H_2O]^+$, 345 $[M-C_{20}–C_{27}]^+$ [2]

^{1}H NMR (J/Hz, CD_3OD): 1.70 (dd, J = 11.9, 13.5, Ha-1), 2.08 (dd, J = 4.0, 11.5, He-1), 3.72 (ddd, J = 3.1, 3.9, 11.9, Ha-2), 3.85 (d, J = 2.8, He-3), 1.60 (Ha-4), 1.76 (dt, J = 3.9, 14.0, He-4), 2.45 (dd, J = 3.7, 12.6, H-5), 5.75 (d, J = 1.0, H-7), 6.29 (dt, J = 2.0, 6.6, H-11), 2.74 (dd, J = 2.5, 17.6, Ha-12), 2.42 (dd, J = 6.8, 18.0, He-12), 1.79 (Ha-15), 1.96 (He-15), 1.80 (Ha-16), 1.99 (Hb-16), 2.50 (t, J = 8.9, H-17), 0.90 (s, CH_3-18), 1.11 (s, CH_3-19), 1.211 (s, CH_3-21), 3.34 (H-22), 1.31 (Ha-23), 1.64 (Hb-23), 1.44 (Ha-24), 1.81 (Hb-24), 1.19 (s, CH_3-26), 1.206 (s, CH_3-27) [2]

^{13}C NMR (CD_3OD) [2]:

Table 1

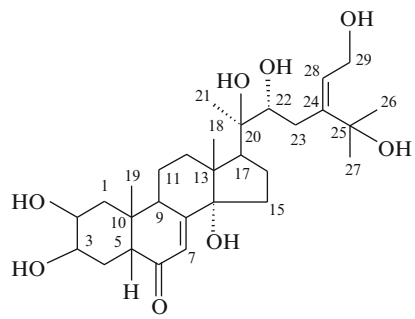
C-1	37.5	C-10	41.1	C-19	31.6
2	68.9	11	134.0	20	78.0
3	68.4	12	39.2	21	21.0
4	35.9	13	48.1	22	78.6
5	51.7	14	84.6	23	27.5
6		15	31.6	24	42.5
7	119.4	16	22.0	25	71.6
8	156.7	17	50.7	26	29.1
9	136.3	18	18.3	27	29.8

References

1. J. Wu, H. Wang, W. Ye, X. Zuo, S. Zhao, Zhongguo yaoke Daxue Xuebao **37**, 487 (2006)
2. A. Hunyadi, A. Gergely, A. Simon, G. Toth, G. Veress, M. Bathori, J. Chrom. Sci. **45**, 76 (2007)

29-Hydroxy-24(28)-Dehydromakisterone C

CAS Registry Number: 423762-74-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Leuzea carthamoides* [1]
$C_{29}H_{46}O_8$: 522.3192
$[\alpha]_D^{20}$ + 32.5° (c 0.24, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3405, 1653 [1]
FAB-MS m/z: 545 (20) $[M + Na]^+$, 523 (26) $[M + H]^+$, 505 (20), 487 (17), 480 (34), 469 (15), 465 (21), 451 (9), 433 (15), 417 (13), 405 (12), 392 (20), 387 (17), 373 (31), 365 (15), 363 (13), 351 (55), 350 (58), 341 (100), 334 (51), 327 (50), 319 (20) [1]
HR-MS m/z: for $C_{29}H_{47}O_8$ $[M + H]^+$ calcd. 523.3279, found 523.3177 [1]
CD (c, MeOH): $\Delta\varepsilon$ = +2.90 (216 nm), $\Delta\varepsilon$ = −3.86 (252 nm), $\Delta\varepsilon$ = +1.53 (329 nm) [1]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.80 (dd, Ha-1), 1.43 (dd, He-1), 3.84 (ddd, Ha-2), 3.95 (bq, He-3), 1.73 (Ha-4), 1.73 (He-4), 2.39 (dd, H-5), 5.81 (d, H-7), 3.16 (ddd, H-9), 1.82 (Ha-11), 1.70 (He-11), 2.15 (dt, Ha-12), 1.88 (He-12), 1.96 (Ha-15), 1.61 (Hb-15), 1.83 (Ha-16), 2.02 (Hb-16), 2.42 (dd, H-17), 0.90 (s, CH_3-18), 0.97 (s, CH_3-19), 1.22 (s, CH_3-21), 3.55 (dd, H-22), 2.31 (Ha-23), 2.16 (Hb-23), 1.42 (s, CH_3-26), 1.36 (s, CH_3-27), 5.43 (bt, J = 6.2, H-28), 4.31 (dd, J = 14.0, 6.2, H-29), 4.28 (dd, J = 14.0, 6.2, H-29) [1]
^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

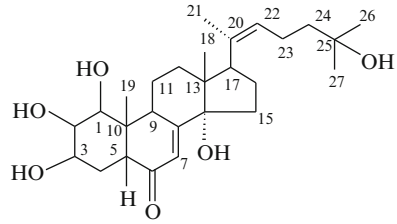
C-1	37.54	C-11	21.61	C-21	21.00
2	68.78	12	32.56	22	78.20
3	68.60	13	49.0	23	38.01
4	32.84	14	85.33	24	147.18
5	51.85	15	31.81	25	73.94
6	206.40	16	21.61	26	30.24
7	122.20	17	50.57	27	30.94
8	167.83	18	18.01	28	128.78
9	35.24	19	24.38	29	60.46
10	39.31	20	77.86		

References

1. K. Vokas, M. Budesinsky, J. Harmatha, Coll. Czech. Chem. Comm. **67**, 124 (2002)

1-Hydroxy-20,22-Didehydrotaxisterone

CAS Registry Number: 938112-72-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Serratula wolffii* [1]
$C_{27}H_{42}O_6$: 462.2981
Mp: 218–220°C [1]
$[\alpha]_D^{28}$ + 10° (c 0.05, MeOH) [1]
UV λ_{max}^{MeOH} nm (log ε): 241 (3.95) [1]
ESI-MS m/z: 501 $[M + K]^+$ (26), 463 $[M + H]^+$ (4), 445 $[M + H–H_2O]^+$ (100), 427 $[M + H–2H_2O]^+$(8), 408 $[M + H–3H_2O]^+$ (2), 391 $[M + H–4H_2O]^+$ (14), 374 (4), 363 (5), 336 (4) [1]
HR-ESI-MS m/z: for $C_{27}H_{43}O_6$ $[M + H]^+$ calcd. 463.2970, found 463.2976 [1]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 3.82 (br, Ha-1), 1.43 (dd, J = 12.2, 13.4, He-1), 3.88 (t, J = 3.1, Ha-2), 4.04 (br, He-3), 1.78 (m, Ha-4), 1.83 (m, He-4), 2.61 (dd, J = 4.5, 12.8, H-5), 5.84 (d, J = 2.5, H-7), 3.10 (t, J = 8.8, H-9), 1.69–1.72 (m, H-11), 2.06 (m, Ha-12), 1.52 (m, Hb-12), 2.05 (m, Ha-15), 1.66 (m, Hb-15), 1.82 (m, Ha-16), 1.95 (ddt, J = 2.2, 9.2, 12.0, Hb-16), 2.89 (t, J = 9.2, H-17), 0.59 (s, CH_3-18), 1.07 (br s, CH_3-19), 1.68 (s, CH_3-21), 5.30 (t, J = 7.0, H-22), 2.13 (m, H-23), 1.50 (m, H-24), 1.20 (s, CH_3-26), 1.20 (s, CH_3-27) [1]
^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

C-1	76.6	C-10	44.0	C-19	20.2
2	68.6	11	22.2	20	134.8
3	71.1	12	31.1	21	18.4
4	33.7	13	48.9	22	127.7
5	47.0	14	84.8	23	24.3

(*continued*)

Table 1 (continued)

6	206.7	15	32.3	24	44.9
7	122.0	16	24.0	25	71.5
8	167.9	17	54.3	26	29.3
9	36.0	18	17.7	27	29.3

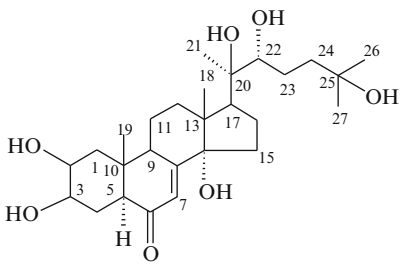
Pharm./Biol.: *Acyrthosiphon pisum* aphid larvae: low oral activity LC_{50} = 48.5 ppm (20-hydroxyecdysone LC_{50} = 1.07 ppm) [1].

References

1. E. Liktor-Busa, A. Simon, G. Toth, G. Fekete, Z. Kele, M. Bathori, J. Nat. Prod. **70**, 884 (2007)

5α-20-Hydroxyecdysone

CAS Registry Number: 35241-82-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Achyranthes fauriei* [1], *Leuzea carthamoides* [2], *Silene italica* ssp. *nemoralis* [3]

$C_{27}H_{44}O_7$: 480.3087

Mp: 278°C [1]

$[\alpha]_D$ + 55.5° (c 0.54, MeOH) [1], $[\alpha]_D^{20}$ + 56.2° (c 0.13, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3400, 1655 [1], 3422, 1651 [2]

UV λ_{max}^{EtOH} nm (log ε): 242 (4.30) [1]

EI-MS m/z: 480 $[M]^+$ [1]

FAB-MS m/z: 503 $[M + Na]^+$ (5), 481 $[M + H]^+$ (100), 463 (51), 445 (84), 427 (38), 363 (12), 347 (24), 329 (28), 301 (21), 277 (39), 257 (49), 215 (46) [2]

HR-MS m/z: for $C_{27}H_{45}O_7$ $[M + H]^+$ calcd. 481.3165, found 481.2829 [2]

CD (c, MeOH): Δε = +4.10 (327 nm), Δε = −11.10 (248 nm) [2]

ORD (c, 0.073, dioxane): $[\varphi]_{450}$ + 660, $[\varphi]_{356}^{peak}$ + 5200, $[\varphi]_{352}^{peak}$ + 5000, $[\varphi]_{342}$ 0, $[\varphi]_{303}^{trough}$ −8200, $[\varphi]_{255}^{trough}$ −23100, $[\varphi]_{242}$ 0, $[\varphi]_{220}$ −24400 [1]

^{1}H NMR (C_5D_5N): 1.21 (s, CH_3-18), 1.41 (s, CH_3-19), 1.59 (s, CH_3-21), 1.39 (s, CH_3-26), 1.39 (s, CH_3-27) [1]

^{1}H NMR (500 MHz, CD_3OD): 1.54 (dd, Ha-1), 2.09 (dd, He-1), 3.96 (dq, Ha-2), 3.58 (ddd, He-3), 1.90 (m, Ha-4), 1.75 (q, He-4), 2.38 (dd, H-5), 5.84 (d, H-7), 2.72 (ddd, H-9), 1.77 (Ha-11), 1.66 (He-11), 2.11 (dt, Ha-12), 1.84 (dd, He-12), 1.95 (Ha-15), 1.58 (Hb-15), 1.71 (Ha-16), 1.97 (Hb-16), 2.37 (m, H-17), 0.88 (s, CH_3-18), 1.02 (s, CH_3-19), 1.19 (s, CH_3-21), 3.34 (dd, H-22), 1.66 (Ha-23), 1.28 (Hb-23), 1.78 (Ha-24), 1.43 (Hb-24), 1.20 (s, CH_3-26), 1.19 (s, CH_3-27) [2]

^{13}C NMR (125 MHz, CD_3OD) [2]:

Table 1

C-1	43.86	C-10	39.23	C-19	15.72
2	70.30	11	21.41	20	77.94
3	72.68	12	32.42	21	21.02
4	24.71	13	49.00	22	78.44
5	55.29	14	85.02	23	27.34
6	203.00	15	31.86	24	42.41
7	123.57	16	21.67	25	71.31
8	166.23	17	50.59	26	29.67
9	48.26	18	17.98	27	28.96

Pharm./Biol.: *Sarcophaga pregrina* bioassay: not so marked biological activity [1], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 3.3 \times 10^{-6}$ M [4, 5].

References

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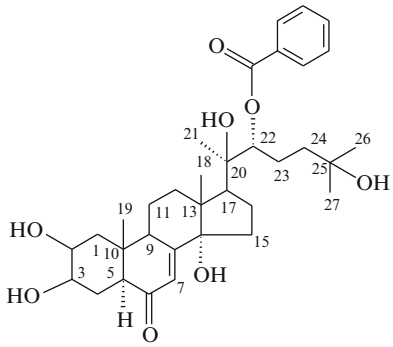
2. K. Vokac, M. Budesinsky, J. Harmata, Coll. Czech. Chem. Comm. **67**, 124 (2002)

3. A. Simon, Z. Pongracz, G. Toth, M. Mak, I. Mathe, M. Bathori, Steroids **69**, 389 (2004)
4. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
5. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

5α-20-Hydroxyecdysone-22-Benzoate

CAS Registry Number: 113814-96-3



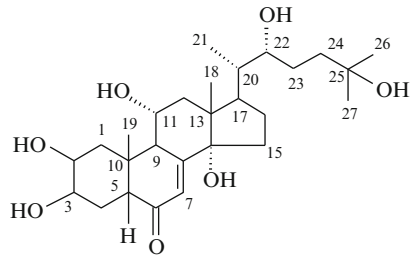
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Silene scabrifolia* [1]
$C_{34}H_{48}O_8$: 584.3349
Mp: 262–264°C (MeOH–H_2O) [1]
$[\alpha]_D^{20}$ + 45.8 ± 2° (c, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3420–3470, 1720, 1710, 1660, 1610, 1580, 1280, 725 [1]
EI-MS m/z: 566 $[M\text{-}H_2O]^+$(0.1), 548 (0.2), 530 (0.3), 515 (0.2), 512 (0.2), 462 (0.7), 444 (1), 426 (6), 411 (2), 408 (6), 393 (2), 363 (2), 345 (6), 329 (2), 327 (2), 301 (8), 300 (9), 250 (7), 122 (44), 105 (100), 99 (22), 81 (23), 77 (50), 69 (24), 55 (24), 51 (20) [1]
^{1}H NMR (100 MHz, C_5D_5N): 4.37 (m, H-2), 3.89 (m, H-3), 6.21 (br s, H-7), 3.60 (m, H-9), 1.21 (s, CH_3-18), 1.44 (s, CH_3-19), 1.79 (s, CH_3-21), 5.77 (m, H-22), 1.34 (s, CH_3-26), 1.34 (s, CH_3-27), Ar: 7.40 (3H), 8.26 (2H) [1]

References

1. Z. Saatov, M.B. Gorovits, N.D. Abdullaev, N.K. Abubakirov, Chem. Nat. Comp. **23**, 563 (1987)

11α-Hydroxyecdysone

CAS Registry Number: 130690-11-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Vitex scabra* [1], *V. strickeri* [2]
$C_{27}H_{44}O_7$: 480.3087
Mp: amorphous [2]
IR (Nujol) ν_{max} cm^{-1}: 3200, 1648 [2]
UV λ_{max}^{MeOH} nm: 299 [2]
FAB-MS m/z: 481 $[M + H]^+$ [2]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.97 (Ha-1), 3.43 (dd, J = 5.0, 12.0, He-1), 4.50 (Ha-2), 4.19 (s, He-3), 1.77 (Ha-4), 2.00 (He-4), 3.02 (dd, J = 2.0, 9.0, H-5), 6.25 (d, J = 2.0, H-7), 3.82 (dd, J = 12.0, 12.0, Ha-9), 4.45 (Ha-11), 2.95 (dd, J = 12.0, 12.0, Ha-12), 2.48 (dd, J = 12.0, 17.0, He-12), 1.86 (Ha-15), 2.02 (Hb-15), 1.59 (Ha-16), 2.23 (Hb-16), 2.64 (H-17), 0.77 (s, CH_3-18), 1.31 (s, CH_3-19), 2.11 (m, H-20), 1.27 (d, J = 7.0, CH_3-21),4.03 (m, H-22), 1.78 (Ha-23), 1.84 (Hb-23), 2.04 (Ha-24), 2.24 (Hb-24), 1.37 (s, CH_3-26), 1.39 (s, CH_3-27) [2]
^{13}C NMR (125 MHz, C_5D_5N) [2]:

Table 1

C-1	39.54	C-10	39.86	C-19	24.90
2	68.39	11	68.77	20	43.51
3	68.14	12	42.93	21	13.60

(*continued*)

Table 1 (continued)

4	32.88	13	47.53	22	73.92
5	52.49	14	83.87	23	25.65
6	204.00	15	32.11	24	42.52
7	122.17	16	26.67	25	69.65
8	163.80	17	48.26	26	30.25
9	42.88	18	16.69	27	30.02

References

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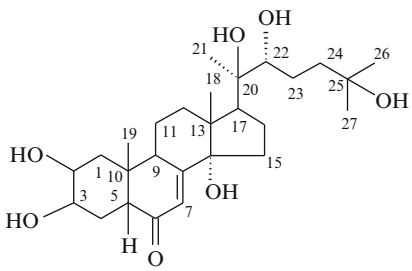
20-Hydroxyecdysone

CAS Registry Number: 5289-74-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Achyranthes aspera* [1–3], *A. bidentata* [4], *A. fauriei* [4–6], *A. japonica* [4, 7], *A. japonica, A. longifolia, A. mollicola* [4], *A. obtusilolia* [4, 8], *A. ogatai* [4], *A. rubrofusca* [4, 9], *Acrostichum aureum* [10], *A. speciosum* [10, 11], *Aerva tomentosa* [12], *Ajuga austarlis, A. bracteosa* [13], *A. chamaepitys* [14], *A. chameacistus* [15], *A. chia* [16–18], *A. ciliate* [19], *A. decumbens* [20, 21], *A. incisa* [20–22], *A. iva* [23–25], *A. japonica* [21], *A. laxmanni*, *A. linearifolia* [13], *A. macrosperma* var. *breviflora* [26], *A. multiflora* [10, 13], *A. nipponensis* [20, 21, 27], *A. remota* [15, 28], *A. reptans* [29, 30], *A. turkestanica* [18, 31, 32], *Anemone nemerosa, A. ranunculoides, A. tuberose* [33], *Asparagus dumosus* [34, 35], *A. falcatus, A. laricinus, A. ramosissimus, A. scandens* [36], *A. filicinus* [37], *Athyrium yokocense* [38, 39], *A. hipponicum* [40], *Atriplex nummularia* [41], *Axyris amaranthoides* [42], *Bassia quinquecuspus* [10], *Blandfordia graudiflora, B. punicea* [43], *Blechnum amabile* [44], *B. minus* [45], *B. nigrum* [46], *B. nipponicum* [44], *B. penna-marina* [45], *B. spicant* L [47], *Boerhaavia diffusa* [48], *Bosea yervamora* [49], *Briza maxima* [50], *Centaurea americana, C. dealbata, C. Rothrockii, C. rupestris* [51], *C. moschata* [52], *Cheilantes seiberi* [10], *Chenopodium album* [53, 54], *Ch. ambrosioides* [53], *Ch. bonus-henricus* [53, 55], *Ch. pallidicaule* [56], *Ch. polyspermum* [53], *Ch. quinoa* [57], *Ch. trigonon* [10], *Coronaria coreacea* [58], *C. flos-cuculi* [59], *Cryosinus hostatus* [40], *Cucubalis baccifer* [60], *Cyathea cooperi* [10], *Cyathula prostrata* [7, 61], *Cyanothis arachnoides* [62], *C. longifolia* [63], *C. vaga* [64, 65], *Cyclosorus acuminatus* [20], *Dacrydium intermedium* [66–68], *D. pierrei* [68], *Dianthus hoeltzeri* [69], *Diplazium sibiricum* [70], *Diploclisia glaucescens* [71, 72], *Doodia aspera* [10], *Dryopteris thelypteris* [73], *Elisanthe viscose* [74], *Eriophyton wallchii* [75], *Fibraurea chloroleuca* [76], *Froelichia floridana* [77], *Gastrolychnis apetala* [74], *Gomphrena celosiodes*, *G. haageana* [78], *Helleborus abchasicus, H. atrorubens, H. bocconei* [79], *H. caucasicus* [80], *H. cyclophyllus, H. dumentorum, H. dumentorum* ssp. *atrorubens*, *H. foetidus, H. guttatus, H. lividus, H. lividus* ssp. *corsicus, H. multifidus, H. niger, H. orientalis* [79], *H. odorus* ssp. Laxus [81], *H. odorus* Waldst and Kit, *H. purpurascens* [81], *H. torquatus* [82], *H. viridis* [79, 81], *H. viridis* ssp. *occidentalis* [79], *H. viridis* ssp. *viridis* [81], *Ipomoea calonyction* [83, 84], *Klaseopsis chinensis* [85], *Kochia scoparia* [86], *Lamium album* [87], *L. barbatum* [88], *L. maculatum, L. purpureum* [87], *Lastrea japonica* [60, 89, 90], *L. thelypteris* [89, 90], *Lemmaphyllum macrophyllum* [91, 92], *Leuzea carthamoides* [93], *Limnanthes alba* [94], *L. douglasii* [95], *Lloydia serotina* [96], *Lychnis arkwrigtii* [97], *L. chalcedonica* [20, 97, 98], *L. cognate* [97], *L. flos-cuculi* [99], *L. fulgens* [97, 100], *L. haageana* [97], *L. miqueliana* [20, 103],

L. sibirica, L. villosula, L. wilfordii [97], *Matteuccia struthiopteris* [73], *Melandrium turkestanicum* [102], *Microsorum maximum, M. punctatum* [103], *M. membranifolium* [104], *Microsorum scolopendria* [105], *Morus spp* [106], *Murdanna triquetra* [107], *Nierembergia hippomanica* [108], *Neocheiropteris ensata* [91], *Onoclea sensibilis* [20, 73, 89], *Onopordum acanthium* [109], *Osmunda asiatica, O. japonica* [89, 110], *O. regalis* [111], *Ourisia caespitosa, O. macrocarpa, O. macrophylla* [112], *Palisota hirsuta* [113], *Pandiaka involucrate* [12], *Paris formosona* [114], *P. luquonensis* [115], *P. polyphylla* [116], *P. quadrifolia* [117], *P. tetraphylla* [20], *P. verticillata* [118], *Paxillus atrotomentosus* [119], *Pellaea falcate* [10], *Penstemon venustus* [120], *Pfaffia iresinoides* [121, 122], *Plenasium banksiifolium* [123], *Pleopeltis thunbergiana* [91, 124], *Phymatodes novaezelandiae* [125], *Podocarpus amarus* [10], *P. andina* [10, 126], *P. campactus* [10], *P. chinensis* [127, 128], *P. dacrydioides* [10, 129], *P. dispermus, P. drougianus* [10], *P. elatus, P. elongata, P. falcate, P. ferrugineus* [10, 129], *P. macrophyllus* [127], *P. nakaii* [130, 131], *P. nivalis* [10], *P. nubigena* [127, 128], *P. spinulosus, P. totara* [10], *Polypodium aureum* [124], *P. japonicum* [20], *P. virginianum* [132], *P. vulgare* [133, 134], *Pteridium aquilinum* [135], *P. aquilinum* var. *latiusculum* [136], *Pteris cretica* [20], *Pulsatilla alpine, P. sulphurea* [137], *Rhagodia baccata* [138], *Rh. spinescens* [10], *Rhaponticum carthamoides* [139–141], *Rh. integrifolium* [142–144], *Rh. lyratum* [139], *Rh. nanum* [145], *Rh. pulchrum, Rh. scariosum* [139], *Rh. uniflorum* [146], *Schizea dichotoma* [10], *Serratula algida, S. centauroides* [147], *S. coronata* [148–150], *S. inermis* [109, 150, 151], *S. komarovii* [152], *S. procumbens, S. quinquefolia* [147], *S. sogdiana* [153], *S. strangulate* [154], *S. tinctoria* [155–157], *S. wolffii* [158], *S. xeranthemoides* [159], *Sesuvium portulacastrum* [1], *Sida acuta* [160], *S. carpinifolia* [161], *S. cordifolia* [162], *S. filicaulis* [160, 163], *S. rhombifolia* [160, 163, 164], *S. spinosa* [165], *Silene acaulis* [166], *S. altaica* [167], *S. antirrhina* [168], *S. apetala* [74], *S. armeria* [74, 167], *S. bashkirorum, S. bellidifolia* [169], *S. bergiana, S. borystenica* [74], *S. brachypoda* [169], *S. brahuica* [170, 171], *S. burchelli, S. campanulata, S. caramanica* [172], *S. catholica* [167], *S. caucasia* [172, 173], *S. chamarensis* [174], *S. chlorantha, S. chlorifolia, S. ciliata* [166, 167, 169, 173], *S. ciliate* var *graefteri* [169], *S. claviformis* [175], *S. coelirosa* [167, 169], *S. colorata*, *S. colorata* ssp. *trichocalysina* [166, 169, 173], *S. coronaria* [166, 173], *S. cretica* [53, 176], *S. damboldtiana, S. densiflora* [172, 173], *S. dioica* [177, 178], *S. disticha* [53, 176], *S. echinata* [179], *S. fetissovii* [74], *S. firma* [176], *S. flavescens* [167], *S. foliosa* [74], *S. frivaldszkyana* [53, 180], *S. fruticosa* [169, 181], *S. gallica, S. gallica* var. *quiquivulnera* [10, 169], *S. gebleriana* [74], *S. gigantea, S. goulimyi* [10, 169], *S. graefferi* [74], *S. graminifolia* [53, 174], *S. guntensis* [182, 183], *S. hifacensis* [169], *S. holopetala, S. incurvifolia* [74], *S. italica* [53, 169, 180, 184], *S. jenisseensis* [53, 174], *S. kungessana* [74], *S. latifolia* [182, 183], *S. linicola* [53, 176], *S. longicalycina* [182, 183], *S. mellifera* [169, 173, 180, 185], *S. micropetala* [53, 176], *S. mollissima* [73], *S. multicaulis* [167], *S. multiflora* [174], *S. nemoralis* [173], *S. nutans* [53, 186, 187], *S. obovata, S. odoratissima, S. oligantha* [74], *S. otites* [172, 178, 186], *S. otites* var. *parviflorus, S. paradoxa, S. parnassica, S. patula, S. portensis* [166, 169, 173, 181], *S. praemixta* [182, 183, 188], *S. pseudotites, S. psevdovelutina* [173], *S. pygmaea* [167], *S. quinquevulnera* [74], *S. radicosa* [169, 172], *S. regia* [168], *S. reichenbachii* [74, 167], *S. repens* [174], *S. roemeri, S. rubella* [169, 172], *S. saxifaga* [74], *S. scabrifolia* [189], *S. schafta, S. schischkinii* [74], *S. sieberi* [169], *S. schmuckeri* [167, 173], *S. secundiflora* [53, 176], *S. sendtneri* [166, 167, 173], *S. sericea* [74], *S. sobolevskajae, S. supina* [173, 174], *S. spergulofolia, S. squamigera, S. stenophylla, S. stylosa, S. sussamyrica* [74], *S. tatarica* [53, 173], *S. thessalonica* [185], *S. tomentella* [190], *S. turczaninovii* [74], *S. viridiflora* [191], *S. wallichiana* [192], *S. wolgensis* [74], *S. zawadskii* [167], *Spinacia oleracea* [55], *Stachyurus himalaicus* var. *himalaicus* [193], *S. praecox* [20, 27], *Stemmacantha uniflora* [194], *Stenochlaena polustrus* [10], *Struthiopteris nipponica* [20], *Tapinella panuoides* [195], *Taxus baccata* [128], *T. chinensis, T. cuspidate* [11, 129, 196], *Tectaria*

sp [10], *Thelypteris japonica* [73], *Trianthema galericulata* [10], *T. portulacastrum* [1], *Trillium erectum* [197], *T. smallii, T. tsconoski* [20], *Trisetum flavescens* [198], *Vitex agnus-castus* [199], *V. canescens* [200], *V. cymosa* [201], *V. fisherii* [202], *V. glabrata* [203], *V. leptobotrys* [72, 204], *V. madiensis* [205, 206], *V. megapotamica* [206–208], *V. pinnata* [206], *V. polygama* [209], *V. rehmanni* [206, 210], *V. scabra* [211], *V. sereti* [206, 210], *V. stickeri* [212, 213], *V. thyrsiflora* [206, 214]

$C_{27}H_{44}O_7$: 480.3087

Mp: 241–242°C (acetone) [69], 230–233°C (acetone) [119], 240–242°C [121], 243°C [133], 246°C (EtOAc-MeOH) [150], 234–235°C (acetone) [159]

$[\alpha]_D^{20}$ + 60.1 ± 2° (c 0.36, MeOH) [69], $[\alpha]_D^{22}$ + 62.1° (c 0.03, $CHCl_3$) [108], $[\alpha]_D^{20}$ + 60.7 ± 2° (c 0.55, MeOH) [117], $[\alpha]_D$ + 61.8° (c, MeOH) [133], $[\alpha]_D^{17}$ + 65.3° (c 1.0, MeOH) [150]

IR (KBr) ν_{max} cm^{-1}: 3560, 2860, 1660, 1640, 1460, 1445, 1320, 1270, 1230, 1215, 1075, 1060, 1030, 885, 682 [108], 3400, 1650 [121], 1642, 1608 [133], 3350–3450, 1660, 1615 [159], 3426, 1658, 1052 [195]

UV λ_{max}^{MeOH} nm: 242, 240, 300 [108], 244 (log ε 4.09) [133], 242 (log ε 3.98) [159]

EI-MS m/z: 462 $[M\text{-}H_2O]^+$ (2), 444 $[M\text{-}2H_2O]^+$ (8), 429 $[M\text{-}2H_2O\text{–}CH_3]^+$ (10), 426 $[M\text{-}3H_2O]^+$ (37), 411 $[M\text{-}3H_2O\text{–}CH_3]^+$ (5), 408 $[M\text{-}4H_2O]^+$ (17), 393 $[M\text{-}4H_2O\text{–}CH_3]^+$ (10), 363 $[M\text{-}117]^+$ (28), 345 (79), 344 (73), 327 (67), 309 (17), 301 (20), 300 (39), 285 (25), 173 (31), 161 (10), 143 (31), 125 (18), 117 (5), 99 (100), 81 (69), 71 (23), 69 (28), 59 (30), 57 (18), 56 (16), 55 (29), 43 (94) [108], 462 $[M\text{-}H_2O]^+$, 444, 426, 408, 393, 363, 345, 327, 301, 300, 99, 81, 69 [117]

FAB-MS m/z: 481 $[M + H]^+$ [4]; 503 $[M + Na]^+$ (25), 481 $[M + H]^+$ (85), 463 $[M + H\text{–}H_2O]^+$ (40), 445 $[M + H\text{–}2H_2O]^+$ (55), 427 $[M + H\text{–}3H_2O]^+$ (26), 309 (100) [195]

HR-MS m/z: for $C_{27}H_{47}O_7$ $[M + H]^+$ calcd. 481.3165, found 481.3233 [119]

^{1}H NMR (250 MHz, J/Hz, C_5D_5N): 1.91 (Ha-1), 2.14 (He-1), 4.17 (m, Ha-2), 4.21 (m, He-3), 1.80 (Ha-4), 2.02 (He-4), 3.01 (H-5), 6.25 (d, J = 2.5, H-7), 3.58 (m, H-9), 1.71 (Ha-11), 1.88 (He-11), 2.58 (ddd, J = 5.0, 13.0, 13.0, Ha-12), 1.95 (He-12), 2.14 (Ha-15), 1.89 (Hb-15), 2.44 (Ha-16), 2.08 (Hb-16), 3.00 (H-17), 1.21 (s, CH_3-18), 1.06 (s, CH_3-19), 1.58 (s, CH_3-21), 3.87 (m, H-22), 1.85 (Ha-23), 2.14 (Hb-23), 2.28 (Ha-24), 1.81 (Hb-24), 1.36 (s, CH_3-26), 1.36 (s, CH_3-27) [215]

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.43 (Ha-1), 1.78 (He-1), 3.83 (ddd, J = 3.0, 3.0, 12.0, Ha-2), 3.94 (ddd, J = 3.0, 3.0, 3.0, He-3), 1.65 (Ha-4), 1.75 (He-4), 2.38 (dd, J = 5.0, 12.0, H-5), 5.80 (d, J = 2.5, H-7), 3.14 (m, H-9), 1.65 (Ha-11), 1.78 (He-11), 2.13 (ddd, J = 5.0, 13.0, 13.0, Ha-12), 1.85 (He-12), 2.00 (Ha-15), 1.55 (Hb-15), 1.95 (Ha-16), 1.75 (Hb-16), 2.39 (m, H-17), 0.89 (s, CH_3-18), 0.96 (s, CH_3-19), 1.18 (s, CH_3-21), 3.33 (dd, J = 2.0, 11.0, H-22), 1.30 (Ha-23), 1.65 (Hb-23), 1.75 (Ha-24), 1.45 (Hb-24), 1.19 (s, CH_3-26), 1.20 (s, CH_3-27) [215]

^{1}H NMR (250 MHz, J/Hz, D_2O): 1.38 (Ha-1), 1.88 (He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.36 (t, H-5), 5.97 (d, J = 2.5, H-7), 3.11 (m, H-9), 1.73 (Ha-11), 1.86 (He-11), 1.96 (Ha-12), 1.90 (Ha-16), 1.75 (Hb-16), 2.34 (m, H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.22 (s, CH_3-21), 3.43 (d, J = 10.0, H-22), 1.31 (Ha-23), 1.66 (Hb-23), 1.24 (s, CH_3-26), 1.24 (s, CH_3-27) [215]

^{1}H NMR (250 MHz, J/Hz, $CDCl_3$): 1.39 (Ha-1), 1.86 (He-1), 3.89 (ddd, J = 3.3, 4.7, 11.7, Ha-2), 4.04 (m, He-3), 1.63 (Ha-4), 1.83 (He-4), 2.43 (dd, J = 4.5, 14.0, H-5), 5.84 (d, J = 2.5, H-7), 2.98 (m, H-9), 1.70 (Ha-11), 1.78 (He-11), 1.90 (Ha-15), 1.50 (Hb-15), 2.00 (Ha-16), 1.75 (Hb-16), 2.33 (m, H-17), 0.86 (s, CH_3-18), 0.98 (s, CH_3-19), 1.21 (s, CH_3-21), 3.44 (d, J = 10.0, H-22), 1.34 (Ha-23), 1.65 (Hb-23), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27) [215]

^{13}C NMR (62.9 MHz, C_5D_5N) [215]: **^{13}C NMR** (62.9 MHz, CD_3OD) [215]:

Table 1

C-1	38.09	C-15	31.88	C-1	37.46	C-15	31.76
2	68.33	16	21.61	2	68.72	16	21.54
3	68.23	17	50.28	3	68.54	17	50.54
4	32.53	18	17.99	4	32.81	18	18.02
5	51.48	19	24.55	5	51.78	19	24.38
6	203.56	20	77.09	6	206.39	20	77.94
7	121.79	21	21.77	7	122.12	21	21.09
8	166.11	22	77.75	8	167.88	22	78.41
9	34.67	23	27.59	9	35.14	23	27.39
10	38.80	24	42.64	10	39.28	24	42.37
11	21.29	25	69.86	11	21.54	25	71.29
12	32.19	26	30.10	12	32.52	26	29.12

(*continued*)

Table 1 (continued)

13	48.27	27	30.15	13	48.65	27	29.61
14	84.42			14	85.26		

Pharm./Biol.: *Brine shrimp* lethality assay ($LD_{50} = 640$ μg/mL) [51], antimicrobial tests: inactive >20 μg/ml; antimalarial test: inactive >4.76 μg/ml; antiprotozoal test: in active >40 μg/ml [164], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 7.5 \times 10^{-9}$ M [150, 216–219], $EC_{50} = 7.6 \times 10^{-9}$ M [220], *Galleria mellonella* bioassay: $ED_{50} = 7.8$ μg/g, *Sarcophaga bullata* bioassay: $ED_{50} = 2.6$ μg/g, *Dermestes vulpinus* bioassay: $ED_{50} = 42.0$ μg/g [221], *Drosophila melanogaster* in vitro bioassay: active [222], anabolic activity [223–237], antidiabetic activity [238–241], antiminflammatory activity [242], antiarrhythmic effect [243–247], antiulcer activity [248, 249], antitumor activity [250–253], antioxidant activity [254–259], antiepileptic effects [260], hypocholesterolemic effects [261, 262], hepatoprotective action [263–267], immunomodulating effects [268–271], sexual activity [272, 273], tonic effect [274–276], protein kinase activity [277–279], cytotoxic active for C6 rat glioma cells [280].

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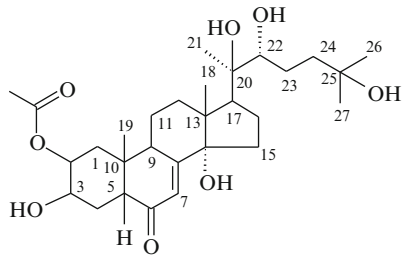
20-Hydroxyecdysone-2-Acetate

CAS Registry Number: 19536-25-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga macrosperma* var. *breviflora* [1], A. *reptans* var. *atropurpurea* [2], *Cyanothis arachinoidae* [3], *Klaseopsis chinensis* [4], *Leuzea carthamoides* [5], *Lychnis flos-cuculi* [6], *Serratula coronata* [7], *S. tinctoria* [8]

$C_{29}H_{46}O_8$: 522.3193

Mp: 145–147°C (EtOAc-petroleum) [9]

IR (KBr) ν_{max} cm^{-1}: 3432, 2964, 1719, 1653, 1446, 1379, 1258, 1150, 1048 [10]

UV λ_{max}^{EtOH} nm (ε): 243 (10700) [9]

EI-MS m/z: 486 $[M\text{-}2H_2O]^+$ (1), 471 (1), 468 (3), 450 (1), 405 (22), 388 (47), 387 (65), 370 (18), 369 (4), 345 (31), 327 (66), 309 (19) [10]

CI-MS m/z: 540, 523 $[M + H]^+$, 505, 487, 469, 405, 387, 345, 329, 327 [6], 540 $[M + NH_4]^+$, 522 $[M]^+$, 506, 498, 480, 422, 388, 308, 274, 222, 176, 122, 116, 94 [7]

TSP-MS m/z: 540 $[M + NH_4]^+$ (7), 523 $[M + H]^+$ (44), 522 $[M]^+$ (51), 504 $[M\text{-}H_2O]^+$ (81), 487 $[M + H\text{–}2H_2O]^+$ (100), 469 $[M + H\text{–}3H_2O]^+$ (55), 463 $[M + H\text{–}CH_3COOH]^+$ (50), 462 $[M\text{-}CH_3COOH]^+$ (30), 445 $[M + H\text{–}H_2O\text{–}CH_3COOH]^+$ (56), 427 $[M + H\text{–}2H_2O\text{–}CH_3COOH]^+$ (98), 389 $[M + H\text{–}H_2O\text{–(C-17/C-20)}]^+$ (44), 362 $[M + H\text{-(C-17/C-20)}]^+$ (44), 346 $[M\text{-}CH_3\text{-(C-17/C-20)}]^+$ (46) [2]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 5.25 (m, Ha-2), 4.29 (m, He-3), 3.04 (H-5), 6.25 (d, J = 2.4, H-7), 3.65 (m, H-9), 2.50 (Ha-12), 3.02 (H-17), 1.20 (s, CH_3-18), 1.07 (s, CH_3-19), 1.57 (s, CH_3-21), 3.86 (m, H-22), 1.38 (s, CH_3-26), 1.38 (s, CH_3-27), 1.93 (s, CH_3COO-2) [2]

^{1}H NMR (J/Hz, $CDCl_3$): 1.55 (Ha-1), 1.82 (He-1), 5.01 (m, Ha-2), 4.11 (m, He-3), 1.60 (Ha-4), 1.85 (He-4), 2.51 (dd, J = 4.0, 13.0, H-5), 5.84 (d, J = 2.5, H-7), 3.09 (m, H-9), 1.70 (Ha-11), 1.80 (He-11), 2.00 (Ha-16), 1.75 (Hb-16), 2.34 (m, H-17), 0.86 (s, CH_3-18), 0.99 (s, CH_3-19), 1.21 (s, CH_3-21), 3.44 (br d, J = 10.0, H-22), 1.35 (Ha-23), 1.65 (Hb-23), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27), 2.08 (s, CH_3COO-2) [6]

^{1}H NMR (500 MHz, J/Hz, D_2O): 5.07 (m, Ha-2), 4.22 (m, He-3), 2.42 (m, H-5), 5.99 (d, J = 2.5, H-7), 3.18 (m, H-9), 2.33 (t, J = 9.0, H-17), 0.87 (s, CH_3-18), 1.03 (s, CH_3-19), 1.24 (s, CH_3-21), 3.43 (d, J = 10.0, H-22), 1.23 (s, CH_3-26), 1.24 (s, CH_3-27), 2.13 (s, CH_3COO-2) [7]

^{13}C NMR (75 MHz, C_5D_5N) [2]:

Table 1

C-1	33.63	C-11	21.06	C-21	21.58
2	72.50	12	31.89	22	77.43
3	65.09	13	47.94	23	27.40
4	32.55	14	84.09	24	42.58
5	51.09	15	31.64	25	69.51
6	202.81	16	21.35	26	29.84
7	121.55	17	49.94	27	30.16

(*continued*)

Table 1 (continued)

8	166.20	18	17.78	$\underline{CH_3}COO$	21.10
9	34.25	19	24.19	$CH_3\underline{COO}$	170.40
10	38.70	20	76.75		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.2 \times 10^{-7}$ M [7], $EC_{50} = 4.0 \times 10^{-7}$ M [11–13].

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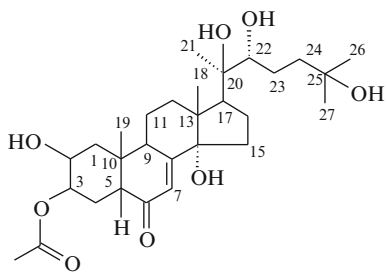
20-Hydroxyecdysone-3-Acetate

CAS Registry Number: 22961-68-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga macrosperma* var. *breviflora* [1], *Ajuga reptans* var. *atropurpurea* [2], *Cyanotis longifolia* [3], *Klaseopsis chinensis* [4], *Leuzea carthamoides* [5], *Lychnis flos-cuculi* [6, 7], *Serratula coronata* [8], *S. tinctoria* [9]

$C_{29}H_{46}O_8$: 522.3193

Mp: 210–211.5°C (EtOAc-petroleum) [10]

IR (KBr) ν_{max} cm^{-1}: 3432, 2964, 1719, 1653, 1446, 1379, 1258, 1150, 1048 [11]

UV λ_{max}^{EtOH} nm (ε): 243 (12200) [10]

EI-MS m/z: 522, 540, 523, 505, 487, 469, 405, 387, 364, 345, 329, 327, 322 [5], 486 $[M\text{-}2H_2O]^+$ (1), 471 (1), 468 (3), 450 (1), 405 (22), 388 (47), 387 (65), 370 (18), 369 (4), 345 (31), 327 (66), 309 (19) [11]

CI-MS m/z: 540 $[M + NH_4]^+$, 523 $[M + H]^+$, 505, 487, 469, 405, 387, 345, 329, 327 [6], 540 $[M + NH_4]^+$, 523 $[M + H]^+$, 505, 487, 469, 405, 387, 345, 329, 327 [7], 540 $[M + NH_4]^+$, 522 $[M]^+$, 506, 498, 480, 422, 388, 308, 274, 222, 176, 122, 116, 94 [8]

TSP-MS m/z: 540 $[M + NH_4]^+$ (60), 523 $[M + H]^+$ (100), 522 $[M]^+$ (37), 505 $[M + H\text{–}H_2O]^+$ (65), 487 $[M + H\text{–}2H_2O]^+$ (48), 469 $[M + H\text{–}3H_2O]^+$ (32), 463 $[M + H\text{–}CH_3COOH]^+$ (22), 462 $[M\text{-}CH_3COOH]^+$ (17), 445 $[M + H\text{–}H_2O\text{–}CH_3COOH]^+$ (21), 427 $[M + H\text{–}2H_2O\text{–}CH_3COOH]^+$ (28), 362 [M + H-(C-17/C-20)]$^+$ (21), 328 $[M\text{-}CH_3\text{–}H_2O\text{-}$(C-17/C-20)]$^+$ (21) [2]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 1.81 (Ha-1), 2.25 (He-1), 4.30 (m, Ha-2), 5.51 (m, He-3), 1.80 (Ha-4), 1.97 (He-4), 2.67 (dd, J = 3.9, 13.2, H-5), 6.24 (d, J = 2.1, H-7), 3.57 (br t, H-9), 2.57 (Ha-12), 3.00 (br t, J = 9.3, H-17), 1.23 (s, CH_3-18), 1.08 (s, CH_3-19), 1.60 (s, CH_3-21), 3.88 (br d, H-22), 1.37 (s, CH_3-26), 1.37 (s, CH_3-27), 1.98 (s, CH_3COO-3) [2]

^{1}H NMR (J/Hz, $CDCl_3$): 1.30 (Ha-1), 1.90 (He-1), 4.02 (m, Ha-2), 5.21 (m, He-3), 1.60 (Ha-4), 1.85 (He-4), 2.30 (H-5), 5.85 (d, J = 2.5, H-7), 3.01 (m, H-9), 1.70 (Ha-11), 1.80 (He-11), 2.00 (Ha-16), 1.75 (Hb-16), 2.33 (m, H-17), 0.87 (s, CH_3-18), 1.01 (s, CH_3-19), 1.21 (s, CH_3-21), 3.44 (d, J = 10.0, H-22), 1.35 (Ha-23), 1.65 (Hb-23), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27), 2.12 (s, CH_3COO-3) [6]

^{1}H NMR (J/Hz, CD_3OD): 1.30 (Ha-1), 1.90 (He-1), 4.02 (m, Ha-2), 5.21 (m, He-3), 1.60 (Ha-4), 1.85 (He-4), 2.30 (H-5), 5.85 (d, J = 2.5, H-7), 3.01

(m, H-9), 1.70 (Ha-11), 1.80 (He-11), 2.00 (Ha-16), 1.75 (Hb-16), 2.33 (m, H-17), 0.87 (s, CH_3-18), 1.01 (s, CH_3-19), 1.21 (s, CH_3-21), 3.44 (d, J = 10.0, H-22), 1.35 (Ha-23), 1.65 (Hb-23), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27), 2.12 (s, CH_3COO-3) [7]

^{1}H NMR (500 MHz, J/Hz, D_2O): 4.13 (m, Ha-2), 5.17 (m, He-3), 2.33 (m, H-5), 5.98 (d, J = 2.5, H-7), 3.12 (m, H-9), 2.33 (m, H-17), 0.87 (s, CH_3-18), 1.03 (s, CH_3-19), 1.24 (s, CH_3-21), 3.43 (d, J = 10.0, H-22), 1.23 (s, CH_3-26), 1.24 (s, CH_3-27), 2.17 (s, CH_3COO-3) [8]

^{13}C NMR (75 MHz, C_5D_5N) [2]:

Table 1

C-1	38.64	C-11	21.05	C-21	21.63
2	66.06	12	31.85	22	77.48
3	71.20	13	47.99	23	27.39
4	29.62	14	84.06	24	42.56
5	51.88	15	31.65	25	69.49
6	202.24	16	21.38	26	29.88
7	121.36	17	50.00	27	30.06
8	166.48	18	17.81	CH_3COO	21.05
9	34.35	19	24.21	CH_3COO	170.56
10	38.48	20	76.77		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.7 \times 10^{-7}$ M [12–14].

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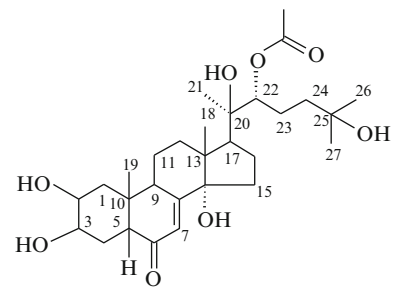
20-Hydroxyecdysone-22-Acetate

CAS Registry Number: 22799-02-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* [1], *Melandrium turkestanicum* [2], *Serratula tinctoria* [3], *S. coronata* [4], *Silene otites* [5]

$C_{29}H_{46}O_8$: 522.3193

Mp: 147–148°C [4], 145–147°C (EtOAc-petroleum) [6], 146–148°C (EtOAc-hexane) [7]

$[\alpha]_D^{15}$ + 49.5° (c 0.96, MeOH) [4]

IR (KBr) ν_{max} cm^{-1}: 3428, 2962, 1714, 1651, 1444, 1377, 1253, 1052 [7]

UV λ_{max}^{EtOH} nm (ε): 243 (10700) [6]

EI-MS m/z: 486 $[M\text{-}2H_2O]^+$ (0.4), 468 (2), 426 (13), 408 (3), 363 (15), 345 (15), 327 (14), 309 (4), 159 (8) [7]

CI-MS m/z: 540 $[M + H + NH_3]^+$, 523 $[M + H]^+$, 505, 487, 463 $[M + H\text{–}CH_3COOH]^+$, 445 $[M + H\text{–}CH_3COOH\text{–}H_2O]^+$, 427, 409, 363 $[M + H\text{-}(C\text{-}17/C\text{-}22)]^+$, 345 [5, 8]

^{1}H NMR (J/Hz, $CDCl_3$): 1.40 (Ha-1), 1.85 (He-1), 3.88 (m, Ha-2), 4.11 (m, He-3), 1.60 (Ha-4), 1.85 (He-4), 2.42 (dd, J = 4.0, 13.0, H-5), 5.84 (d, J = 2.5, H-7), 2.98 (m, H-9), 1.60 (Ha-11), 1.75 (He-11), 2.35 (m, H-17), 0.79 (s, CH_3-18), 0.97 (s, CH_3-19), 1.20 (s, CH_3-21), 4.84 (br d, J = 10.0, H-22), 1.50 (Ha-23), 1.70 (Hb-23), 1.22 (s, CH_3-26), 1.26 (s, CH_3-27), 2.10 (s, CH_3COO-22) [5]

^{1}H NMR (250 MHz, J/Hz, D_2O): 3.99 (m, Ha-2), 4.07 (m, He-3), 5.97 (d, J = 2.5, H-7), 3.11 (m, H-9), 0.86 (s, CH_3-18), 1.00 (s, CH_3-19), 1.34 (s, CH_3-21), 4.85 (d, H-22), 1.21 (s, CH_3-26), 1.21 (s, CH_3-27), 2.16 (s, CH_3COO-22) [6]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.19 (m, Ha-2), 4.23 (br s, He-3), 3.03 (m, H-5), 6.24 (d, J = 2.0, H-7), 3.59 (m, H-9), 2.97 (m, H-17), 1.16 (s, CH_3-18), 1.05 (s, CH_3-19), 1.62 (s, CH_3-21), 5.50 (br d, J = 9.5, H-22), 1.32 (s, CH_3-26), 1.33 (s, CH_3-27), 2.01 (s, CH_3COO-22) [7]

^{13}C NMR (75.0 MHz, CD_3OD) [4]:

Table 1

C-1	37.32 (t)	C-11	21.52 (t)	C-21	21.28 (q)
2	68.69 (d)	12	32.56 (t)	22	80.66 (d)
3	68.49 (d)	13		23	26.20 (t)
4	32.83 (t)	14	85.19 (s)	24	41.55(t)
5	51.74 (d)	15	31.78 (t)	25	71.46 (s)
6	206.47 (s)	16	21.52 (t)	26	28.97 (q)
7	122.20 (d)	17	50.87 (d)	27	29.49 (q)
8	167.97 (s)	18	18.13 (q)	CH_3COO	21.28 (q)
9	35.05 (d)	19	24.45 (q)	CH_3COO	173.42 (s)
10	39.26 (s)	20	77.53 (s)		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 2.0 \times 10^{-7}$ M [4], $EC_{50} = 4.0 \times 10^{-6}$ M [9], *Musca domestica* bioassay: $EC_{50} = 2.1 \times 10^{-5}$ M [10].

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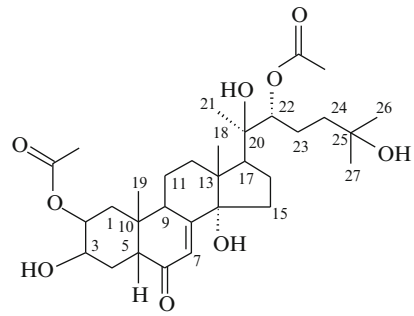
20-Hydroxyecdysone-2,22-Diacetate

CAS Registry Number: 22798-97-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula tinctoria* [1]

$C_{31}H_{48}O_9$: 564.3298

Mp: 160–162°C (EtOAc-hexane) [2]

IR (KBr) ν_{max} cm^{-1}: 3428, 2968, 1717, 1657, 1445, 1377, 1317, 1250, 1150, 1121, 1049, 948 [2]

EI-MS m/z: 486 $[M\text{-}AcOH\text{–}H_2O]^+$ (0.5), 471 (1), 468 (2), 453 (3), 405 (16), 388 (10), 387 (8), 345 (25), 327 (22), 309 (8), 292 (29), 291 (11), 159 (9) [2]

^{1}H NMR (250 MHz, J/Hz, $CDCl_3$): 5.02 (m, H-2), 4.12 (m, H-3), 2.52 (dd, J = 4.5, 14.0, H-5), 5.86 (d, J = 2.5, H-7), 3.09 (m, H-9), 2.35 (m, H-17), 0.84 (s, CH_3-18), 0.99 (s, CH_3-19), 1.26 (s, CH_3-21), 4.86 (dd, J = 2.0, 10.0, H-22), 1.21 (s, CH_3-26), 1.23 (s, CH_3-27), Other: 2.08 (s, CH_3COO-2), 2.10 (s, CH_3COO-22) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 5.23 (m, H-2), 4.28 (br s, H-3), 3.02 (dd, J = 4.3, 13.4, H-5), 6.21 (d, J = 2.1, H-7), 3.62 (m, H-9), 2.94 (m, H-17), 1.14 (s, CH_3-18), 1.05 (s, CH_3-19), 1.59 (s, CH_3-21), 5.48 (br d, J = 9.0, H-22), 1.34 (s, CH_3-26), 1.35 (s, CH_3-27), Other: 1.91 (s, CH_3COO-2), 2.01 (s, CH_3COO-22) [2]

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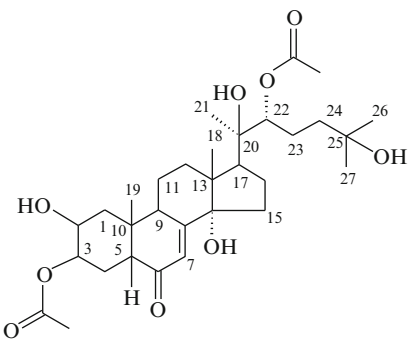
2. A. Suksamrarn, P. Pattanaprateep, Tetrahedron **51**, 10633 (1995)

20-Hydroxyecdysone-3,22-Diacetate

CAS Registry Number: 22798-99-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula tinctoria* [1]

$C_{31}H_{48}O_9$: 564.3298

^{1}H NMR (250 MHz, J/Hz, $CDCl_3$): 4.00 (m, H-2), 5.20 (m, H-3), 2.30 (H-5), 5.84 (d, J = 2.5, H-7), 3.01 (m, H-9), 2.34 (m, H-17), 0.84 (s, CH_3-18), 1.01 (s, CH_3-19), 1.24 (s, CH_3-21), 4.84 (dd, J = 2.0, 10.0, H-22), 1.21 (s, CH_3-26), 1.23 (s, CH_3-27), Other: 2.11 (s, CH_3COO-3), 2.10 (s, CH_3COO-22) [1]

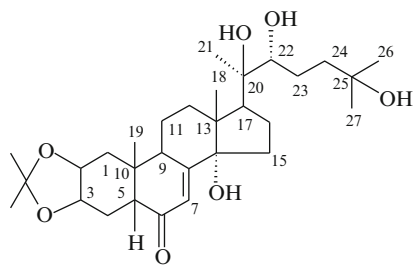
^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.29 (m, H-2), 5.42 (br s, H-3), 2.64 (dd, J = 4.0, 13.5, H-5), 6.19 (d, J = 2.1, H-7), 3.53 (m, H-9), 2.94 (m, H-17), 1.14 (s, CH_3-18), 1.05 (s, CH_3-19), 1.59 (s, CH_3-21), 5.48 (br d, J = 9.0, H-22), 1.31 (s, CH_3-26), 1.32 (s, CH_3-27), Other: 1.96 (s, CH_3COO-3), 2.00 (s, CH_3COO-22) [2]

References

1. D. Rudel, M. Bathori, J. Gharbi, J.P. Girault, I. Racz, K. Melis, K. Szendrei, R. Lafont, Planta Med. **58**, 358 (1992)
2. A. Suksamrarn, P. Pattanaprateep, Tetrahedron **51**, 10633 (1995)

20-Hydroxyecdysone-2,3-Acetonide

CAS Registry Number: 113866-76-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga turkestanica* [1], *Cyanotis arachnoidea* [2], *Rhaponticum carthamoides* [3, 4], *Silene scabrifolia* [5]

$C_{30}H_{48}O_7$: 520.3400

Mp: 232–233°C (EtOAc–MeOH) [4], 242–244°C (EtOAc) [5], 269–271°C [6]

$[\alpha]_D^{20}$ + 56.4 ± 2° (c 0.9, MeOH) [4], $[\alpha]_D^{20}$ + 59.2 ± 2° (c 0.3, MeOH) [5]

IR (KBr) ν_{max} cm^{-1}: 3460–3500, 1643 [4], 3458, 2966, 1641, 1449, 1379, 1243, 1224, 1150, 1057 [6]

UV λ_{max}^{EtOH} nm (log ε): 244 (4.08) [4]

EI-MS m/z: 520 $[M]^+$ (1), 505 (7), 502 (2), 487 (3), 484 (2), 469 (5), 466 (4), 451 (4), 403 (72), 385 (100), 371 (7), 368 (6), 360 (7), 345 (10), 327 (36), 309 (9),269 (13), 143 (12), 99 (36), 81 (24) [4], 466 $[M\text{-}3H_2O]^+$ (2), 403 (16), 386 (21), 385 (25), 269 (17), 161 (14), 117 (5), 99 (100) [6]

^{1}H NMR (500 MHz, J/Hz, Me_2CO-d_6): 4.23 (m, Ha-2), 4.24 (m, He-3), 5.70 (d, J = 2.7, H-7), 2.96 (ddd, J = 2.7, 7.0, 11.6, H-9), 2.45 (t, J = 9.0, H-17), 0.91 (s, CH_3-18), 0.96 (s, CH_3-19), 1.19 (s, CH_3-21), 3.36 (br d, J = 2.0, 10.3, H-22), 1.18 (s, CH_3-26), 1.17 (s, CH_3-27), Other: 1.26 and 1.42 (s, 2,3-iPr) [3]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 5.99 (br s, H-7), 1.04 (s, CH_3-18), 0.88 (s, CH_3-19), 1.42 (s, CH_3-21), 1.23 (s, CH_3-26), 1.23 (s, CH_3-27), Other: 1.23 and 1.42 (s, 2,3-iPr) [4]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.17 (m, H-2), 4.08 (m, H-3), 2.55 (m, H-5), 6.20 (d, J = 2.0, H-7), 3.15 (m, H-9), 3.00 (t, J = 8.9, H-17), 1.19 (s, CH_3-18), 0.99 (s, CH_3-19), 1.60 (s, CH_3-21), 3.87 (br d, J = 8.1, H-22), 1.35 (s, CH_3-26), 1.35 (s, CH_3-27), Other: 1.31 and 1.55 (s, 2,3-iPr) [6]

^{1}H NMR (300 MHz, J/Hz, DMSO-d_6): 1.12 (Ha-1), 1.87 (He-1), 4.20 (m, H-2), 4.20 (m, H-3), 1.50 (Ha-4), 1.82 (He-4), 2.11 (dd, J = 5.0, 12.0, H-5), 5.64 (br s, H-7), 2.81 (dd, J = 8.0, 12.0, H-9), 1.48 (Ha-11), 1.65 (He-11), 2.03 (ddd, J = 4.0, 13.0, 13.0, Ha-12), 1.75 (He-12), 1.48 (Ha-15), 1.80 (Hb-15), 1.65 (Ha-16), 1.85 (Hb-16), 2.27 (dd, J = 8.5, 10.0, H-17), 0.78 (s, CH_3-18), 0.88 (s, CH_3-19), 1.07 (s, CH_3-21), 3.13 (d, J = 10.0, H-22), 1.12 (Ha-23), 1.47 (Hb-23), 1.65 (Ha-24), 1.28 (Hb-24), 1.07 (s, CH_3-26), 1.08 (s, CH_3-27), Other: 1.28 and 1.41 (s, 2,3-iPr) [7]

^{1}H NMR (300 MHz, J/Hz, $CDCl_3$): 4.25 (m, H-2), 4.25 (m, H-3), 2.32 (m, H-5), 5.83 (d, J = 2.5, H-7), 2.84 (ddd, J = 2.5, 9.0, 12.0, H-9), 2.32 (m, H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.22 (s, CH_3-21), 3.48 (d, J = 10.0, H-22), 1.27 (s, CH_3-26), 1.27 (s, CH_3-27), Other: 1.33 and 1.50 (s, 2,3-iPr) [7]

^{13}C NMR (125.7 MHz, CD_3OD) [7]: **^{13}C NMR** (75 MHz, DMSO-d_6) [7]:

Table 1

C-1	38.7	C-15	31.7	C-1	37.3	C-15	30.2
2	73.5	16	21.5	2	71.4	16	20.4
3	73.2	17	50.5	3	71.2	17	48.7
4	27.7	18	18.0	4	26.0	18	17.1
5	52.5	19	24.0	5	50.5	19	23.2
6	205.6	20	77.9	6	201.6	20	75.7
7	121.8	21	21.0	7	120.1	21	21.9
8	167.2	22	78.4	8	164.8	22	76.2
9	35.7	23	27.3	9	33.9	23	26.1
10	38.9	24	42.9	10	37.2	24	41.4
11	21.6	25	71.3	11	20.1	25	68.7
12	32.5	26	29.7	12	30.9	26	29.0
13		27	28.9	13	47.1	27	29.9
14	85.2	2,3-iPr	109.5,	14	82.9	2,3-iPr	107.3,
			28.8,				26.4,
			26.6				28.4

^{13}C NMR (75 MHz, $CDCl_3$) [7]:

Table 2

C-1	37.6	C-11	20.6	C-21	20.7
2	72.2	12	31.2	22	76.7
3	71.7	13	47.7	23	26.1
4	26.7	14	84.8	24	40.8
5	50.8	15	31.6	25	70.6
6	202.8	16	20.5	26	29.3
7	121.5	17	49.1	27	30.0
8	163.3	18	17.4	2,3-iPr	108.3
9	34.6	19	23.6		26.3
10	37.8	20	76.9		28.5

Pharm./Biol.: *Sarcophaga bullata* bioassay: inactive [7].

References

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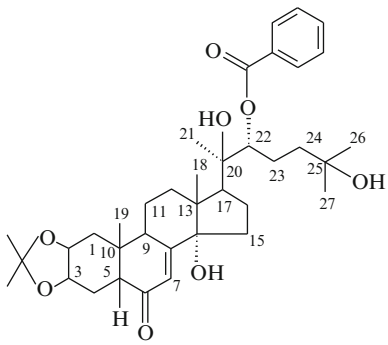
20-Hydroxyecdysone-2,3-Acetonide-22-Benzoate

CAS Registry Number: 103654-40-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene scabrifolia* [1, 2]

$C_{37}H_{52}O_8$: 624.3662

Mp: 258–260°C (MeOH–H_2O), 242–244°C ($CHCl_3$) [1, 2]

$[\alpha]_D^{20}$ + 34.2 ± 2° (c 0.60, MeOH) [1], $[\alpha]_D^{20}$ + 33.3 ± 2° (c 0.66, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3455, 1725, 1710, 1645, 1610, 1585, 1265, 715 [2]

EI-MS m/z: 624 $[M]^+$ (0.02), 609 (15), 591 (0.9), 573 (0.9), 502 (0.9), 487 (4), 466 (22), 451 (21), 403 (46), 385 (21), 327 (21), 290 (22), 267 (22), 163 (28), 139 (37), 126 (53), 122 (52), 105 (100), 99 (37), 81 (22), 77 (23), 59 (22), 43 (52) [2]

^{1}H NMR (100 MHz, J/Hz, $CDCl_3$): 4.20 (m, He-2), 4.20 (m, He-3), 5.80 (br m, H-7), 0.84 (s, CH_3-18), 0.93 (s, CH_3-19), 1.32 (s, CH_3-21), 5.13 (m, H-22), 1.18 (s, CH_3-26), 1.18 (s, CH_3-27), Other: Ar: 7.47 (m, 3H), 8.00 (m, 2H) [2]

Pharm./Biol.: *Galleria mellonela* bioassay: EC_{50} = 31.2 μg/g, *Sarcophaga bullata* bioassay: EC_{50} = 104 μg/g [3].

References

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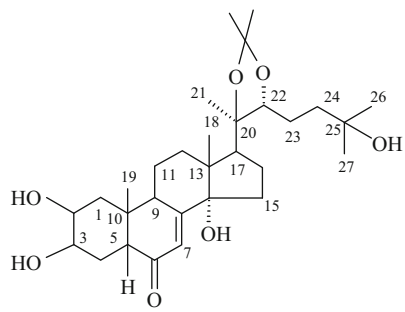
3. K. Slama, N.K. Abubakirov, M.B. Gorovits, U.A. Baltaev, Z. Saatov, Insect Biochem. Mol. Biol. **23**, 181 (1993)

20-Hydroxyecdysone-20,22-Acetonide

CAS Registry Number: 22798-96-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum carthamoides* [1, 2], *Serratula coronata* [3], *S. strangulata* [4], *S. wolffii* [5], *Sida spinosa* [6], *Silene scabrifolia* [7], *Stachyurus himalaicus* var. *himalaicus* [8], *Vitex strickeri* [9]

$C_{30}H_{48}O_7$: 520.3400

Mp: 227–229°C (EtOAc–MeOH) [2], 220–222°C (EtOAc-hexane) [5], 221–222°C (EtOAc-hexane) [7], 222–224°C [10], 222.5–223.5°C (acetone-petroleum) [11]

$[\alpha]_D^{20}$ + 60.1 ± 2° (c 1.3, MeOH) [2], $[\alpha]_D^{20}$ + 58.9 ± 2° (c 0.32, MeOH) [5], $[\alpha]_D^{20}$ + 59.2 ± 2° (c 0.32, MeOH) [7], $[\alpha]_D^{19}$ + 60° (c 0.5, MeOH) [11]

IR (KBr) ν_{max} cm^{-1}: 3400–3465, 1660 [2], 3400–3460, 1660 [7], 3420, 2974, 1649, 1454, 1377, 1216, 1170, 1103, 1057, 1001, 877 [10]

UV λ_{max}^{EtOH} nm: 243 (log ε 4.01) [2], 244 (log ε 4.00) [7], 242 (ε 12300) [11]

EI-MS m/z: 520 $[M]^+$, 505 (2), 502 (1), 487 (4), 469 (5), 445 (4), 427 (29), 409 (13), 363 (100), 353 (15), 345 (26), 329 (10), 327 (9), 320 (4), 300 (32), 201 (13), 143 (11), 99 (19), 81 (26) [2], 486 $[M\text{-}2H_2O]^+$ (2), 426 (10), 396 (23), 363 (15), 345 (23), 328 (24) [5], 487 $[M\text{-}CH_3\text{–}H_2O]^+$ (0.4), 469 (0.5), 363 (5), 143 (17), 125 (15) [10]

FAB-MS m/z: 521 $[M + H]^+$ [9]

CI/D m/z: 538 $[M + NH_4]^+$, 521 $[M + H]^+$, 503 $[M + H\text{–}H_2O]^+$, 490, 480, 464, 447, 429, 413, 394, 391, 380, 364, 279, 230, 212, 178, 136, 124 [3]

^{1}H NMR (500 MHz, J/Hz, $Me_2CO\text{-}d_6$): 3.82 (m, Ha-2), 3.90 (m, He-3), 2.33 (dd, J = 6.0, 11.5, H-5), 5.72 (d, J = 2.7, H-7), 3.16 (ddd, J = 2.7, 7.0, 11.7, H-9), 2.37 (dd, J = 8.0, 9.5, H-17), 0.83 (s, CH_3-18), 0.93 (s, CH_3-19), 1.18 (s, CH_3-21), 3.48 (t, J = 3.0, H-22), 1.18 (s, CH_3-26), 1.17 (s, CH_3-27), Other: 1.36 and 1.30 (s, 20,22-iPr) [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.38 (t, J = 13.4, Ha-1), 1.88 (m, He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (t, Ha-4), 1.75 (t, He-4), 2.36 (t, H-5), 5.98 (d, J = 2.5, H-7), 3.11 (m, H-9), 1.71 (m, Ha-11), 1.86 (m, He-11), 1.95 (m, Ha-12), 1.75 (m, He-12), 2.05 (m, Ha-15), 1.65 (m, Hb-15), 1.95 (m, Ha-16), 2.02 (m, Hb-16), 2.27 (t, J = 9.0, H-17), 0.831 (s, CH_3-18), 1.00 (s, CH_3-19), 1.25 (s, CH_3-21), 3.88 (m, H-22), 1.58 (m, Ha-23), 1.58 (m, Hb-23), 1.70 (m, Ha-24), 1.60 (m, Hb-24), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27), Other: 1.42 and 1.49 (s, 20,22-iPr) [3]

^{1}H NMR (300 MHz, J/Hz, CD_3OD): 1.48 (Ha-1), 1.82 (He-1), 3.77 (Ha-2), 3.90 (He-3), 1.69 (Ha-4), 1.75 (He-4), 2.26 (dd, J = 5.0, 10.5, H-5), 5.75 (d, J = 2.5, H-7), 3.16 (ddd, J = 2.2, 7.0, 10.2, H-9), 1.69 (Ha-11), 1.82 (He-11), 2.05 (ddd, J = 4.4, 12.0, 12.0, Ha-12), 1.87 (He-12), 1.98 (Ha-15), 1.53 (Hb-15), 1.92 (Ha-16), 1.75 (Hb-16), 2.33 (dd, J = 6.0, 9.5, H-17), 0.76 (s, CH_3-18), 1.12 (s, CH_3-19), 0.90 (s, CH_3-21), 3.54 (br d, H-22), 1.36 (dddd, J = 4.3, 10.8, 13.8, 16.0, Ha-23), 1.72 (Hb-23), 1.80 (Ha-24), 1.45 (Hb-24), 1.14 (s, CH_3-26), 1.22 (s, CH_3-27), Other: 1.26 and 1.33 (s, 20,22-iPr) [6]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.89 (Ha-1), 1.94 (He-1), 3.95 (m, Ha-2), 4.22 (m, He-3), 1.76 (Ha-4), 2.02 (He-4), 3.00 (dd, J = 5.0, 12.0, H-5), 6.25 (H-7), 3.55 (m, H-9), 1.72 (Ha-11), 1.88 (He-11), 2.50 (ddd, J = 5.0, 10.0, 10.0, Ha-12), 2.10 (He-12), 1.90 (Ha-15), 2.10 (Hb-15), 2.24 (Ha-16), 2.12 (Hb-16), 2.77 (H-17), 1.02 (s, CH_3-18), 1.34 (s, CH_3-19), 1.06 (s, CH_3-21), 4.15 (m, H-22), 1.90 (Ha-23), 2.16 (Hb-23), 2.10 (Ha-24), 1.74 (Hb-24), 1.33 (s, CH_3-26), 1.37 (s, CH_3-27), Other: 1.46 and 1.55 (s, 20,22-iPr) [9]

^{1}H NMR (300 MHz, J/Hz, $CDCl_3$): 3.80 (m, Ha-2), 4.03 (br s, He-3), 2.39 (m, H-5), 5.84 (d, J = 2.1, H-7), 2.97 (m, H-9), 2.39 (m, H-17), 0.78 (s, CH_3-18), 0.96 (s, CH_3-19), 1.15 (s, CH_3-21), 3.60 (m, H-22), 1.20 (s, CH_3-26), 1.29 (s, CH_3-27), Other: 1.32 and 1.36 (s, 20,22-iPr) [10]

^{13}C NMR (125.7 MHz, CD_3OD) [1]: **^{13}C NMR** (125 MHz, D_2O) [3]:

Table 1

C-1	37.4	C-16	22.4	C-1	36.4 (t)	C-16	
2	68.7	17	50.5	2	68.3 (d)	17	50.3 (d)
3	68.5	18	17.7	3	68.2 (d)	18	18.0 (q)
4	32.9	19	24.5	4	32.3 (t)	19	24.2 (q)
5	51.8	20	85.9	5	51.4 (d)	20	87.3 (s)
6	206.5	21	22.6	6		21	22.3 (q)
7	122.1	22	83.3	7	122.1 (d)	22	83.4 (d)
8	167.7	23	24.7	8		23	24.6 (t)
9	35.1	24	42.2	9	34.9 (d)	24	41.7 (t)
10	39.2	25	71.1	10	39.1 (s)	25	72.7 (s)
11	21.5	26	29.5	11		26	28.5 (q)
12	32.3	27	29.3	12	31.8 (t)	27	29.1 (q)
13		20,22-iPr	26.6	13	47.9 (s)	20,22-iPr	27.3 (q)
14	85.3		28.8	14	86.4 (s)		29.4 (q)
15	31.7		109.5	15	31.4 (t)		109.0 (s)

^{13}C NMR (125 MHz, C_5D_5N) [9]:

Table 2

C-1	38.01	C-11	21.05	C-21	22.40
2	68.12	12	32.43	22	85.57
3	68.07	13	47.88	23	24.39
4	31.72	14	84.18	24	42.17
5	51.36	15	31.66	25	69.24
6	203.50	16	22.11	26	30.07
7	121.81	17	50.03	27	29.87
8	165.42	18	17.29	20,22-iPr	27.17
9	34.45	19	24.44		29.42
10	38.62	20	82.12		106.91

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.1 \times 10^{-6}$ M [3], *Sarcophaga bullata* bioassay: $ED_{50} = 0.3$ µg/g [12].

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2. U.A. Baltaev, N.K. Abubakirov, Chem. Nat. Comp. **23**, 565 (1987)
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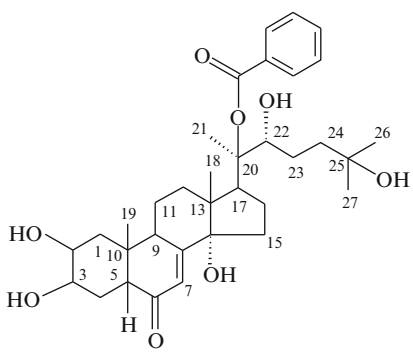
20-Hydroxyecdysone-20-Benzoate

CAS Registry Number: 114317-60-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene tatarica* [1]

$C_{34}H_{48}O_8$: 584.3349

Mp: 232–233°C (EtOAc–CH_3OH) [1]

$[\alpha]_D^{20}$ + 34.4 ± 2° (c 0.9, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3400–3480, 1710, 1665, 1610, 1590, 1287, 720 [1]

UV λ_{max}^{EtOH} nm (log ε): 232 (4.08) [1]

EI-MS m/z: 485 (5), 470 (1), 468 (1), 452 (2), 444 (5), 439 (15), 426 (35), 411 (10), 408 (5), 393 (5), 353 (5), 301 (5), 122 (100), 105 (90), 77 (40) [1]

^{1}H NMR (60 MHz, C_5D_5N): 4.10 (m, H-2), 4.10 (m, H-3), 6.12 (br s, H-7), 3.45 (m, H-9), 1.08 (s, CH_3-18), 0.97 (s, CH_3-19), 1.65 (s, CH_3-21), 3.66 (m, H-22), 1.22 (s, CH_3-26), 1.22 (s, CH_3-27) [1]

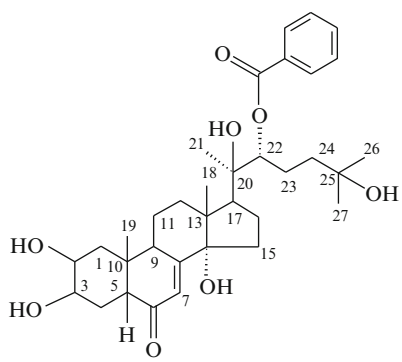
Pharm./Biol.: *Galleria mellonella* bioassay: ED_{50} = 15.6 μg/g, *Sarcophaga bullata* bioassay: ED_{50} = 2.6 μg/g [2].

References

1. U.A. Baltaev, V.N. Darmogray, N.K. Abubakirov, Chem. Nat. Comp. **23**, 706 (1987)
2. K. Slama, N.K. Abubakirov, M.B. Gorovits, U.A. Baltaev, Z. Saatov, Insect. Biochem. Molec. Biol. **23**, 181 (1993)

20-Hydroxyecdysone-22-Benzoate

CAS Registry Number: 103654-38-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene otites* [1], *S. scabrifolia* [2], *S. wallichiana* [3]

$C_{34}H_{48}O_8$: 584.3349
Mp: 202–205°C (MeOH-H_2O) [2, 3]
$[\alpha]_D^{20}$ + 45.0 ± 2° (c 1.1, MeOH) [2, 3]
IR (KBr) ν_{max} cm^{-1}: 3420–3470, 1660, 1710, 1285, 1610, 1587, 720 [2]
UV λ_{max}^{EtOH} nm (log ε): 235 (4.36) [2]
EI-MS m/z: 584 $[M]^+$ (0.02), 566 (0.1), 548 (0.2), 533 (0.4), 530 (0.3), 462 (0.8), 445 (7), 444 (23), 429 (23), 427 (39), 426 (84), 411 (56), 408 (23), 393 (24), 375 (24), 363 (39), 357 (24), 353 (25), 345 (24), 329 (24), 327 (23), 315 (24), 301 (56), 300 (54), 251 (39), 250 (84), 249 (80), 232 (24), 231 (24), 152 (80), 126 (81), 122 (81), 109 (56), 105 (100), 99 (52), 81 (52), 77 (53), 69 (52), 59 (52), 51 (53), 43 (53) [2]
^{1}H NMR (100 MHz, $CDCl_3$): 3.94 (m, Ha-2), 3.94 (m, He-3), 5.78 (br s, H-7), 0.83 (s, CH_3-18), 0.89 (s, CH_3-19), 1.33 (s, CH_3-21), 5.06 (m, H-22), 1.11 (s, CH_3-26), 1.11 (s, CH_3-27), Other: Ar: 7.39 (m, 3H), 7.99 (m, 2H) [2]
^{1}H NMR (C_5D_5N): 4.0–4.3 (m, H-2), 4.0–4.3 (m, H-3), 6.22 (br s, H-7), 3.60 (m, H-9), 1.21 (s, CH_3-18), 1.10 (s, CH_3-19), 1.78 (s, CH_3-21), 5.76 (m, H-22), 1.32 (s, CH_3-26), 1.32 (s, CH_3-27), Other: Ar: 7.40 (3H), 8.27 (2H) [3]
^{13}C NMR (C_5D_5N) [3]:

Table 1

C-1	37.9	C-12	31.7	C-23	26.2
2	68.1	13	48.2	24	41.8
3	68.1	14	84.1	25	69.2
4	32.4	15	32.0	26	29.6
5	51.3	16	22.5	27	30.0
6	203.4	17	50.6	COO	167.0
7	121.8	18	17.8	1′	131.8
8	165.8	19	24.4	2′, 6′	130.0
9	34.4	20	76.6	3′, 5′	128.7
10	38.7	21	21.1	4′	133.0
11	21.6	22	81.3		

Pharm./Biol.: *Galleria mellonela* bioassay: 7.8 µg/g, *Sarcophaga bullata* bioassay: 2.6 µg/g [4].

References

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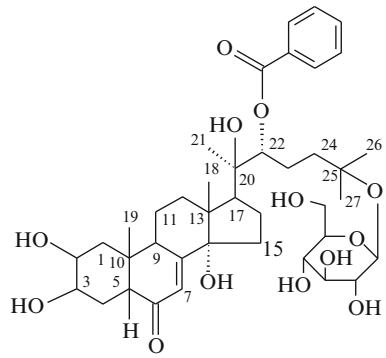
2. Z. Saatov, M.B. Gorovits, S. Melibaev, N.K. Abubakirov, Chem. Nat. Comp. **22**, 71 (1986)
3. Z. Saatov, N.D. Abdullaev, M.B. Gorovits, N.K. Abubakirov, Chem. Nat. Comp. **26**, 301 (1990)
4. K. Slama, N.K. Abubakirov, M.B. Gorovits, U.A. Baltaev, Z. Saatov, Insect Biochem. Mol. Biol. **23**, 181 (1993)

20-Hydroxyecdysone-22-Benzoate-25-Glucoside

CAS Registry Number: 128552-87-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Silene otites* [1]
$C_{40}H_{58}O_{13}$: 746.3877
CI-MS m/z: 747 $[M + H]^+$, 729, 643, 625, 607, 463, 445, 427, 363, 345 [1]
^{1}H NMR (J/Hz, CD_3OD): 3.82 (m, Ha-2), 3.94 (m, He-3), 2.37 (dd, J = 5.0, 12.0, H-5), 5.81 (d, J = 2.0, H-7), 3.10–3.20 (H-9), 2.46 (m, H-17), 0.88 (s, CH_3-18), 0.95 (s, CH_3-19), 1.41 (s, CH_3-21), 5.14 (br d, J = 10.0, H-22), 1.22 (s, CH_3-26), 1.22 (s, CH_3-27), Other: C_6H_5CO: 7.49 (t, J = 7.0, 2H), 8.08 (t, J = 7.0, 2H), 7.61 (t, J = 7.0, 1H), β-D-Glcp′: 4.41 (d, J = 7.6, H-1), 3.12 (H-2), 3.78 (dd, J = 2.2, 12.3, Ha-6), 3.62 (Hb-6) [1]

References

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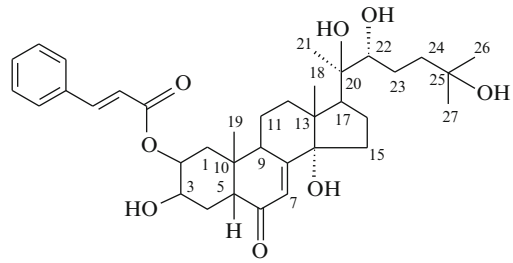
20-Hydroxyecdysone-2-Cinnamate

CAS Registry Number: 38147-15-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Dacrydium intermedium* [1, 2]

$C_{36}H_{50}O_8$: 610.3505

Mp: 254–256°C [1], 258–260°C [2]

IR (KBr) ν_{max} cm^{-1}: 1700, 1645 [1], 3400, 1700, 1646 [2]

UV λ_{max}^{EtOH} nm (ε): 276 (21000), 237 (20100), 223 (19200) [1]

EI-MS m/z: 610 $[M]^+$, 592 $[M\text{-}H_2O]^+$, 574 $[M\text{-}2H_2O]^+$, 556 $[M\text{-}3H_2O]^+$, 494 [M-116 (side chain)]$^+$, 426 [M-148 (cinnamic acid) - 36]$^+$, 345 [M-148-117]$^+$, 324, 148 (cinnamic acid), 147 (base peak) (cinnamoyl-oxy), 131 (cinnamoyl) [1, 2]

HR-MS m/z: for $C_{36}H_{44}O_5$ $[M\text{-}3H_2O]^+$ calcd. 556 [2]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 5.42 (m, Ha-2), 4.37 (m, He-3), 6.25 (H-7), 1.21 (s, CH_3-18), 1.11 (s, CH_3-19), 1.57 (s, CH_3-21), 1.38 (s, CH_3-26), 1.38 (s, CH_3-27), 7.38 (Ar), 6.60 (d, J = 16.0, vinylic), 7.92 (d, J = 16.0, vinylic) [2]

Pharm./Biol.: *Musca* bioassay: 1/10th the moulting hormone activity of 20-hydroxyecdysone [1].

References

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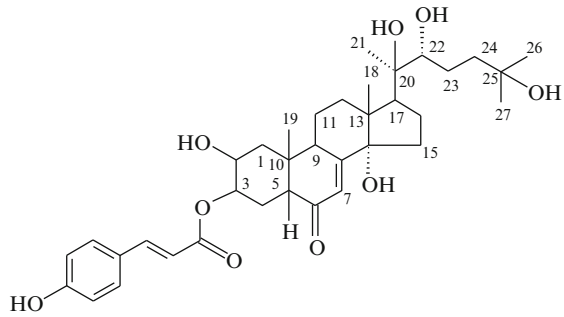
20-Hydroxyecdysone-3-p-Coumarate

CAS Registry Number: 83462-53-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Dacrydium intermedium* [1]

$C_{36}H_{50}O_9$: 626.3454

Mp: 265–267°C [1]

IR (KBr) ν_{max} cm^{-1}: 3400, 1720, 1645 [1]

UV λ_{max}^{EtOH} nm (ε): 315 (22500), 300 (19000), 250 (sh.), 238 (19000), 212 (12800) [1]

EI-MS m/z: 608 $[M\text{-}H_2O]^+$, 590 $[M\text{-}2H_2O]^+$, 572 $[M\text{-}3H_2O]^+$, 510 [M-116 (side chain)]$^+$, 345, 327, 147 (base peak) (coumaroyl) [1]

HR-MS m/z: for $C_{36}H_{44}O_6$ $[M\text{-}3H_2O]^+$ calcd. 572 [1]

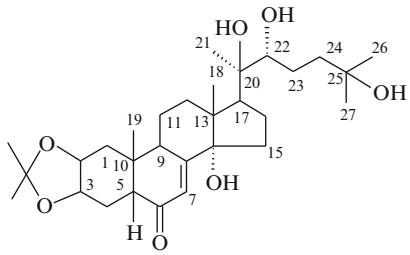
^{1}H NMR (100 MHz, J/Hz, CD_3OD): 4.10 (m, Ha-2), 5.26 (m, He-3), 5.85 (H-7), 0.90 (s, CH_3-18), 1.03 (s, CH_3-19), 1.16 (s, CH_3-21), 1.16 (s, CH_3-26), 1.16 (s, CH_3-27), Other: 6.83 (d, J = 9.0, Ar), 7.50 (d, J = 9.0, Ar), 6.43 (d, J = 16.0, vinylic), 7.71 (d, J = 16.0, vinylic) [1]

References

1. G.B. Russel, P.G. Fenemore, D.H.S. Horn, E.J. Middleton, Aust. J. Chem. **25**, 1935 (1972)

20-Hydroxyecdysone-2,3;20,22-Diacetonide

CAS Registry Number: 22798-98-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotis arachnoidea* [1], *Leuzea carthamoides* [2], *Serratula coronata* [3], *S. wolffii* [4]

$C_{33}H_{52}O_7$: 560.3713

Mp: 230–232°C (acetone-ether) [4], 233–234°C (acetone-hexane) [5], 234–236°C (dec.) (acetone-petroleum) [6]

$[\alpha]_D^{20}$ + 36.8 ± 2° (c 0.30, MeOH) [4], $[\alpha]_D^{19}$ + 37° (c 0.5) [6]

IR (KBr) ν_{max} cm^{-1}: 3404, 2966, 1640, 1444, 1378, 1315, 1243, 1224, 1151, 1062, 951, 753 [5]

UV λ_{max}^{EtOH} nm (ε): 242 (11700) [6]

EI-MS m/z: 560 (1), 545 (12), 527 (10), 509 (5), 403 (100), 385 (25), 341 (20) [1], 545 $[M + CH_3]^+$ (4), 527 (3), 509 (2), 467 (7), 403 (7), 143 (20), 125 (28) [5]

FAB-MS m/z: 583 (20), 561 $[M + H]^+$ (20), 543 (25), 485 (28), 427 (10) [2]

^{1}H NMR (500 MHz, J/Hz, Me_2CO-d_6): 4.23 (m, Ha-2), 4.25 (m, He-3), 5.71 (d, J = 2.7, H-7), 2.95 (ddd, J = 2.7, 7.0, 12.0, H-9), 2.37 (dd, J = 8.5, 9.5, H-17), 0.83 (s, CH_3-18), 0.95 (s, CH_3-19), 1.18 (s, CH_3-21), 3.68 (dd, J = 5.2, 7.5, H-22), 1.18 (s, CH_3-26), 1.17 (s, CH_3-27), Other: 1.25 and 1.42 (s, 2,3-iPr), 1.30 and 1.36 (s, 20,22-iPr) [2]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.16 (m, H-2), 4.09 (br s, H-3), 2.54 (dd, J = 4.7, 12.5, H-5), 6.18 (d, J = 2.2, H-7), 3.15 (m, H-9), 2.75 (t, J = 8.3, H-17), 0.98 (s, CH_3-18), 0.97 (s, CH_3-19), 1.54 (s, CH_3-21), 3.93 (dd, J = 2.5, 9.5, H-22), 1.32 (s, CH_3-26), 1.32 (s, CH_3-27), Other: 1.34 and 1.53 (s, 2,3-iPr), 1.30 and 1.44 (s, 20,22-iPr) [5]

^{1}H NMR (300 MHz, J/Hz, $CDCl_3$): 4.23 (m, H-2), 4.26 (br s, H-3), 2.36 (dd, J = 4.7, 12.5, H-5), 5.83 (d, J = 2.2, H-7), 2.80 (m, H-9), 2.22 (t, J = 8.0, H-17), 0.78 (s, CH_3-18), 0.98 (s, CH_3-19), 1.16 (s, CH_3-21), 3.65 (dd, J = 2.5, 9.5, H-22), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27), Other: 1.33 and 1.41 (s, 2,3-iPr), 1.33 and 1.49 (s, 20,22-iPr) [5]

^{13}C NMR (125.7 MHz, CD_3OD) [2]:

Table 1

C-1	38.7	C-11	21.6	C-21	22.6
2	73.5	12	32.3	22	83.3
3	73.1	13		23	24.7
4	27.7	14	85.2	24	42.2
5	52.5	15	31.6	25	71.1
6	205.6	16	21.4	26	29.5
7	121.8	17	50.5	27	29.4
8	166.9	18	17.7	2,3-iPr	26.6, 28.8, 109.5
				20,22-iPr	27.2, 29.0, 108.0
9	35.8	19	24.0		
10	38.8	20	85.3		

Pharm./Biol.: *Drosophila melanogaster* bioassay: inactive [7].

References

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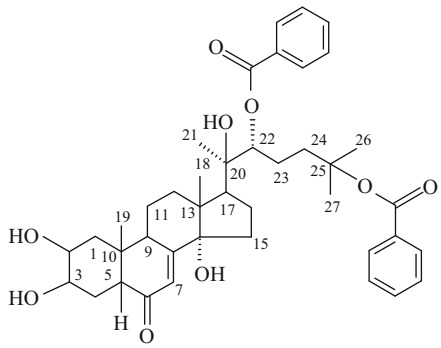
20-Hydroxyecdysone-22,25-Dibenzoate

CAS Registry Number: 148031-28-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene scabrifolia* [1]

$C_{41}H_{52}O_9$: 688.3611

Mp: amorphous [1]

$[\alpha]_D^{20}$ + 80.1 ± 2° (c 0.22, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3460–3520, 1720, 1670, 1295, 1610, 1590, 730 [1]

UV λ_{max}^{EtOH} nm (log ε): 235 (4.10) [1]

EI-MS m/z: 548 $[M\text{-}C_6H_5COOH\text{–}H_2O]^+$ (0.8), 530 (1), 515 (0.2), 512 (0.2), 479 (0.2), 467 (0.2), 462 (0.4), 461 (0.4), 450 (2.8), 444 (5), 426 (28), 408 (30), 393 (13), 375 (30), 363 (42), 357 (28), 345 (28), 329 (13), 327 (14), 301 (30), 300 (30), 250 (50), 163 (30), 122 (98), 105 (100), 99 (17), 81 (30), 77 (54), 51 (50) [1]

^{1}H NMR (C_5D_5N): 3.9–4.3 (m, H-2), 3.9–4.3 (m, H-3), 6.22 (br s, H-7), 3.52 (m, H-9), 1.18 (s, CH_3-18), 1.06 (s, CH_3-19), 1.73 (s, CH_3-21), 5.66 (m, H-22), 1.54 (s, CH_3-26), 1.54 (s, CH_3-27), Other: Ar: 7.39 (6H), 8.25 (4H) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

C-1	37.9	C-12	31.8	C-23	25.4
2	68.0	13	48.0	24	39.1

(*continued*)

Table 1 (continued)

3	68.0	14	83.8	25	82.3
4	32.2	15	31.8	26	25.6
5	51.4	16	22.2	27	25.9
6	202.2	17	50.4	COO	166.9
7	121.0	18	17.5	1′	131.7, 131.7
8	165.5	19	24.3	2′, 6′	129.8, 130.1
9	34.3	20	76.5	3′, 5′	128.8, 128.8
10	38.7	21	21.2	4′	133.0, 133.1
11	21.5	22	80.9		

Pharm./Biol.: *Galleria mellonela* bioassay: EC_{50} = 31.2 μg/g, *Sarcophaga bullata* bioassay: EC_{50} = 104 μg/g [2].

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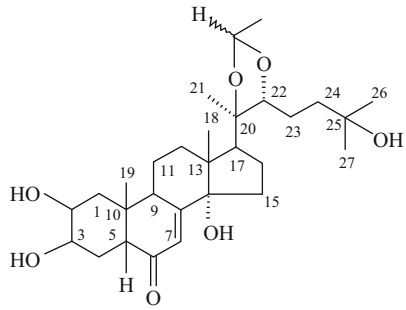
2. K. Slama, N.K. Abubakirov, M.B. Gorovits, U.A. Baltaev, Z. Saatov, Insect Biochem. Mol. Biol. **23**, 181 (1993)

20-Hydroxyecdysone-20,22-O-R-Ethylidene

CAS Registry Number: 802986-10-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula coronata* [1]

$C_{29}H_{46}O_7$: 506.3243

CI-MS m/z: 524 $[M + H + NH_3]^+$, 507 $[M + H]^+$, 489, 471, 463, 445, 427, 411, 409, 391, 370, 346, 279, 272, 246, 299, 187, 160, 143, 124, 99 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.38 (t, J = 13.4, Ha-1), 1.88 (m, He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (t, Ha-4), 1.75 (t, He-4), 2.36 (t, H-5), 5.97 (d, J = 2.5, H-7), 3.11 (m, H-9), 1.73 (m, Ha-11), 1.86 (m, He-11), 1.95 (m, Ha-12), 1.75 (m, He-12), 1.65 (m, Ha-15), 2.05 (m, Hb-15), 1.88 (m, Ha-16), 1.74 (m, Hb-16), 2.31 (t, J = 9.0, H-17), 0.86 (s, CH_3-18), 1.00 (s, CH_3-19), 1.25 (s, CH_3-21), 3.85 (m, H-22), 1.63 (m, Ha-23), 1.63 (m, Hb-23), 1.75 (m, Ha-24), 1.75 (m, Hb-24), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27), Other: –OC(Me)O: 1.40 (d, J = 5.0), min: 1.35 (d, J = 5.0), OCHO: 5.16 (q, J = 5.0), min: 5.36 (q, J = 5.0) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

C-1	36.1 (t)	C-11		C-21	24.9 (q)
2	68.5 (d)	12	31.7 (t)	22	86.1 (d)
3	68.5 (d)	13	48.2 (s)	23	
4	32.3 (t)	14	86.1 (s)	24	41.7 (t)
5	51.4 (d)	15		25	72.8 (s)
6		16		26	29.0 (q)
7	122.1 (d)	17	51.1 (d)	27	29.0 (q)
8		18	18.0 (q)	$CHCH_3$	102.5 (d)
9	34.9 (d)	19	24.3 (q)		21.3 (q)
10	39.1 (s)	20	87.3 (s)		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.3 \times 10^{-7}$ M [1].

References

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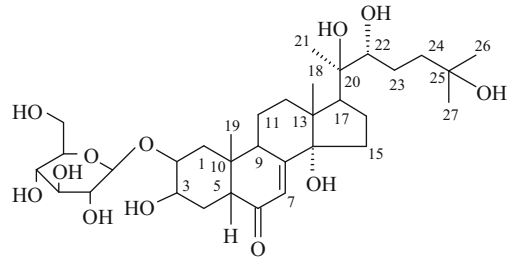
20-Hydroxyecdysone-2-Glucoside

CAS Registry Number: 163916-39-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Sida filicaulis* [1], *Xerophyllum tenax* [2]

$C_{33}H_{54}O_{12}$: 642.3615

Mp: 180–183°C [3]

IR (KBr) ν_{max} cm^{-1}: 3420, 1652, 1050, 1031 [3]

UV λ_{max}^{MeOH} nm (log ε): 244 (4.09), 320 (3.15) [2]

EI-MS m/z: 463 $[M\text{-}C_6H_{11}O_6]^+$, 462, 446, 444, 443, 428, 427, 426, 408, 376, 368, 346, 345, 344, 330, 329, 328, 327, 326, 302, 301, 300, 285, 284, 267, 266, 189, 188, 179 $[C_6H_{11}O_6]^+$, 178, 177, 163, 159, 113, 99, 69, 55 [2]

FAB-MS m/z (glycerol): 641 $[M\text{-}H]^-$, 479 [2]

FAB-MS m/z: 665 $[M + Na]^+$, 647 $[M + Na–H_2O]^+$, 643 $[M + H]^+$, 625 $[M + H–H_2O]^+$ [3]

HR-MS m/z: for $C_{33}H_{55}O_{12}$ $[M + H]^+$ calcd. 643.3694, found 643.3656 [3]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.94 (Ha-1), 2.16 (He-1), 4.29 (m, Ha-2), 4.36 (m, He-3), 2.04 (Ha-4), 1.80 (He-4), 2.96 (H-5), 6.23 (d, J = 2.3, H-7), 1.72 (Ha-11), 1.89 (He-11), 2.46 (ddd, J = 5.0, 13.0, 13.0, Ha-12), 1.92 (He-12), 2.14 (Ha-15), 1.90 (Hb-15), 2.43 (Ha-16), 2.04 (Hb-16), 2.94 (H-17), 1.19 (s, CH_3-18), 1.03 (s, CH_3-19), 1.58 (s, CH_3-21), 3.87 (br d, J = 10.0, H-22), 2.12 (Ha-23), 1.85 (Hb-23), 2.28 (Ha-24), 1.83 (Hb-24), 1.39 (s, CH_3-26), 1.39 (s, CH_3-27), Other: β-D-Glcp′:

5.02 (d, J = 7.9, H-1), 4.05 (t, J = 8.0, H-2), 4.32 (H-3), 4.25 (t, J = 9.0, H-4), 4.00 (m, H-5), 4.36 (Ha-6), 4.54 (d, J = 11.8, Hb-6) [2]

^{1}H NMR (500 MHz, J/Hz, acetone-d_6): 4.00 (ddd, J = 3.0, 4.0, 12.0, Ha-2), 4.13 (br q, J = 3.0, He-3), 2.33 (dd, J = 6.0, 10.5, H-5), 5.71 (d, J = 2.5, H-7), 3.14 (m, H-9), 2.45 (t, J = 9.0, H-17), 0.910 (s, CH_3-18), 0.945 (s, CH_3-19), 1.196 (s, CH_3-21), 3.36 (dd, J = 1.5, 10.0, H-22), 1.179 (s, CH_3-26), 1.170 (s, CH_3-27), Other: β-D-Glcp′: 4.53 (d, J = 7.8, H-1), 3.18 (dd, J = 7.8, 9.0, H-2), 3.40 (t, J = 9.0, H-3), 3.36 (t, J = 9.0, H-4), 3.32 (m, J = 2.5, 5.0, 9.0, H-5), 3.84 (dd, J = 2.5, 11.5, Ha-6), 3.67 (dd, J = 5.0, 11.5, Hb-6) [3]

^{13}C NMR (100 MHz, C_5D_5N) [2]: **^{13}C NMR** (125.7 MHz, CD_3OD) [3]:

Table 1

C-1	35.9	C-18	17.8	C-1	36.11	C-18	18.05
2	75.8	19	24.2	2	76.40	19	24.23
3	64.6	20	76.8	3	65.98	20	77.92
4	31.3	21	21.6	4	32.10	21	21.05
5	51.3	22	77.5	5	51.84	22	78.42
6	202.9	23	27.6	6	206.16	23	27.33
7	121.7	24	42.6	7	122.11	24	42.38
8	166.0	25	69.5	8	168.14	25	71.29
9	34.4	26	30.0	9	34.99	26	29.71
10	38.6	27	30.1	10	39.51	27	28.95
11	20.9	Glc′-1	101.7	11	21.50	Glc′-1	102.68
12	31.9	2	75.4	12	32.47	2	75.19
13	48.0	3	78.7	13	48.57	3	77.87
14	84.1	4	71.6	14	85.23	4	71.64
15	31.6	5	78.6	15	31.74	5	77.97
16	21.4	6	62.7	16	21.38	6	62.71
17	50.0			17	50.52		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.3 \times 10^{-4}$ M [2], $EC_{50} = 2.0 \times 10^{-4}$ M [4], $EC_{50} = 2.0 \times 10^{-5}$ M [5–7].

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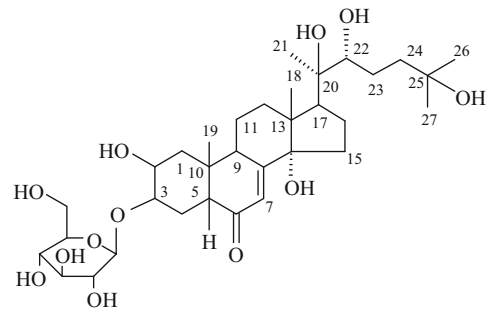
20-Hydroxyecdysone-3-Glucoside

CAS Registry Number: 128365-93-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Asparagus scandens* [1], *Helleborus orientalis* [2], *H. torquatus* [3], *Sida filicaulis* [4], *S. rhombifolia* [4, 5], *Silene otites* [6], *Trisetum flavescens* [7]

$C_{33}H_{54}O_{12}$: 642.3615

Mp: 297–300°C (MeOH) [8]

IR (KBr) ν_{max} cm^{-1}: 3404, 1770, 1577, 1087 [2], 3419, 1660, 1051 [8]

EIS-MS m/z: 647.3 $[M + Na–H_2O]^+$, 503.2 [aglycone + Na]$^+$ [2]

FAB-MS m/z: 623.3 $[M–H–H_2O]^-$ [2], 665 $[M + Na]^+$, 647 $[M + Na–H_2O]^+$, 643 $[M + H]^+$, 625 $[M + H–H_2O]^+$ [8]

HR-MS m/z: for $C_{33}H_{55}O_{12}$ $[M + H]^+$ calcd. 643.3694, found 643.3658 [8]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 4.02 (dt, J = 5.0, 11.5, Ha-2), 4.13 (br q, J = 2.0, He-3), 2.38 (m, H-5), 5.80 (d, J = 2.5, H-7), 3.15 (m, H-9), 2.38 (m, H-17), 0.88 (s, CH_3-18), 0.96 (s, CH_3-19), 1.18 (s, CH_3-21), 3.30 (m, H-22), 1.19 (s, CH_3-26), 1.19 (s, CH_3-27), Other: β-D-Glcp′: 4.48 (d, J = 8.0, H-1), 3.20 (t, J = 8.5, H-2), 3.36 (t, J = 9.0, H-3), 3.33

(t, J = 9.8, H-4), 3.30 (m, H-5), 3.69 (dd, J = 5.2, 11.8, Ha-6), 3.87 (d, J = 10.0, Hb-6) [6]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.11 (dt, J = 3.0, 3.0, 12.3, Ha-2), 4.31 (br q, J = 3.0, He-3), 2.93 (dd, J = 3.5, 13.3, H-5), 6.21 (d, J = 2.3, H-7), 3.53 (m, H-9), 2.98 (t, J = 9.0, H-17), 1.170 (s, CH_3-18), 0.858 (s, CH_3-19), 1.576 (s, CH_3-21), 3.87 (dd, J = 1.0, 9.6, H-22), 1.374 (s, CH_3-26), 1.374 (s, CH_3-27), Other: β-D-Glcp′: 4.90 (d, J = 7.8, H-1), 4.03 (dd, J = 7.8, 9.0, H-2), 4.22 (t, J = 9.0, 9.0, H-3), 4.18 (t, J = 9.0, 9.0, H-4), 3.92 (ddd, J = 2.2, 5.8, 9.0, H-5), 4.53 (dd, J = 2.2, 11.7, Ha-6), 4.30 (dd, J = 5.8, 11.7, Hb-6) [8]

^{13}C NMR (125.7 MHz, CD_3OD) [6]: **^{13}C NMR** (125.7 MHz, C_5D_5N) [8]:

Table 1

C-1	36.1	C-18	18.1	C-1	38.99	C-18	17.99
2	66.0	19	24.2	2	68.34	19	24.12
3	76.4	20	77.9	3	77.39	20	77.03
4	32.5	21	21.1	4	30.80	21	21.80
5	51.9	22	78.4	5	51.41	22	77.73
6	206.2	23	27.4	6	203.56	23	27.56
7	122.1	24	42.4	7	121.69	24	42.73
8	168.1	25	71.7	8	166.75	25	69.79
9	35.0	26	29.0	9	34.35	26	30.12
10	39.5	27	29.7	10	38.73	27	30.04
11	21.5	Glc′-1	102.7	11	21.15	Glc′-1	103.98
12	32.1	2	75.2	12	32.03	2	75.03
13	48.4	3	77.9	13	48.15	3	78.74
14	85.3	4	71.3	14	84.30	4	71.73
15	31.7	5	78.0	15	31.80	5	78.54
16	21.4	6	62.7	16	21.57	6	62.70
17	50.5			17	50.20		

Pharm./Biol.: Antimicrobial tests: inactive > 20 μg/ml; antimalarial test: inactive >4.76 μg/ml; antiprotozoal test: in active >40 μg/ml [5], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.3 \times 10^{-5}$ M [9–12].

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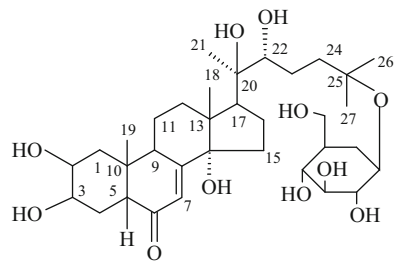
20-Hydroxyecdysone-25-Glucoside

CAS Registry Number: 116424-80-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Asparagus scandens* [1], *Pfaffia iresinoides* [2], *Silene otites* [3], *Trisetum flavescens* [4]

$C_{33}H_{54}O_{12}$: 642.3615

Mp: 158–163°C [5]

$[\alpha]_D^{15}$ + 26.0° (c 1.5, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3450, 1650 [1], 3420, 1652, 1052 [5]

UV λ_{max}^{EtOH} nm (log ε): 243 (4.02) [2]

FAB-MS m/z: 665 $[M + Na]^+$, 647 $[M + Na–H_2O]^+$, 643 $[M + H]^+$, 625 $[M + H–H_2O]^+$ [5]

HR-MS m/z: for $C_{33}H_{54}O_{12}$ $[M + H]^+$ calcd. 643.3694, found 643.3656 [5]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 2.99 (dd, J = 4.0, 13.2, H-5), 6.21 (d, J = 2.2, H-7), 3.55 (br t, J = 9.0,

H-9), 2.52 (dt, J = 4.2, 13.2, Ha-12), 2.42 (q, J = 10.4, Ha-16), 2.94 (t, J = 8.8, H-17), 1.18 (s, CH_3-18), 1.04 (s, CH_3-19), 1.56 (s, CH_3-21), 3.83 (br d, J = 9.4, H-22), 1.31 (s, CH_3-26), 1.37 (s, CH_3-27), Other: β-D-Glcp′: 5.00 (d, J = 7.6, H-1) [2]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 3.85 (m, Ha-2), 3.92 (m, He-3), 5.72 (d, J = 2.5, H-7), 3.16 (m, H-9), 2.46 (t, J = 9.0, H-17), 0.910 (s, CH_3-18), 0.939 (s, CH_3-19), 1.192 (s, CH_3-21), 3.35 (br d, J = 10.0, H-22), 1.245 (s, CH_3-26), 1.216 (s, CH_3-27), Other: β-D-Glcp′: 4.50 (d, J = 7.7, H-1), 3.14 (dd, J = 7.7, 9.0, H-2), 3.41 (t, J = 9.0, H-3), 3.24 (t, J = 9.0, H-4), 3.31 (ddd, J = 2.5, 6.7, 9.0, H-5), 3.84 (dd, J = 2.5, 11.7, Ha-6), 3.58 (dd, J = 6.7, 11.7, Hb-6) [5]

^{13}C NMR (100 MHz, C_5D_5N) [2]: **^{13}C NMR** (125.7 MHz, CD_3OD) [5]:

Table 1

C-1	37.9	C-18	17.9	C-1	37.36	C-18	18.06
2	68.1	19	24.4	2	68.70	19	24.40
3	68.0	20	76.9	3	68.51	20	77.96
4	32.4	21	21.7	4	32.86	21	21.06
5	51.4	22	77.7	5	51.78	22	78.41
6	203.7	23	26.6	6	206.44	23	26.69
7	121.7	24	39.8	7	122.17	24	40.10
8	166.1	25	77.4	8	167.92	25	78.67
9	34.4	26	27.5	9	122.17	26	27.35
10	38.6	27	27.6	10	39.27	27	27.35
11	21.1	Glc′-1	98.8	11	21.46	Glc′-1	98.66
12	32.0	2	75.5	12	32.50	2	75.30
13	48.1	3	78.7	13	49.00	3	78.19
14	84.3	4	72.1	14	85.37	4	71.87
15	31.7	5	78.5	15	31.76	5	79.00
16	21.4	6	63.4	16	21.46	6	63.13
17	50.0			17	50.43		

Pharm./Biol.: *Lucilia cuprina* test: ca 1/100 to 20-hydroxyecdysone [2], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 8.5 \times 10^{-6}$ M [6–9].

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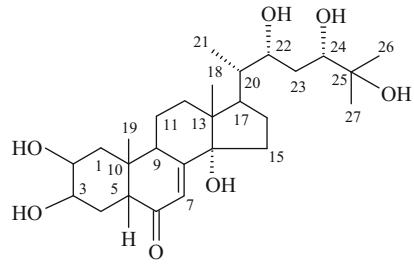
7. M. Bathori, J.P. Girault, H. Kalasz, I. Mathe, L. Dinan, R. Lafont, Arch. Insect Biochem. Physiol. **41**, 1 (1999)
8. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
9. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

24-Hydroxyecdysone

CAS Registry Number: 156558-81-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polypodium vulgare* [1]

$C_{27}H_{44}O_7$: 480.3087

TSP-MS m/z: 498 $[M + H + NH_3]^+$, 481 $[M + H]^+$, 463 $[M + H–H_2O]^+$, 445 $[M + H–2H_2O]^+$, 427 $[M + H–3H_2O]^+$ [1]

^{1}H NMR (J/Hz, C_5D_5N): 4.13 (Ha-2), 4.20 (He-3), 3.01 (dd, J = 15.0, 3.8, H-5), 6.22 (d, J = 2.4, H-7), 3.54 (m, Ha-9), 2.98 (t, J = 8.4, H-17), 0.68 (s, CH_3-18), 1.05 (s, CH_3-19), 1.26 (d, J = 6.6, CH_3-21), 4.08 (H-22), 4.41 (d, J = 2.4, H-24), 1.49 (s, CH_3-26), 1.43 (s, CH_3-27) [1]

^{13}C NMR (C_5D_5N): [1]:

Table 1

C-1	37.97	C-10	38.73	C-19	24.52
2	68.14	11	21.09	20	42.54
3	68.08	12	31.36	21	13.80
4	32.50	13	47.56	22	74.93
5	51.44	14	83.77	23	30.67
6	203.69	15	31.95	24	80.85

(*continued*)

Table 1 (continued)

7	121.61	16	26.64	25	72.31
8	165.70	17	48.17	26	26.74
9	34.48	18	15.81	27	25.54

References

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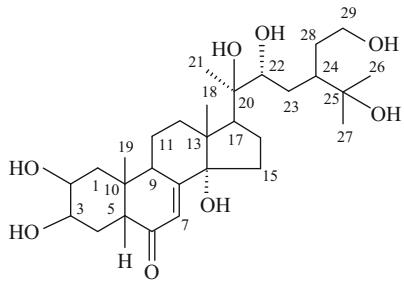
24-(2-Hydroxyethyl)-20-Hydroxyecdysone

CAS Registry Number: 573951-21-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula strangulata* [1]

$C_{29}H_{48}O_8$: 524.3349

Mp: 242–244°C [1]

$[\alpha]_D^{24}$ + 65.2° (c 0.04, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3387, 1642 [1]

UV λ_{max}^{EtOH} nm (log ε): 252 (4.00) [1]

FAB-MS m/z: 525 $[M + H]^+$, 510, 507, 492, 389, 371, 189, 171, 145, 127 [1]

HR-EI-MS m/z: for $C_{29}H_{48}O_8$ $[M]^+$ calcd. 524.3349, found 524.3341 [1]

^{1}H NMR (J/Hz, DMSO-d_6): 1.70–1.84 (m, He-1), 3.81–3.85 (m, Ha-2), 3.92–3.96 (m, He-3), 1.61–1.68 (m, Ha-4), 1.70–1.84 (m, He-4), 2.37 (dd, J = 5.0, 12.0, H-5), 5.61 (s, H-7), 3.14–3.18 (m, H-9), 1.61–1.68 (Ha-11), 1.70–1.84 (m, He-11), 2.10–2.16 (m, Ha-12), 1.84–1.90 (m, He-12), 1.97–2.03 (m, Ha-15), 1.52–1.58 (m, Hb-15), 1.97–2.03 (m, Ha-16), 1.70–1.84 (m, Hb-16), 2.27–2.41 (m, H-17), 0.89 (s, CH_3-18), 0.96 (s, CH_3-19), 1.19 (s, CH_3-21), 3.41–3.44 (m, H-22), 1.41–1.45 (m, Ha-23), 1.52–1.58 (m, Hb-23), 1.45–1.55 (m, H-24), 1.20 (s, CH_3-26), 1.21 (s, CH_3-27), 1.37–1.40 (m, 2H-28), 3.20–3.26 (m, 2H-29) [1]

^{13}C NMR (DMSO-d_6) [1]:

Table 1

C-1	36.59	C-11	20.04	C-21	20.92
2	66.56	12	30.26	22	75.60
3	66.74	13	46.62	23	26.06
4	31.49	14	82.95	24	36.55
5	50.50	15	30.82	25	68.66
6	202.59	16	20.22	26	28.97
7	120.41	17	48.65	27	29.92
8	165.15	18	17.07	28	41.34
9	33.15	19	23.81	29	66.06
10	37.58	20	76.18		

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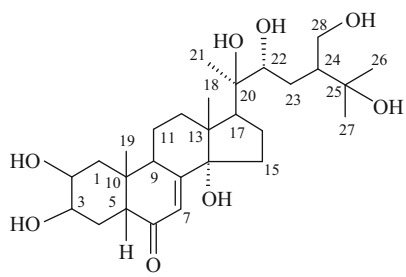
20-Hydroxy-24-Hydroxymethylecdysone

CAS Registry Number: 556064-20-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Sida spinosa* [1]
$C_{28}H_{46}O_8$: 510.3192
Mp: amorphous [1]
IR (KBr) ν_{max} cm^{-1}: 3505–3375, 1662, 1033 [1]
EI-MS m/z: 460 $[M-51]^+$ (2), 446 (3), 363 (37), 345 (49), 327 (27), 301 (15), 269 (17), 250 (49), 231 (16), 191 (13), 183 (11), 173 (27), 165 (9), 147 (28), 129 (18), 81 (100) [1]
FAB-MS m/z: 511 $[M + H]^+$ [1]
^{1}H NMR (300 MHz, J/Hz, DMSO): 1.26 (t, J = 9.0, Ha-1), 1.60 (He-1), 3.60 (Ha-2), 3.74 (He-3), 1.48 (Ha-4), 1.60 (He-4), 2.20 (dd, J = 13.0, 4.0, H-5), 5.63 (d, J = 2.5, H-7), 3.03 (ddd, J = 9.0, 7.2, 2.0, H-9), 1.55 (Ha-11), 1.78 (He-11), 2.06 (ddd, J = 13.0, 13.0, 4.8, Ha-12), 1.74 (He-12), 1.80 (Ha-15), 1.50 (Hb-15), 1.88 (Ha-16), 1.64 (Hb-16), 2.22 (t, J = 8.0, H-17), 0.76 (s, CH_3-18), 0.83 (s, CH_3-19), 1.05 (s, CH_3-21), 3.15 (br d, J = 10.0, Hb-22), 1.45 (ddd, Ha-23), 1.57 (Hb-23), 1.75 (Ha-24), 1.03 (s, CH_3-26), 1.06 (s, CH_3-27), 3.30 (dd, J = 11.0, 3.2, CH_2OH-28), 3.37 (dd, J = 11.0, 4.8, CH_2OH-28) [1]
^{13}C NMR (75 MHz, DMSO) [1]:

Table 1

C-1	36.8 (t)	C-11	20.5 (t)	C-21	21.8 (q)
2	66.8 (d)	12	31.7 (t)	22	76.2 (d)
3	67.0 (d)	13	47.1 (s)	23	31.1 (t)
4	31.9 (t)	14	83.2 (s)	24	48.9 (d)
5	48.9 (d)	15	30.6 (t)	25	69.0 (s)
6	203.0 (s)	16	20.3 (t)	26	30.4 (q)
7	120.7 (d)	17	50.4 (d)	27	29.2 (q)
8	165.5 (s)	18	17.4 (q)	28	63.3 (t)
9	33.4 (d)	19	24.6 (q)		
10	37.9 (s)	20	76.0 (s)		

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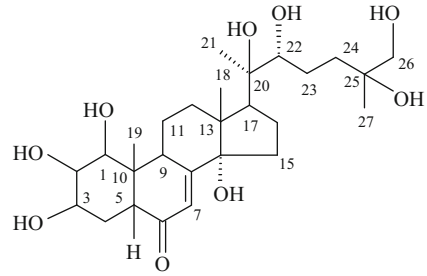
26-Hydroxyintegristerone A

CAS Registry Number: 1236198-93-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Silene fridvaldszkyana* [1]
$C_{27}H_{44}O_9$: 512.2985
UV λ_{max}^{EtOH} nm: 242 [1]
CI-MS m/z: 530 $[M + H + NH_3]^+$, 512 $[M]^+$ (100), 494, 477, 459, 378, 360, 180 [1]
^{1}H NMR (J/Hz, D_2O): 3.93 (br s, He-1), 4.05 (t, J = 3.0, Ha-2), 4.15 (br s, He-3), 1.82 (Ha-4), 1.82 (He-4), 2.63 (br t, J = 9.2, H-5), 6.00 (d, J = 2.1, H-7), 3.04 (br s, H-9), 1.77 (Ha-11), 1.78 (He-11), 1.96 (Ha-12), 1.96 (He-12), 1.67 (Ha-15), 2.06 (m, Hb-15), 1.88 (Ha-16), 1.78 (Hb-16), 2.32 (t, J = 9.9, H-17), 0.88 (s, CH_3-18), 1.10 (br s, CH_3-19), 1.24 (s, CH_3-21), 3.43 (d, J = 10.0, H-22), 1.34 (Ha-23), 1.66 (Hb-23), 1.76 (Ha-24), 1.48 (td, J = 13.4, 3.9, Hb-24), 3.47 (CH_2OH-26), for 2 epimers: 1.17 and 1.18 (s, CH_3-27) [1]
^{13}C NMR (D_2O) [1]:

Table 1

C-1	76.9	C-10	45.0	C-19	21.4
2	69.8	11	22.7	20	80.5
3	71.5	12	33.5	21	22.1
4	34.3	13	49.7	22	79.8
5	47.8	14	87.6	23	27.7
6	n.d.	15	32.8	24	38.0
7	123.6	16	22.5	25	75.7
8	n.d.	17	51.7	26	71.3
9	37.0	18	19.5	27 (2 epimers)	24.4 and 24.9

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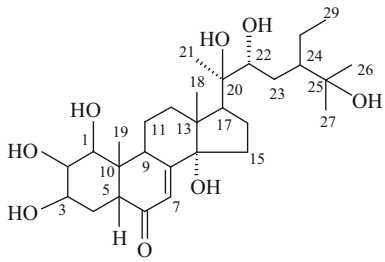
1β-Hydroxymakisterone C

CAS Registry Number: 1042045-46-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{29}H_{48}O_8$: 524.3349

$[\alpha]_D^{20}$ + 50.8° (c 0.17, EtOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3370, 1650, 1076, 1063 [1]

ESI-MS m/z: 525 $[M + H]^+$, 507 $[M + H–H_2O]^+$, 489 $[M + H–2H_2O]^+$, 471 $[M + H–3H_2O]^+$, 453 $[M + H–4H_2O]^+$, 387, 363, 345, 319, 171, 127 [1]

HR-ESI-MS m/z: for $C_{29}H_{48}O_8Na$ $[M + Na]^+$ calcd. 547.3247, found 547.3251 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 2.82 (Ha-1), 3.87 (t, J = 3.1, 3.1, Ha-2), 4.04 (He-3), 1.80 (Ha-4), 1.80 (He-4), 2.61 (dd, J = 4.5, 12.5, H-5), 5.83 (d, J = 2.5, H-7), 3.08 (bt, Ha-9), 1.78 (Ha-11), 1.70 (He-11), 2.10 (dt, J = 5.0, 13.0, 13.0, Ha-12), 1.87 (He-12), 1.99 (Ha-15), 1.62 (He-15), 1.76 (Ha-16), 2.03 (Hb-16), 2.41 (dd, J = 8.5, 9.5, H-17), 0.910 (s, CH_3-18), 1.079 (s, CH_3-19), 1.196 (s, CH_3-21), 3.41 (dd, J = 1.7, 10.8, H-22), 1.56 (Ha-23), 1.41 (Hb-23), 1.47 (Ha-24), 1.105 (s, CH_3-26), 1.215 (s, CH_3-27), 1.57 (Ha-28), 1.15 (Hb-28), 1.015 (t, J = 7.4, 7.4, CH_3-29) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

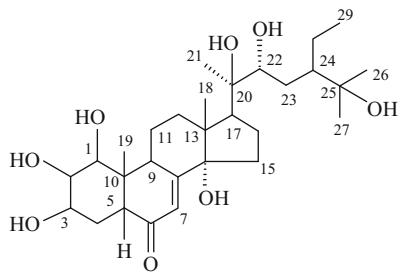
C-1	76.45	C-11	21.91	C-21	20.95
2	68.47	12	32.49	22	77.22
3	71.00	13	49.00	23	33.04
4	33.52	14	85.04	24	50.29
5	46.78	15	31.82	25	74.12
6	205.55	16	21.51	26	25.60
7	122.16	17	50.45	27	29.09
8	167.23	18	18.04	28	25.97
9	35.63	19	20.03	29	14.35
10	43.80	20	77.98		

References

1. M. Budesinsky, K. Vokas, J. Harmatha, J. Cvacka, Steroids **73**, 502 (2008)

26-Hydroxymakisterone C

CAS Registry Number: 1042045-44-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{29}H_{48}O_8$: 524.3349

$[\alpha]_D^{20}$ + 64.0° (c 0.075, EtOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3409, 1654, 1056 [1]

ESI-MS m/z: 525 $[M + H]^+$, 507 $[M + H–H_2O]^+$, 489 $[M + H–2H_2O]^+$, 471 $[M + H–3H_2O]^+$, 453 $[M + H–4H_2O]^+$ [1]

HR-ESI-MS m/z: for $C_{29}H_{48}O_8Na$ $[M + Na]^+$ calcd. 547.3247, found 547.3276 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (Ha-1), 1.43 (He-1), 3.84 (ddd, J = 3.0, 4.2, 12.0, Ha-2), 3.95 (q,

J = 3.0, He-3), 1.68-1.76 (Ha-4), 1.68-1.76 (He-4), 2.39 (dd, J = 4.8, 12.8, H-5), 5.81 (d, J = 2.6, H-7), 3.16 (m, J = 2.6, 7.0, 11.5, Ha-9), 1.80 (Ha-11), 1.71 (He-11), 2.13 (dt, J = 5.0, 13.0, 13.0, Ha-12), 1.87 (He-12), 1.96 (Ha-15), 1.62 (He-15), 1.78 (Ha-16), 2.04 (Hb-16), 2.39 (dd, J = 8.8, 10.0, H-17), 0.896 (s, CH_3-18), 0.967 (s, CH_3-19), 1.196 (s, CH_3-21), 3.45 (dd, J = 2.4, 10.8, H-22), 1.45 (Ha-23), 1.37 (Hb-23), 1.66 (Ha-24), 3.58 (d, J = 11.7, Ha-26), 3.35 (d, J = 11.7, He-26), 1.061 (s, CH_3-27), 1.79 (Ha-28), 1.20 (Hb-28), 1.030 (t, J = 7.4, 7.4, CH_3-29) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

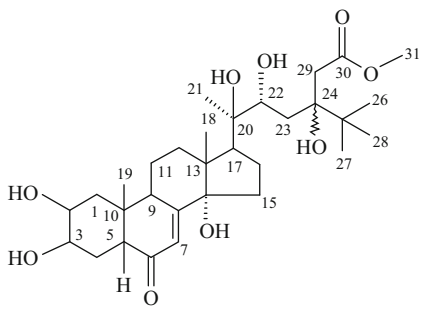
Table 1

C-1	37.36	C-11	21.63	C-21	20.82
2	68.71	12	32.49	22	77.57
3	68.51	13	49.17	23	33.40
4	32.87	14	85.19	24	45.30
5	51.80	15	31.81	25	76.41
6	206.44	16	21.63	26	69.08
7	122.14	17	50.39	27	21.01
8	167.86	18	18.03	28	25.04
9	35.10	19	24.41	29	14.30
10	39.26	20	77.91		

References

1. M. Budesinsky, K. Vokas, J. Harmatha, J. Cvacka, Steroids **73**, 502 (2008)

24-Hydroxy-25-Methyl-Makisterone C-30-Methylate



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *reptans* [1]

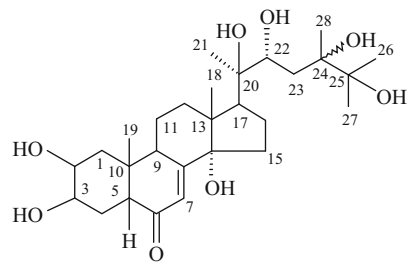
$C_{31}H_{50}O_9$: 566.3454

References

1. M. Bathori, A. Hunyadi, A. Simon, G. Toth, L. Polgar, I. Mathe, in *55th International Congress & Annual Meeting of the Society for Medicinal Plant Research*, Graz, 2007, p. 378, 942

25-Hydroxypanuosterone

CAS Registry Number: 220617-97-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cucubalis baccifer* (1), *Tapinella panuoides* (2, 3)

$C_{28}H_{46}O_8$: 510.3192

Mp: 248–256°C (MeOH) (3)

IR (KBr) ν_{max} cm^{-1}: 3406, 1653 (3)

FAB-MS m/z: 533 $[M + Na]^+$ (60), 511 $[M + H]^+$ (27), 493 (23), 457 (42), 311 (100) (3)

HR-MS m/z: for $C_{28}H_{47}O_8$ $[M + H]^+$ calcd. 511.3271, found 511.3131 (3)

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (dd, J = 13.5, 4.5, Ha-1), 1.43 (dd, J = 13.0, 12.0, He-1), 3.84 (ddd, J = 12.0, 4.5, 3.0, Ha-2), 3.95 (q, J = 3.0, He-3), 1.76 (Ha-4), 1.69 (He-4), 2.38 (dd, J = 13.0, 4.4, H-5), 5.82 (d, J = 2.5, H-7), 3.15 (ddd, J = 10.0, 7.0, 2.5, H-9), 1.70 (Ha-11), 1.79 (He-11),

2.13 (dt, J = 13.0, 13.0, 4.5, Ha-12), 1.87 (He-12), 1.95 (Ha-15), 1.59 (Hb-15), 2.02 (Ha-16), 1.88 (Hb-16), 2.34 (t, J = 9.0, H-17), 0.899 (s, CH_3-18), 0.969 (s, CH_3-19), 1.207 (s, CH_3-21), 3.73 (d, J = 9.2, H-22), 1.83 (d, J = 14.6, Ha-23), 1.53 (dd, J = 14.6, 9.3, Hb-23), 1.257 (s, CH_3-26), 1.242 (s, CH_3-27), 1.199 (s, CH_3-28) (3)

^{13}C NMR (125 MHz, CD_3OD) (3):

Table 1

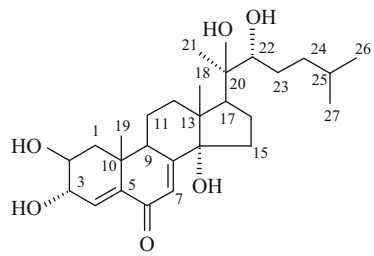
C-1	37.37	C-11	21.51	C-21	20.69
2	68.72	12	32.41	22	74.02
3	68.53	13		23	39.96
4	32.84	14	85.48	24	76.27
5	51.80	15	31.79	25	77.51
6	204.46	16	21.32	26	25.25
7	122.29	17	50.00	27	25.25
8	167.84	18	17.96	28	22.41
9	35.13	19	24.39		
10	39.30	20	77.91		

References

1. Y.X. Cheng, J. Zhou, N.H. Tan, Z.T. Ding, Acta Bot. Sin. **43**, 316 (2001)
2. K. Vokas, M. Budesinsky, J. Harmatha, in *XIth Ecdysone Workshop*, Ceske Budejovice, Abstracts, 1994, p. 119
3. K. Vokas, M. Budesinsky, J. Harmatha, J. Kohoutova, Phytochemistry **49**, 2109 (1998)

14-Hydroxypinnasterol

CAS Registry Number: 104406-80-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Laurencia pinnata* [1]

$C_{27}H_{42}O_6$: 462.2981

Mp: 210–212°C (MeOH–H_2O) [1]

$[\alpha]_D^{22}$ + 39° (c 0.35, MeOH)

IR (KBr) ν_{max} cm^{-1}: 3450, 1685, 1655, 1075 [1]

UV λ_{max}^{EtOH} nm (log ε): 256 (3.88) [1]

FD-MS m/z: 462 $[M]^+$, 444, 351, 317, 145 [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.21 (ddd, J = 10.0, 7.0, 3.5, Ha-2), 4.64 (dd, J = 7.0, 2.0, He-3), 6.79 (d, J = 2.0, H-4), 6.28 (d, J = 2.0, H-7), 3.54 (ddd, J = 12.0, 7.0, 2.0, Ha-9), 2.94 (t, J = 9.0, Ha-17), 1.22 (s, CH_3-18), 1.26 (s, CH_3-19), 1.59 (s, CH_3-21), 3.83 (d, J = 11.0, Hb-22), 0.84 (d, J = 6.7, CH_3-26), 0.85 (d, J = 6.7, CH_3-27) [1]

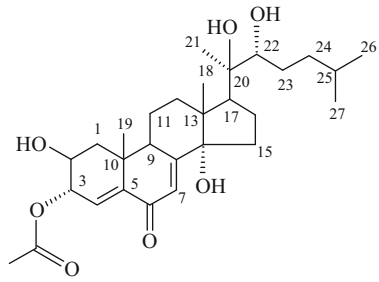
Pharm./Biol.: *Sarcophaga* test: ED_{50} = 0.25 µg [1].

References

1. A. Fukuzawa, M. Miyamoto, Y. Kumagai, T. Masamune, Phytochemistry **25**, 1305 (1986)

14-Hydroxypinnasterol-3-Acetate

CAS Registry Number: 104387-08-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Laurencia pinnata* [1]

$C_{29}H_{44}O_7$: 504.3087

Mp: (Oil) [1]

$[\alpha]_D^{20}$ + 92° (c 0.5, $CHCl_3$) [1]

IR ($CHCl_3$) ν_{max} cm^{-1}: 3455, 1680, 1643, 1270 [1]

UV λ_{max}^{EtOH} nm (log ε): 255 (4.00) [1]

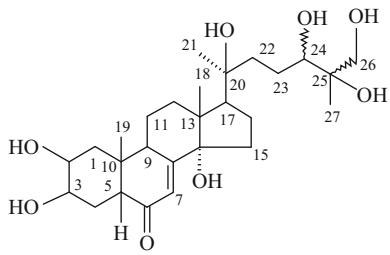
FD-MS m/z: 505 $[M + H]^+$, 487, 486, 145, 101 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.23 (ddd, J = 10.0, 7.0, 3.5, Ha-2), 5.76 (dd, J = 7.0, 2.0, He-3), 6.41 (d, J = 2.0, H-4), 6.31 (d, J = 2.5, H-7), 2.94 (t, J = 9.0, H-17), 1.20 (s, CH_3-18), 1.26 (s, CH_3-19), 1.60 (s, CH_3-21), 3.83 (d, J = 10.0, Hb-22), 0.84 (d, J = 6.4, CH_3-26), 0.85 (d, J = 6.4, CH_3-27), 6.52 (br s, OH) [1]

References

1. A. Fukuzawa, M. Miyamoto, Y. Kumagai, T. Masamune, Phytochemistry **25**, 1305 (1986)

26-Hydroxypinnatasterone

CAS Registry Number:
351343-09-4 (25R)
351343-11-8 (25S)



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Vitex cymosa* [1]
$C_{27}H_{44}O_8$: 496.3036
$[\alpha]_D^{25}$ + 36.0° (c 0.1, MeOH) [1]
EI-MS m/z: 460 (1), 442 (5), 363 (5), 345 (12), 327 (11), 301 (8), 285 (5), 267 (8), 259 (5), 225 (6), 211 (6), 173 (10), 129 (9), 115 (36), 105 (8), 97 (18), 91 (10), 69 (34), 55 (25), 43 (100) [1]
FAB-MS m/z: 519 (100), 497 (31), 460 (60), 385 (34), 363 (48), 301 (18) [1]
^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.25 (Ha-2), 4.25 (He-3), 3.02 (dd, J = 13.0, 4.0, H-5), 6.28 (d, J = 1.7, H-7), 3.69 (m, H-9), 3.07 (t, J = 9.0, H-17), 1.24 (s, CH_3-18), 1.08 (s, CH_3-19), 1.59, 1.60 (s, CH_3-21), 3.89 (br dd, J = 10.0, 3.0, H-24), 4.25 (CH_2OH-26), 1.49, 1.50 (s, CH_3-27) [1]
^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

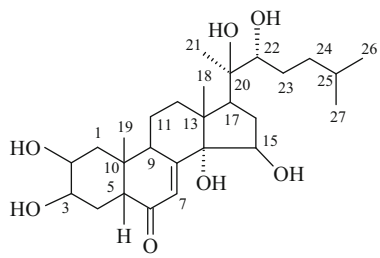
C-1	37.8	C-10	38.5	C-19	24.3
2	67.9	11	20.9	20	76.7
3	67.8	12	31.8	21	21.5
4	32.3	13	47.9	22	37.4
5	51.2	14	84.0	23	26.5
6	203.3	15	31.6	24	77.5
7	121.4	16	21.3	25	71.4
8	166.0	17	49.9	26	64.6
9	34.2	18	17.7	27	24.5

References

1. T.C. Santos, F. Delle Monache, S.G. Leitao, Fitoterapia **72**, 215 (2001)

15-Hydroxyponasterone A

CAS Registry Number: 1026800-42-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Leuzea carthamoides* [1]
$C_{27}H_{44}O_7$: 480.3087
$[\alpha]_D^{20}$ + 41.2° (c 0.17, EtOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3585, 3563, 3370, 1646, 1055, 1008, 988 [1]
ESI-MS m/z: 481 $[M + H]^+$, 463 $[M + H–H_2O]^+$, 445 $[M + H–2H_2O]^+$, 427 $[M + H–3H_2O]^+$, 409 $[M + H–4H_2O]^+$, 401 $[M + H–C_3H_8–2H_2O]^+$, 329, 311, 299 [1]
HR-ESI-MS m/z: for $C_{27}H_{44}O_7Na$ $[M + Na]^+$ calcd. 503.2985, found 503.2990 [1]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (Ha-1), 1.43 (He-1), 3.81 (ddd, J = 3.0, 4.2, 12.2, Ha-2), 3.96 (q,

J = 3.0, He-3), 1.79 (Ha-4), 1.72 (He-4), 2.37 (dd, J = 4.4, 13.2, H-5), 6.47 (d, J = 2.6, H-7), 3.13 (ddd, J = 2.6, 7.0, 11.5, Ha-9), 1.75–1.80 (Ha-11), 1.75–1.80 (He-11), 2.11 (td, J = 5.0, 13.0, 13.0, Ha-12), 1.85 (He-12), 4.13 (m, Ha-15), 1.92 (Ha-16), 2.24 (Hb-16), 2.25 (H-17), 1.137 (s, CH_3-18), 1.002 (s, CH_3-19), 1.188 (s, CH_3-21), 3.30 (dd, J = 1.5, 11.0, Hb-22), 1.48 (Ha-23), 1.22 (Hb-23), 1.51 (Ha-24), 1.22 (Hb-24), 1.57 (H-25), 0.908 (d, J = 6.5, CH_3-26), 0.920 (d, J = 6.5, CH_3-27) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

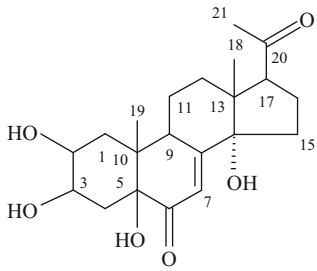
C-1	37.40	C-10	39.58	C-19	24.22
2	68.66	11	21.28	20	77.58
3	68.59	12	34.01	21	21.00
4	32.70	13	47.48	22	77.92
5	51.47	14	85.19	23	37.62
6	206.68	15	76.84	24	30.38
7	124.56	16	35.59	25	29.22
8	165.77	17	49.96	26	22.73
9	35.17	18	18.11	27	23.42

References

1. M. Budesinsky, K. Vokas, J. Harmatha, J. Cvacka, Steroids **73**, 502 (2008)

5β-Hydroxypoststerone

CAS Registry Number: 1236073-68-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotus longifolia* [1]

$C_{21}H_{30}O_6$: 378.2042

CI-MS m/z: 396 $[M + NH_4]^+$, 379 $[M + H]^+$, 361 $[M + H\text{-}H_2O]^+$ [1]

^{1}H NMR (J/Hz, D_2O): 1.72 (Ha-1), 1.82 (He-1), 4.15 (m, Ha-2), 4.14 (m, He-3), 1.89 (Ha-4), 2.07 (He-4), 6.02 (d, J = 2.2, H-7), 3.20 (m, H-9), 1.78 (Ha-11), 1.96 (He-12), 1.92 (Ha-12), 2.19 (He-12), 2.12 (Ha-15), 1.76 (Hb-15), 1.92 (Ha-16), 2.22 (Hb-16), 3.33 (dd, J = 9.5, 7.9, H-17), 0.65 (s, CH_3-18), 0.94 (s, CH_3-19), 2.26 (s, CH_3-21) [1]

^{13}C NMR (D_2O) [1]:

Table 1

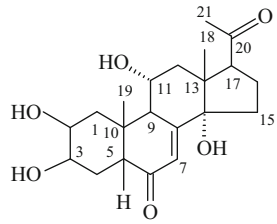
C-1	35.3	C-8	n.d.	C-15	34.0
2	70.2	9	41.0	16	24.0
3	71.6	10	47.8	17	62.3
4	37.9	11	24.3	18	19.9
5	83.1	12	32.9	19	19.1
6	n.d.	13	51.4	20	220.4
7	123.6	14	88.1	21	34.5

References

1. S. Crouzet, A. Maria, L. Dinan, R. Lafont, J.P. Girault, Arch. Insect Biochem. Physiol. **72**, 194 (2009)

11α-Hydroxypoststerone

CAS Registry Number: 730978-47-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula wolffii* [1]

$C_{21}H_{30}O_6$: 378.2042

Mp: 174–176°C [1]

$[\alpha]_D^{28}$ + 12° (c 0.1, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3320, 1718, 1653 [1]

UV λ_{max}^{MeOH} nm (log ε): 240 (4.116) [1]

FAB-MS m/z: 379 $[M + H]^+$ (100), 361 $[M + H\text{–}H_2O]^+$ (88), 343 $[M + H\text{–}2H_2O]^+$ (40), 325 $[M + H\text{–}3H_2O]^+$ (10), 299 (11), 282 (32), 277 (13), 249 (80), 231 (20) [1]

HR-ESI-MS m/z: for $C_{21}H_{30}O_6$ $[M]^+$ calcd. 378.2042, found 378.2045 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 2.60 (dd, J = 4.2, 13.0, Ha-1), 1.38 (t, J = 12.3, He-1), 4.015 (dt, J = 3.8, 11.8, Ha-2), 3.96 (q, J = 2.9, He-3), 1.775 (td, J = 2.4, 13.6, H-4), 2.345 (dd, J = 4.1, 13.1, H-5), 5.807 (d, J = 2.7, H-7), 3.18 (dd, J = 2.7, 8.9, H-9), 4.08 (ddd, J = 5.8, 8.9, 10.8, H-11), 2.406 (t, J = 11.4, Ha-12), 2.08 (dd, J = 5.8, 12.0, He-12), 3.36 (dd, J = 8.1, 9.4, H-17), 0.61 (s, CH_3-18), 1.05 (s, CH_3-19), 2.16 (s, CH_3-21) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

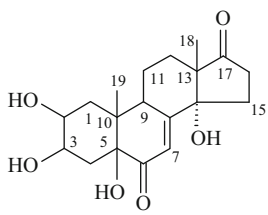
C-1	39.2	C-8	164.4	C-15	32.3
2	69.1	9	43.1	16	22.4
3	68.7	10	40.1	17	60.0
4	33.5	11	69.4	18	18.4
5	53.0	12	42.3	19	24.8
6	206.6	13	48.6	20	212.3
7	123.3	14	84.8	21	31.6

References

1. A. Hinyadi, C. Toth, A. Simon, M. Mak, Z. Kele, I. Mathe, M. Bathori, J. Nat. Prod. **67**, 1070 (2004)

5β-Hydroxyrubrosterone

CAS Registry Number: 144405-74-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula tinctoria* [1]

$C_{19}H_{26}O_6$: 350.1729

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.80 (Ha-1), 2.1 (He-1), 4.00 (m, He-2), 3.95 (m, Ha-3), 1.75 (Ha-4), 1.75 (He-4), 5.97 (d, J = 2.5, H-7), 3.20 (m, Ha-9), 1.70 (Ha-11), 1.90 (He-11), 2.10 (Ha-12), 1.60 (He-12), 2.30 (Ha-15), 2.05 (Hb-15), 2.50 (Ha-16), 2.30 (Hb-16), 0.88 (s, CH_3-18), 0.95 (s, CH_3-19) [1]

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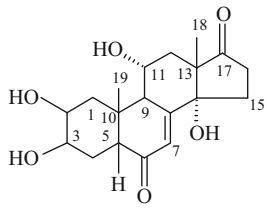
11α-Hydroxyrubrosterone

CAS Registry Number: 661474-66-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotis arachnoidea* [1]

$C_{19}H_{26}O_6$: 350.1729

Mp: 251–253°C [1]

$[\alpha]_D^{20}$ + 1.07° (c, MeOH) [1]

EI-MS m/z: 350 $[M]^+$ (18), 332 $[M\text{-}H_2O]^+$ (77), 314 $[M\text{-}2H_2O]^+$ (25), 304 $[M\text{-}H_2O\text{–}CO]^+$ (23), 286 $[M\text{-}2H_2O\text{–}CO]^+$ (21), 271 $[M\text{-}2H_2O\text{–}CO\text{–}CH_3]^+$ (22), 249 (35), 227 (64), 185 (93), 161 (48), 91 (97), 77 (63), 69 (41), 55 (100), 43 (90) [1]

HR-EI-MS m/z: for $C_{19}H_{26}O_6$ $[M]^+$ calcd. 350.1729, found 350.1718 [1]

^{1}H NMR (J/Hz, C_5D_5N): 3.41 (dd, J = 4.0, 12.6, Ha-1), 2.02 (m, He-1), 4.54 (m, Ha-2), 4.54 (m, He-3), 3.08 (m, H-5), 6.32 (d, J = 2.2, H-7), 3.82 (dd, J = 2.2, 8.6, H-9), 4.21 (m, Ha-11), 2.46 (m, Ha-12), 3.05 (m, He-12), 2.62 (m, Ha-15), 2.62 (m, Hb-15), 2.24 (m, Ha-16), 2.31 (m, Hb-16), 0.90 (s, CH_3-18), 1.29 (s, CH_3-19) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

C-1	39.7	C-8	161.3	C-15	33.7
2	68.1	9	43.5	16	29.1

(*continued*)

Table 1 (continued)

3	68.0	10	39.8	17	216.5
4	32.9	11	68.3	18	17.9
5	52.7	12	36.2	19	24.9
6	203.7	13	53.3		
7	122.6	14	79.5		

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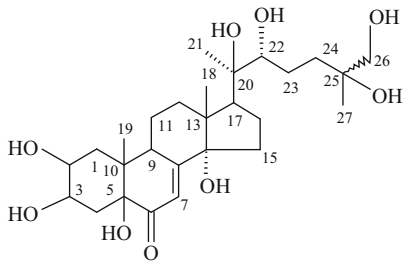
26-Hydroxypolypodine B

CAS Registry Number: 121043-41-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Lychnis flos-culculi* [1], *Silene fridvaldszkyana* [2], *S. nutans* [1], *S. viridiflora* [3, 4]

$C_{27}H_{44}O_9$: 512.2985

Mp: 236–238°C (EtOAc-acetone) [3]

$[\alpha]_D^{23}$ + 34.0 ± 2° (c 0.3, MeOH) [3]

IR (KBr) ν_{max} cm^{-1}: 3443–3368, 1687 [3]

EI-MS m/z: 512 $[M]^+$ [3]

CI-MS m/z: 513 $[M + H]^+$, 495, 477, 459, 441, 396, 379, 363, 361, 345 [1]

^{1}H NMR (J/Hz, CD_3OD): 3.94 (m, Ha-2), 3.97 (m, He-3), 5.84 (d, J = 2.5, H-7), 3.14 (m, H-9), 2.35 (m, H-17), 0.88 (s, CH_3-18), 0.90 (s, CH_3-19), 1.20 (s, CH_3-21), 3.33 (br d, J = 10.0, H-22), 3.35 (s, CH_2OH-26), 1.14 and 1.15 (s, CH_3-27) [1]

^{1}H NMR (J/Hz, $CDCl_3$): 4.17 (m, Ha-2), 4.17 (m, He-3), 6.05 (d, J = 2.5, H-7), 2.37 (m, H-17), 0.92 (s, CH_3-18), 0.99 (s, CH_3-19), 1.29 (s, CH_3-21), 3.18 (m, H-22), 3.51 (s, CH_2OH-26), 1.21 (s, CH_3-27) [3]

^{13}C NMR (125 MHz, CD_3OD) [4]:

Table 1

C-1	34.4	C-10	45.6	C-19	17.1
2	68.6	11	22.6	20	78.0
3	70.4	12	32.7	21	21.2
4	36.3	13	48.9	22	78.6
5	80.4	14	85.2	23	26.7
6	202.5	15	31.9	24	37.3
7	120.7	16	21.6	25	73.8
8	167.7	17	50.6	26	70.9
9	39.1	18	18.2	27	23.7

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.8 \times 10^{-7}$M [5].

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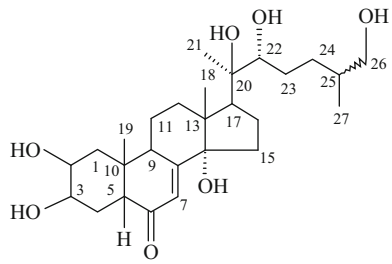
Inokosterone

CAS Registry Number: 15130-85-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Achyranthes bidentata, A. faureiei, A. japonica, A. japonica* var. *hachijoensis, A. longifolia, A. rubrofusca* [1–3], *Lamium album* [4], *Leuzea carthamoides* [5], *Lychnis miqueliana* [6], *Microsorum maximum, M. membranifolium* [7], *M. scolopendria* [8], *Morus* sp [9], *Polypodium vulgare* [10], *Serratula coronata* [11], *Silene disticha* [12], *Vitex megapotamica* [13, 14], *Woodwardia japonica, W. orietalis* var. *formosana, W. takeoi, W. unigemmata* [15]

$C_{27}H_{44}O_7$: 480.3087

Mp: 255°C (MeOH–EtOAc) [3]

IR (KBr) ν_{max} cm^{-1}: 3400, 1640 [3]

EI-MS m/z: 462 $[M\text{-}H_2O]^+$, 444 $[M\text{-}2H_2O]^+$, 426 $[M\text{-}3H_2O]^+$, 411 $[M\text{-}H_2O\text{–}CH_3]^+$, 363 $[M\text{-}117]^+$, 345 $[M\text{-}117\text{-}H_2O]^+$, 301 $[M\text{-}161\text{-}H_2O]^+$ [3]

HR-FAB-MS m/z: for $C_{27}H_{43}O_7$ $[M\text{-}H]^-$ calcd. 479.3008, found (for C-25 epimer-1): 479.3004, found (for C-25 epimer-2): 479.3001 [16]

TSP-MS m/z: 498 $[M + NH_4]^+$, 481 $[M + H]^+$, 463 $[M + H + H_2O]^+$, 445 $[M + H + 2H_2O]^+$, 427 $[M + H + 3H_2O]^+$ [10]

^{1}H NMR (J/Hz, C_5D_5N): 4.18 (m, Ha-2), 4.10 (m, He-3), 6.19 (s, H-7), 3.50–4.00 (m, H-9), 1.16 (s, CH_3-18), 1.05 (s, CH_3-19), 1.52 (s, CH_3-21), 3.50–4.00 (m, H-22), 3.50–4.00 (m, H-26), 1.01 (d, J = 6.0, CH_3-27) [3]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.18 (Ha-2), 4.23 (He-3), 3.02 (dd, J = 4.5, 15.0, H-5), 6.26 (d, J = 2.0, H-7), 3.66 (d, J = 6.3, H-9), 2.96 (t, J = 9.0, H-17), 1.22 (s, CH_3-18), 1.05 (s, CH_3-19), 1.57 (s, CH_3-21), 3.86 (d, J = 9.6, H-22), 3.62 (m, Ha-26), 3.76 (m, Hb-26), 1.03 (d, J = 6.9, CH_3-27) [10]

^{1}H NMR (100 MHz, C_5D_5N): 1.22 (s, CH_3-18), 1.08 (s, CH_3-19), 1.58 (s, CH_3-21), 1.48 (s, CH_3-27) [16]

^{1}H NMR (J/Hz, C_5D_5N) (for C-25 epimer-1): 4.17 (m, Ha-2), 4.23 (m, He-3), 3.01 (dd, J = 3.8, 13.2, H-5), 6.25 (d, J = 2.4, H-7), 3.59 (m, H-9), 2.94 (t, J = 9.1, H-17), 1.217 (s, CH_3-18), 1.067 (s, CH_3-19), 1.577 (s, CH_3-21), 3.86 (br d, J = 9.7, H-22), 3.64 (dd, J = 6.1, 10.3, Ha-26), 3.72 (dd, J = 5.8, 10.3, Hb-26), 1.040 (d, J = 6.1, CH_3-27) [16]

^{13}C NMR (C_5D_5N) [3]: **^{13}C NMR** (75 MHz, C_5D_5N) [10]:

Table 1

C-1	37.9	C-15	32.0	C-1	38.02	C-15	31.83
2	68.0	16	21.6	2	68.11	16	21.53
3	68.0	17	50.0	3	68.19	17	50.10
4	32.2	18	17.8	4	32.52	18	17.97
5	51.3	19	24.4	5	51.47	19	24.52
6	203.3	20	76.7	6	203.61	20	76.82
7	121.6	21	21.1	7	121.72	21	21.72
8	165.9	22	77.2, 77.4	8	166.24	22	77.30
9	34.4	23	30.1	9	34.47	23	30.29
10	38.6	24	31.7, 32.0	10	38.74	24	32.10
11	21.4	25	36.4, 36.7	11	21.15	25	36.82
12	31.7	26	67.3, 68.0	12	32.10	26	67.35
13	48.1	27	17.0, 17.8	13	48.15	27	17.92
14	84.1			14	84.22		

Pharm./Biol.: *Musca domestica* bioassay: C-25 epimer-1 EC_{50} = 3.39 × 10^{-5}M, C-25 epimer-2 EC_{50} = 7.37 × 10^{-5}M [16], *Drosophila melanogaster* B_{II} bioassay: EC_{50} = 1.5 × 10^{-7}M (for C-25 epimer-1), EC_{50} = 2.7×10^{-7}M (for C-25 epimer-2) [17], EC_{50} = 1.1×10^{-7}M [18], high anabolic activity [19, 20], antidiabetic activity [21].

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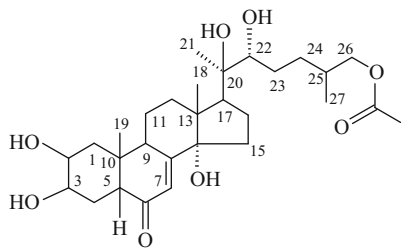
Inokosterone-26-Acetate

CAS Registry Number: 899428-75-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula coronata* [1]

$C_{29}H_{46}O_8$: 522.3192

CI-MS m/z: 540 $[M + H + NH_3]^+$, 522 $[M]^+$, 505, 498, 480, 464, 434, 416, 352, 308, 291, 220, 176, 153, 116 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.38 (t, J = 13.4, Ha-1), 1.88 (m, He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.34 (t, H-5), 5.97 (d, J = 2.0, H-7), 3.11 (m, H-9), 1.73 (Ha-11), 1.86 (He-11), 1.95 (Ha-12), 1.75 (He-12), 1.65 (Ha-15), 2.05 (Hb-15), 1.76 (Ha-16), 1.88 (Hb-16), 2.31 (t, J = 9.0, H-17), 0.86 (s, CH_3-18), 1.00 (s, CH_3-19), 1.22 (s, CH_3-21), 3.43 (dd, J = 10.0, 1.0, H-22), 1.24 (Ha-23), 1.65 (Hb-23), 1.27 (Ha-24), 1.65 (Hb-24), 1.87 (m, H-25), 4.05 (dd, J = 11.0, 6.0, Ha-26), 3.95 (dd, J = 11.0, 6.5, Hb-26), 0.96 (d, J = 6.9, CH_3-27), 2.17 (s, CH_3COO-26) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

C-1	36.6 (t)	C-11	21.3 (t)	C-21	20.7 (q)
2	68.5 (d)	12	32.0 (t)	22	78.2 (d)
3	68.2 (d)	13	48.3 (s)	23	29.1 (t)
4	32.4 (t)	14	86.1 (s)	24	31.5 (t)
5	51.7 (d)	15	31.5 (t)	25	33.2 (d)
6	209.8 (s)	16	21.3 (t)	26	71.2 (t)
7	122.1 (d)	17	50.3 (d)	27	17.3 (q)
8		18	18.0 (q)	CH_3COO	21.7 (q)
9	34.9 (d)	19	24.2 (q)		
10	39.3 (s)	20	79.3 (s)		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 6.0 \times 10^{-8}$M.

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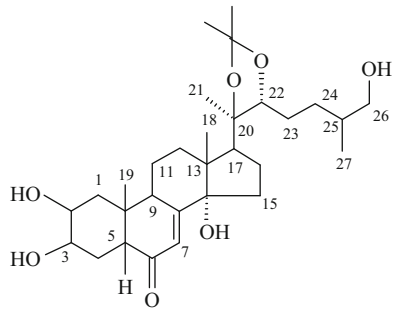
Inokosterone-20,22-Acetonide

CAS Registry Number: 915217-20-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{30}H_{48}O_7$: 520.3400

$[\alpha]_D^{20}$ + 42.9° (c 0.29, EtOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3429, 1655, 1109, 1055 [1]

FAB-MS m/z: 543 $[M + Na]^+$ (45), 521 $[M + H]^+$ (80), 503 $[M + H–H_2O]^+$ (100), 445 (20), 427 (15), 329 (20), 301 (22), 279 (12), 249 (19) [1]

HR-ESI-MS m/z: for $C_{30}H_{48}O_7Na$ $[M + Na]^+$ calcd. 543.3290, found 543.3282 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.78 (dd, J = 4.3, 13.2, Ha-1), 1.43 (dd, J = 12.0, 13.2, He-1), 3.83 (ddd, J = 3.2, 4.3, 12.0, Ha-2), 3.95 (q, J = 3.0, He-3), 1.68-1.78 (Ha-4), 1.68–1.78 (He-4), 2.38 (dd, J = 4.7, 12.8, H-5), 5.82 (d, J = 2.6, H-7), 3.15 (ddd, J = 2.6, 7.0, 11.5, Ha-9), 1.80 (Ha-11), 1.69 (He-11), 2.11 (td, J = 4.8, 13.0, 13.0, Ha-12), 1.85 (He-12), 1.96 (Ha-15), 1.63 (Hb-15), 1.86 (Ha-16), 2.04 (Hb-16), 2.29 (dd, J = 8.2, 9.6, H-17), 0.826 (s, CH_3-18), 0.963 (s, CH_3-19), 1.162 (s, CH_3-21), 3.69 (dd, J = 2.9, 9.4, Hb-22), 1.47 (Ha-23), 1.47 (Hb-23), 1.68 (Ha-24), 1.15 (Hb-24), 1.63 (H-25), 3.36 (dd, J = 5.8, 10.7, Ha-26), 3.43 (dd, J = 6.4, 10.7, Ha-26), 0.937 (d, J = 6.6, CH_3-27), Other: 1.32 and 1.39 (20,22-iPr) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

C-1	37.35	C-11	21.51	C-21	22.54
2	68.72	12	32.32	22	83.13
3	68.49	13	48.44	23	27.43
4	32.87	14	85.34	24	32.05
5	51.77	15	31.72	25	37.01
6	206.43	16	22.43	26	68.23
7	122.15	17	50.46	27	17.04
8	167.56	18	17.69	20,22-iPr	29.36
9	35.14	19	24.45		27.19
10	39.21	20	85.75		107.98

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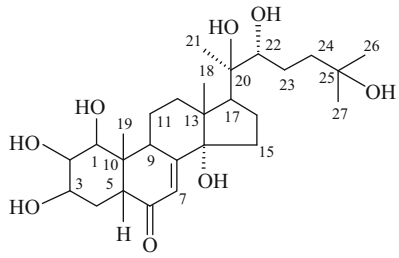
1. M. Budesinsky, K. Vokas, J. Harmatha, J. Cvacka, Steroids **73**, 502 (2008)

Integristerone A

CAS Registry Number: 66450-91-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1], *Lychnis chalcedonica, L. wilfordii* [2], *Melandrium turkestanicum* [3], *Rhaponticum carthamoides* [4], *R. integrifolium* [5], *R. nanum* [6], *Serratula inermis* [7], *S. komarovii* [8], *S. wolffii* [9], *S. xeranthemoides* [10], *Silene brahuica* [11], *S. claviformis* [12], *S. fridvaldszkyana*, *S. gigantea*, *S. repens* [13], *S. italica* ssp. *nemoralis* [14], *S. linicola* [15], *S. nutans, S. otites* [16], *S. tomentella* [17], *S. viridiflora* [18], *S. wallichiana* [19], *Stemmacantha uniflora* [20]

$C_{27}H_{44}O_8$: 496.3036

Mp: 245–246°C (EtOAc–MeOH) [3], 243.5–245°C (EtOAc–MeOH) [4], 244–246°C (EtOAc–MeOH) [6], 246–248°C (EtOAc) [10, 15]

$[\alpha]_D^{20}$ + 35.6 ± 2° (c 0.32, MeOH) [3], $[\alpha]_D^{20}$ + 35.5 ± 2° (c 0.94, MeOH) [4], $[\alpha]_D^{20}$ + 33.5 ± 2° (c 0.81, MeOH) [6], $[\alpha]_D^{20}$ + 39.4° (c 1.2, MeOH) [10], $[\alpha]_D^{24}$ + 36.0 ± 2° (c 1.02, MeOH) [11], $[\alpha]_D^{22}$ + 36.2 ± 2° (c 0.32, MeOH) [12], $[\alpha]_D^{20}$ + 36.1 ± 2° (c 0.43, MeOH) [17]

IR (KBr) ν_{max} cm^{-1}: 3355, 1646 [1], 3480, 3350, 1670 [7], 3350–3480, 1670 [10], 3400, 1660 [15, 17]

UV λ_{max}^{EtOH} nm: 245 (ε 10600) [7], 245 (log ε 4.09) [10], 245 (log ε 4.00) [17]

EI-MS m/z: 496 $[M]^+$, 478, 460, 442, 424, 409, 391, 379, 374, 368, 361 (100), 343, 325, 316, 301, 283, 143, 125, 99, 81, 69 [6], 478 (14), 460(20), 442 (94), 424 (33), 409 (10), 391 (6), 379 (15), 374 (12), 368 (42), 361 (100), 343 (90), 325 (30), 316 (25), 301 (15), 283 (24), 143 (12), 125 (12), 99 (49), 81 (27), 69 (27) [11], 478 $[M\text{-}H_2O]^+$ (3), 460 (4), 445 (10), 442 (18), 427 (11), 409 (7), 391 (4), 379 (73), 374 (5), 368 (17), 361 (74), 343 (100), 325 (43), 316 (17), 304 (7), 283 (41), 143 (60), 135 (61), 99 (35), 81 (34) [17]

FAB-MS m/z: 497 $[M + H]^+$ (21), 480 (50), 479 (54), 461 (97), 443 (59), 407 (25), 387 (40), 379 (27), 363 (31), 345 (43), 319 (44), 317 (45), 299 (38), 255 (42), 243 (45), 227 (61), 211 (100) [1]

HR-MS m/z: for $C_{27}H_{43}O_7$ $[M + H\text{–}H_2O]^+$ calcd. 479.3009, found 479.2941 [1]

^{1}H NMR (500 MHz, CD_3OD): 3.82 (H-1), 3.87 (Ha-2), 4.04 (He-3), 1.80 (Ha-4), 1.75 (He-4), 2.61 (dd, H-5), 5.80 (d, H-7), 3.08 (br t, H-9), 1.79 (Ha-11), 1.70 (He-11), 2.11 (Ha-12), 1.87 (He-12), 2.00 (Ha-15), 1.60 (Hb-15), 1.73 (Ha-16), 1.97 (Hb-16), 2.39 (dd, H-17), 0.90 (s, CH_3-18), 0.91 (s, CH_3-19), 1.19 (s, CH_3-21), 3.22 (dd, H-22), 1.66 (Ha-23), 1.29 (Hb-23), 1.78 (Ha-24), 1.43 (Hb-24), 1.20 (s, CH_3-26), 1.19 (s, CH_3-27) [1]

^{1}H NMR (100 MHz, C_5D_5N): 6.14 (br s, H-7), 1.10 (s, CH_3-18), 1.29 (s, CH_3-19), 1.45 (s, CH_3-21), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27) [10]

^{1}H NMR (100 MHz, C_5D_5N): 4.30 (m, H-1, 2, 3), 6.17 (br s, H-7), 3.57 (m, H-9), 1.19 (s, CH_3-18), 1.40 (s, CH_3-19), 1.58 (s, CH_3-21), 3.77 (m, H-22), 1.39 (s, CH_3-26), 1.39 (s, CH_3-27) [17]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

C-1	76.43	C-10		C-19	20.01
2	70.98	11	21.91	20	77.89
3	68.50	12	32.54	21	21.05
4	43.80	13	49.00	22	78.43
5	46.79	14	85.10	23	27.36
6	205.57	15	31.80	24	42.38
7	122.17	16	21.40	25	71.29
8	167.19	17	50.58	26	29.70
9	35.65	18	18.02	27	28.97

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.8 \times 10^{-7}$ M [21], *Galleria mellonella* bioassay: ED_{50} = 15.6 μg/g, *Sarcophaga bullata* bioassay: ED_{50} = 15.6 μg/g [22], *Drosophila melanogaster in vitro* bioassay: inactive [23].

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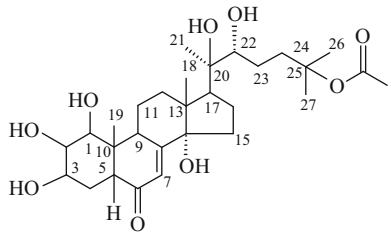
Integristerone A-25-Acetate

CAS Registry Number: 269739-15-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1]

$C_{29}H_{46}O_9$: 538.3141

Mp: 198–200°C (MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3400, 1730, 1655, 1244 [1]

EI-MS m/z: 442 $[M\text{-}CH_3COOH + 2H_2O]^+$ (5), 427 (3.5), 424 (3.5), 409 (3.5), 391 (4), 379 (23), 361 (100), 343 (60), 325 (41), 283 (39), 143 (41), 125 (44), 99 (44), 81 (96) [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N D_2O): 4.30–4.38 (m, He-1), 4.30–4.38 (m, Ha-2), 4.30–4.38 (m, He-3), 6.30 (s, H-7), 3.60 (m, H-9), 3.00 (t, J = 9.1, H-17), 1.26 (s, CH_3-18), 1.43 (s, CH_3-19), 1.63 (s, CH_3-21), 3.87 (d, J = 9.4, H-22), 1.44 (s, CH_3-26), 1.50 (s, CH_3-27), 1.96 (s, CH_3COO-25) [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N D_2O): 4.31 (br s, He-1), 4.24 (br s, Ha-2), 4.31 (br s, He-3), 3.30 (m, H-5), 6.27 (br s, H-7), 3.58 (m, H-9), 2.96 (t, J = 9.0, H-17), 1.22 (s, CH_3-18), 1.41 (s, CH_3-19), 1.59 (s, CH_3-21), 3.83 (br d, J = 9.8, H-22), 1.41 (s, CH_3-26), 1.47 (s, CH_3-27), 1.93 (s, CH_3COO-25) [2]

^{13}C NMR (125 MHz, C_5D_5N) [2]:

Table 1

C-1	77.7	C-11	23.0	C-21	23.2
2	70.0	12	33.6	22	79.1
3	72.2	13	47.7	23	31.6
4	33.3	14	85.7	24	40.9
5	48.1	15	31.2	25	84.0
6	205.5	16		26	27.7
7	123.3	17	51.8	27	27.9
8	166.9	18	19.5	CH_3COO	23.9
9	36.6	19	22.0	CH_3COO	172.0
10	45.5	20	78.5		

References

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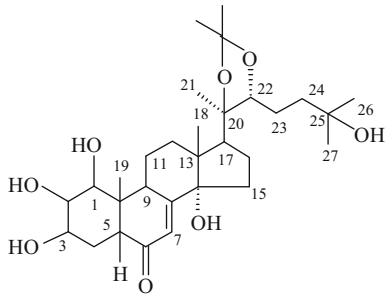
Integristerone A-20,22-Acetonide

CAS Registry Number: 245323-25-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{30}H_{48}O_8$: 536.3349

$[\alpha]_D^{20}$ + 31.6° (c 0.23, EtOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3401, 1655, 1077, 1062 [1]

ESI-MS m/z: 537 $[M + H]^+$, 519 $[M + H\text{–}H_2O]^+$, 501 $[M + H\text{–}2H_2O]^+$, 479 $[M + H\text{–}C_3H_6O]^+$, 461

[M + H–C_3H_8O–H_2O]$^+$, 443 [M + H–C_3H_8O–2H_2O]$^+$, 425 [M + H–C_3H_8O–3H_2O]$^+$ [1]

HR-ESI-MS m/z: for $C_{30}H_{48}O_8Na$ [M + Na]$^+$ calcd. 559.3247, found 559.3243 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 3.82 (Ha-1), 3.87 (t, J = 3.1, 3.1, Ha-2), 4.04 (He-3), 1.81 (Ha-4), 1.78 (He-4), 2.61 (dd, J = 4.4, 12.4, H-5), 5.84 (d, J = 2.4, H-7), 3.07 (br t, Ha-9), 1.73 (Ha-11), 1.70 (He-11), 2.09 (td, J = 5.0, 13.0, Ha-12), 1.83 (He-12), 1.97 (Ha-15), 1.62 (Hb-15), 1.87 (Ha-16), 2.04 (Hb-16), 2.31 (dd, J = 8.4, 9.2, H-17), 0.840 (s, CH_3-18), 1.074 (s, CH_3-19), 1.175 (s, CH_3-21), 3.68 (dd, J = 3.5, 8.2, Hb-22), 1.52 (Ha-23), 1.52 (Hb-23), 1.73 (Ha-24), 1.49 (Hb-24), 1.195 (s, CH_3-26), 1.204 (s, CH_3-27) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

C-1	76.41	C-10	43.75	C-19	20.07
2	68.49	11	21.89	20	85.83
3	70.98	12	32.31	21	22.58
4	33.49	13	49.0	22	83.30
5	46.79	14	85.15	23	24.70
6	205.58	15	31.74	24	42.21
7	122.18	16	22.33	25	71.11
8	166.85	17	51.53	26	29.34
9	35.68	18	17.67	27	29.49

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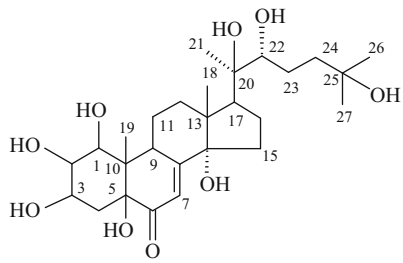
Integristerone B

CAS Registry Number: 68556-60-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1], *Rhaponticum integrifolium* [2]

$C_{27}H_{44}O_9$: 512.2985

Mp: 186–190°C (EtOAc–MeOH) [2]

$[\alpha]_D^{20}$ + 43.6 ± 2° (c 0.55, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3300–3500, 1680, 1635 [1], 3484, 1671 [1]

UV λ_{max}^{EtOH} nm (log ε): 240 (4.10) [2]

EI-MS m/z: 476 [M-2H_2O]$^+$ (3), 458 (11), 440 (13), 422 (5), 416 (5), 395 (3), 390 (65), 384 (6), 377 (26), 372 (10), 359 (17), 354 (19), 341 (19), 332 (7), 324 (21), 323 (4), 273 (65), 272 (74), 256 (47), 255 (94), 229 (40), 228 (53), 227 (38), 143 (18), 125 (20), 99 (100), 81 (53), 69 (48) [2]

FAB-MS m/z: 535 [M + Na]$^+$ (5), 513 [M + H]$^+$ (11), 495 (2), 477 (2), 459 (1), 201 (6), 185 (13), 149 (17), 135 (14), 125 (16), 109 (22), 99 (42), 93 (68), 81 (59), 69 (100) [1]

HR-MS m/z: for $C_{27}H_{45}O_9$ [M + H]$^+$ calcd. 513.3064, found 513.3090 [1]

CD (c, 0.10, dioxane): Δε = +2.1 (328 nm), Δε = −1.6 (255 nm) [2]

^{1}H NMR (100 MHz, C_5D_5N): 4.23 (m, H-1), 4.23 (m, H-2), 4.23 (m, H-3), 6.17 (br s, H-7), 3.45 (m, H-9), 1.09 (s, CH_3-18), 1.43 (s, CH_3-19), 1.43 (s, CH_3-21), 3.73 (m, H-22), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27) [2]

^{1}H NMR (500 MHz, CD_3OD): 3.90 (br d, Ha-1), 4.00 (t, Ha-2), 4.12 (br q, He-3), 2.14 (dd, Ha-4), 1.90 (dd, He-4), 5.88 (d, H-7), 3.08 (ddd, H-9), 1.82 (Ha-11), 1.75 (He-11), 2.10 (Ha-12), 1.86 (He-12), 1.98 (Ha-15), 1.59 (Hb-15), 1.74 (Ha-16), 1.98 (Hb-16), 2.38 (dd, H-17), 0.91 (s, CH_3-18), 1.14 (s, CH_3-19), 1.19 (s, CH_3-21), 3.32 (dd, H-22), 1.65 (Ha-23), 1.27 (Hb-23), 1.80 (Ha-24), 1.43 (Hb-24), 1.20 (s, CH_3-26), 1.19 (s, CH_3-27) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

C-1	76.06	C-10	47.81	C-19	13.95
2	69.05	11	22.63	20	77.87
3	70.01	12	32.61	21	21.02
4	37.57	13	48.46	22	78.42
5	80.36	14	84.97	23	27.34
6	202.33	15	31.79	24	42.37

(*continued*)

Table 1 (continued)

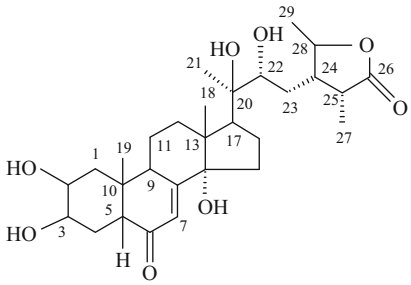
7	120.37	16	21.40	25	71.31
8	166.63	17	50.48	26	29.72
9	39.71	18	18.02	27	28.94

References

1. K. Vokas, M. Budesinsky, J. Harmatha, Coll. Czech. Chem. Comm. **67**, 124 (2002)
2. U.A. Baltaev, M.B. Gorovits, N.D. Abdullaev, Ya.V. Rashkes, M.R. Yagudaev, N.K. Abubakirov, Chem. Nat. Comp. **14**, 388 (1978)

Isocyasterone

CAS Registry Number: 54082-42-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyathula capitata* [1, 2]

$C_{29}H_{44}O_8$: 520.3036

Mp: amorphous [1]

IR (KBr) ν_{max} cm^{-1}: 1755, 1650 [1, 2]

UV λ_{max}^{MeOH} nm (log ε): 242 (4.05) [1, 2]

EI-MS m/z: 502 $[M\text{-}H_2O]^+$, 363, 345, 327, 201, 183, 157, 113 [1, 2]

CD (c, dioxane): $[\theta]_{341} + 4.77 \times 10^3$; $[\theta]_{248} - 10.5 \times 10^3$ [1]

^{1}H NMR (100 MHz, C_5D_5N): 6.16 (d, H-7), 1.16 (s, CH_3-18), 1.04 (s, CH_3-19), 1.52 (s, CH_3-21), 1.24 (d, CH_3-27), 1.19 (d, CH_3-29) [1]

Pharm./Biol.: *Sarcophaga peregrine* bioassay: highly active [2].

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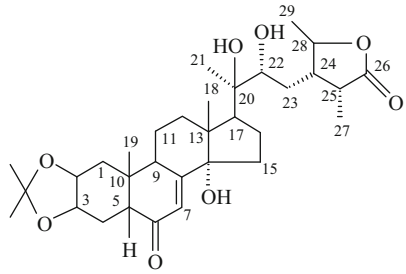
Isocyasterone-2,3-Acetonide

CAS Registry Number: 860303-34-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyathula officinalis* [1]

$C_{32}H_{48}O_8$: 560.3349

Mp: 260–262°C [1]

$[\alpha]_D^{25}$ + 42.2° (c 0.12, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3458, 1754, 1656 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (3.98) [1]

ESI-MS m/z: 559 $[M\text{-}H]^-$, 583 $[M + Na]^+$, 1143 $[2M + Na]^+$ [1]

HR-ESI-MS m/z: for $C_{32}H_{47}O_8$ $[M\text{-}H]^-$ calcd. 559.3270, found 559.3271 [1]

^{1}H NMR (J/Hz, C_5D_5N): 4.18 (m, Ha-2), 4.08 (br s, He-3), 2.56 (d, J = 12.0, H-5), 6.19 (s, H-7), 3.58 (br s, H-9), 2.48 (q, J = 11.2, Ha-16), 3.13 (t, J = 9.0, H-17), 1.18 (s, CH_3-18), 0.99 (s, CH_3-19), 1.59 (s, CH_3-21), 3.80 (d, J = 10.8, H-22), 3.19 (q, J = 7.8, H-25), 1.25 (d, J = 7.8, CH_3-27), 4.63 (q, J = 6.6, H-28), 1.26 (d, J = 6.6, CH_3-29), Other: 1.54 and 1.30 (s, 2,3-iPr) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

C-1	38.0 (t)	C-11	20.9 (t)	C-21	21.1 (q)
2	72.2 (d)	12	31.4 (t)	22	74.8 (d)

(*continued*)

Table 1 (continued)

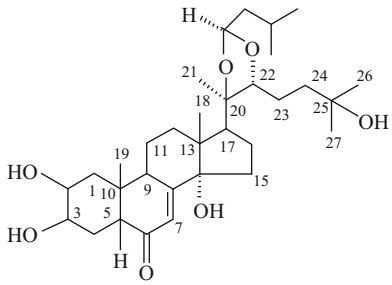
3	71.9 (d)	13	48.1 (s)	23	26.4 (d)
4	26.7 (t)	14	83.8 (s)	24	39.6 (d)
5	51.3 (d)	15	31.7 (t)	25	26.4 (d)
6	202.0 (s)	16	21.4 (t)	26	179.8 (s)
7	121.8 (d)	17	49.7 (d)	27	12.6 (q)
8	165.1 (s)	18	17.5 (q)	28	78.4 (d)
9	34.8 (d)	19	23.6 (q)	29	17.3 (q)
10	37.8 (s)	20	76.5 (s)	20,22-iPr	28.6 (q)
					26.4 (q)
					107.9 (s)

References

1. R. Zhou, B.G. Li, G.L. Zhang, J. Asian Nat. Prod. Res. **7**, 245 (2005)

20,22-Isovaleriate-5β-Cholest-7-en-2β,3β,14α,20R,22R,25-Hexahydroxy-6-on

CAS Registry Number: 404589-62-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene claviformis* [1]

$C_{32}H_{52}O_7$: 548.3713

CI-MS m/z: 566 $[M + H + NH_3]^+$, 549 $[M + H]^+$, 531 $[M + H–H_2O]^+$, 464, 462, 447, 445, 429, 427 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.38 (Ha-1), 1.88 (He-1), 3.99 (m, Ha-2), 4.08 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.36 (t-like, H-5), 5.98 (d, J = 2.0, H-7), 3.11 (m, H-9), 1.73 (Ha-11), 1.86 (He-11), 1.96 (Ha-12), 1.96 (He-12), 2.05 (Ha-15), 1.68 (Hb-15), 1.95 (Ha-16), 1.95 (Hb-16), 2.32 (t, J = 8.1, H-17), 0.85 (s, CH_3-18), 1.00 (s, CH_3-19), 1.27 (s, CH_3-21), 3.82 (m, H-22), 1.55 (Ha-23), 1.73 (Hb-23), 1.55 (Ha-24), 1.55 (Hb-24), 1.237 (s, CH_3-26), 1.241 (s, CH_3-27), Other: 5.29 (t, J = 5.1, H), 1.54 (H), 1.75 (H), 0.943 (d, J = 6.5, CH_3), 0.948 (d, J = 6.5, CH_3) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

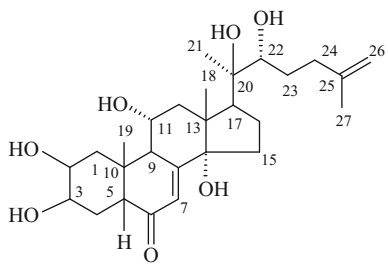
C-1	36.4	C-12	31.9	C-23	
2		13	47.9	24	41.4
3	68.2	14		25	72.7
4	32.3	15		26	28.7
5	51.3	16		27	28.7
6		17	50.7	Other: a	102.7
7		18	17.8	b	24.1
8		19	24.2	c	44.0
9	34.9	20	86.4	d-CH_3	23.3
10	34.9	21	20.1	d'-CH_3	23.3
11		22	83.2		

References

1. Z. Sadikov, Z. Saatov, M. Garcia, J.P. Girault, R. Lafont, Chem. Nat. Comp. **37**, 262 (2001)

Isovitexirone

CAS Registry Number: 160262-51-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotis arachnoidea* [1], *C. longifolia* [2], *Leuzea carthamoides* [3, 4]
$C_{27}H_{42}O_7$: 478.2930
IR (KBr) ν_{max} cm^{-1}: 3391, 1653, 1581 [3, 4]
EI-MS m/z: 478 (0), 461 (1), 442 (2), 426 (2), 408 (1), 393 (1), 379 (1), 361 (7), 360 (8), 343 (28), 325 (15), 267 (20), 171 (25), 69 (37), 55 (42), 43 (100), 41 (70) [3]
FAB-MS m/z: 501$[M + Na]^+$ (56), 479 $[M + H]^+$ (65), 461 (100), 443 (22), 278 (56) [4]
HR-MS m/z: for $C_{27}H_{43}O_7$ $[M + H]^+$ calcd. 479.3009, found 479.2993 [4]
^{1}H NMR (500 MHz, J/Hz, $(CH_3)_2CO$-d_6): 4.00 (ddd, J = 3.5, 4.0, 11.7, Ha-2), 3.89 (m, J = 3.0, He-3), 2.64 (dd, J = 4.4, 12.5, H-5), 5.71 (d, J = 2.6, H-7), 3.16 (dd, J = 2.6, 9.0, H-9), 2.45 (t, J = 9.1, H-17), 0.89 (s, CH_3-18), 1.02 (s, CH_3-19), 1.20 (s, CH_3-21), 3.38 (dd, J = 1.5, 10.6, H-22), 4.70 (br s, 2H-26), 1.72 (br s, CH_3-27) [3]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 2.58 (dd, Ha-1), 1.36 (dd, He-1), 4.00 (ddd, Ha-2), 3.54 (dq, He-3), 1.77 (Ha-4), 1.68 (He-4), 2.32 (dd, H-5), 5.79 (d, H-7), 3.14 (dd, H-9), 4.09 (ddd, He-11), 2.20 (dd, Ha-12), 2.14 (dd, He-12), 1.95 (Ha-15), 1.56 (Hb-15), 1.70 (Ha-16), 1.95 (Hb-16), 2.40 (H-17), 0.86 (s, CH_3-18), 1.05 (s, CH_3-19), 1.20 (s, CH_3-21), 3.35 (dd, H-22), 1.68 (Ha-23), 1.32 (Hb-23), 2.27 (Ha-24), 2.06 (Hb-24), 4.72 (um, H-26), 4.58 (um, H′-26), 1.74 (br s, CH_3-27) [4]
^{13}C NMR (125.7 MHz, CD_3OD) [4]:

Table 1

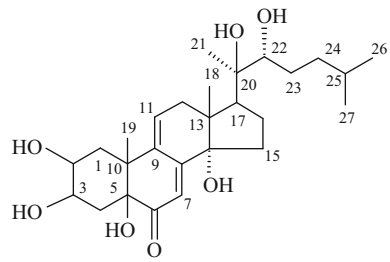
C-1	39.89	C-10	39.06	C-19	24.61
2	69.21	11	69.50	20	77.65
3	68.55	12	43.76	21	30.84
4	33.28	13	49.00	22	77.05
5	52.77	14	84.40	23	20.97
6	206.66	15	31.81	24	36.21
7	122.72	16	21.46	25	146.87
8	165.71	17	50.26	26	110.75
9	42.92	18	18.86	27	22.70

References

1. C. Tan, J. Wang, X. Li, Y. Du, X. Bai, Zhongguo Yaoxue Zazhi **40**, 1537 (2005)
2. S. Crouzet, A. Maria, L. Dinan, R. Lafont, J.P. Girault, Arch. Insect Biochem. Physiol. **72**, 194 (2009)
3. J. Pis, M. Bydesinsky, K. Vokas, V. Laudova, J. Harmatha, Phytochemistry **37**, 707 (1994)
4. K. Vokas, M. Budesinsky, J. Harmatha, Coll. Czech. Chem. Comm. **67**, 124 (2002)

Kaladasterone

CAS Registry Number: 52591-06-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Ipomoea calonyction* [1–3]
$C_{27}H_{42}O_7$: 478.2930
Mp: 242–243°C (MeOH-acetone) [1, 2]
$[\alpha]_D^{24}$ + 79.3° (c, MeOH) [1, 2]
IR (KBr) ν_{max} cm^{-1}: 3200–3600, 1652, 1605 [1]
UV λ_{max}^{MeOH} nm (ε): 298 (10800) [1]
EI-MS m/z: 478 $[M]^+$, 460, 445, 442, 377, 359 (100), 341, 323, 305, 145, 109, 105, 99, 91, 85, 83, 81 [1, 3]
HR-MS m/z: for $C_{27}H_{42}O_7$ $[M]^+$ calcd. 478.2930, found 478.2941 [1]
CD (c, 1.76, dioxane): Δε = +8.7 (314 nm), Δε = 0 (322 nm), Δε = −12.8 (301 nm), Δε = 0 (260 nm), Δε = +13.5 (249 nm), Δε = 0 (239 nm), Δε = −2.98 (221 nm) [3]
^{1}H NMR (J/Hz, DMSO-d_6): 5.65 (s, H-7), 6.18 (m, H-11), 0.73 (s, CH_3-18), 0.96 (s, CH_3-19), 1.06 (s, CH_3-21), 0.86 (d, J = 6.0, CH_3-26), 0.86 (d, J = 6.0, CH_3-27) [1, 2]
^{13}C NMR (C_5D_5N) [1, 3]:

Table 1

C-1	38.6	C-10	45.4	C-19	17.9
2	67.9	11	132.9	20	76.5

(*continued*)

Table 1 (continued)

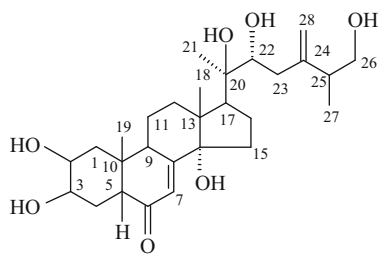
3	69.5	12	38.6	21	21.2
4	35.2	13	47.4	22	76.8
5	79.7	14	83.2	23	30.2
6	201.1	15	31.3	24	37.0
7	116.8	16	21.5	25	28.2
8	156.0	17	49.9	26	22.4
9	137.4	18	26.3	27	23.2

References

1. L. Canonica, B. Danieli, G. Ferrari, M.A. Haimova, J. Krepinsky, Experientia **29**, 1062 (1973)
2. L. Canonica, B. Danieli, G. Ferrari, J. Krepinsky, I. Weisz-Vincze, Phytochemistry **14**, 525 (1975)
3. L. Canonica, B. Danieli, G. Ferrari, J. Krepinsky, M.A. Haimova, Gazz. Chim. Ital. **107**, 123 (1975)

Kancollosterone

CAS Registry Number: 848656-10-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Chenopodium quinoa* [1]

$C_{28}H_{44}O_7$: 492.3087

Mp: amorphous [1]

$[\alpha]_D^{23}$ + 25.1° (c 0.001, MeOH)

IR (KBr) ν_{max} cm^{-1}: 3426, 1658, 1052 [1]

ESI-MS m/z: 491 $[M\text{-}H]^-$ [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.16 (ddd, J = 3.2, 4.0, 12.0, Ha-2), 4.22 (q, J = 2.9, He-3), 6.26 (d, J = 2.6, H-7), 3.59 (ddd, J = 2.6, 7.0, 11.2, H-9), 1.22 (s, CH_3-18), 1.06 (s, CH_3-19), 1.58 (s, CH_3-21), 4.08 (dd, J = 1.7, 11.0, H-22), 3.86 (m, CH_2OH-26), 1.36 (s, CH_3-27), 5.65 (d, J = 1.5, Ha-28), 5.27 (d, J = 1.5, Hb-28) [1]

^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

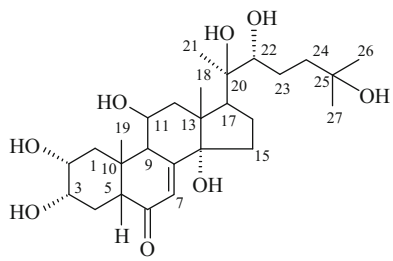
C-1	37.8	C-11	21.1	C-21	21.7
2	67.7	12	31.7	22	77.8
3	66.6	13	48.1	23	27.6
4	32.4	14	84.3	24	150.2
5	51.4	15	31.9	25	42.7
6	203.8	16	21.6	26	69.6
7	121.3	17	50.3	27	29.5
8	166.5	18	17.9	28	109.9
9	34.5	19	24.5		
10	38.3	20	77.0		

References

1. I. Dini, G.C. Tenore, A. Dini, Food Chemistry **92**, 125 (2005)

Lesterone

CAS Registry Number: 256509-87-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{27}H_{44}O_8$: 496.3036

Mp: amorphous [1]

IR (KBr) ν_{max} cm^{-1}: 3360–3470, 1650 [1]

EI-MS m/z: 460 $[M\text{-}2H_2O]^+$, 442 $[M\text{-}3H_2O]^+$, 424 $[M\text{-}4H_2O]^+$, 409 $[M\text{-}4H_2O\text{–}Me]^+$, 406

$[M\text{-}5H_2O\text{–}Me]^+$, 388 $[M\text{-}6H_2O]^+$, 379 $[M\text{-}117]^+$, 373 $[M\text{-}6H_2O\text{–}Me]^+$, 361 $[M\text{-}117\text{-}H_2O]^+$, 343 $[M\text{-}117\text{-}2H_2O]^+$, 325 $[M\text{-}117\text{-}3H_2O]^+$, 99 $[C_6H_{11}O]^+$, 81 $[C_8H_9]^+$ [1]

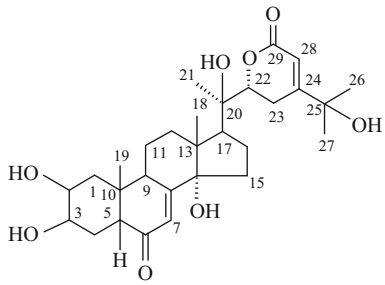
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.14 (q, J = 3.5, H-2), 4.25 (dt, J = 12.0, 4.0, H-3), 6.11 (br s, H-7), 3.53 (m, H-9), 4.04 (dq, H-11), 2.81 (t, H-17), 1.01 (s, CH_3-18), 1.05 (s, CH_3-19), 1.44 (s, CH_3-21), 3.72 (dd, H-22), 1.24 (s, CH_3-26), 1.24 (s, CH_3-27) [1]

References

1. E.B. Borovikova, U.A. Baltaev, Chem. Nat. Comp. **35**, 182 (1999)

Leuzeasterone

CAS Registry Number: 424788-97-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{29}H_{42}O_8$: 518.2879

$[\alpha]_D^{20}$ + 51.6° (c 0.41, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3340, 1705, 1653 [1]

FAB-MS m/z:, 519 (19), 501 (79), 485 (15), 465 (7), 347 (9), 331 (11) 329 (11), 303 (75), 276 (22), 185 (100)

HR-MS m/z: for $C_{29}H_{43}O_8$ $[M + H]^+$ calcd. 519.2958, found 519.3046

CD (c, MeOH): Δε = +7.41 (206 nm), Δε = −1.00 (237 nm), Δε = +1.29 (267 nm), Δε = +1.29 (329 nm) [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (Ha-1), 1.44 (He-1), 3.84 (ddd, Ha-2), 3.95 (br q, He-3), 1.73 (Ha-4), 1.70 (He-4), 2.39 (dd, H-5), 5.82 (d, H-7), 3.17 (H-9), 1.82 (Ha-11), 1.71 (He-11), 2.21 (Ha-12), 1.83 (He-12), 2.00 (Ha-15), 1.64 (Hb-15), 1.77 (Ha-16), 2.01 (Hb-16), 2.49 (dd, H-17), 0.90 (s, CH_3-18), 0.97 (s, CH_3-19), 1.35 (s, CH_3-21), 4.23 (dd, H-22), 2.62 (dd, Ha-23), 2.40 (ddd, Hb-23), 1.40 (s, CH_3-26), 1.38 (s, CH_3-27), 6.02 (d, H-28) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

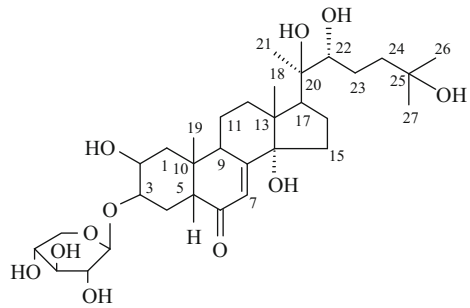
C-1	37.35	C-11	21.49	C-21	21.42
2	68.70	12	32.42	22	84.90
3	68.51	13	49.00	23	26.45
4	32.82	14	85.30	24	169.78
5	51.78	15	31.78	25	72.65
6	206.40	16	21.54	26	28.38
7	122.34	17	50.52	27	27.77
8	168.22	18	18.20	28	113.16
9	35.05	19	24.38	29	167.50
10	39.30	20	76.46		

References

1. K. Vokac, M. Budesinsky, J. Harmata, Coll. Czech. Chem. Comm. **67**, 124 (2002)

Limnantheoside A

CAS Registry Number: 188358-79-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Limnanthes alba* [1], *L. douglasii* [2]
$C_{32}H_{52}O_{11}$: 612.3509
Mp: amorphous [1]
UV λ_{max}^{EtOH} nm (log ε): 241 (3.96) [2]
CI-MS m/z: 630 $[M + H + NH_3]^+$, 613 $[M + H]^+$, 595 $[M + H–H_2O]^+$, 559 $[577\text{-}H_2O]^+$, 541 $[559\text{-}H_2O]^+$, 496, 481 $[M + H–C_5H_8O_4]^+$, 463, 461, 445, 427, 363, 345, 301 [2]
LSI-MS m/z: 613 $[M + H]^+$ [1]
^{1}H NMR (500 MHz, J/Hz, D_2O): 1.46 (t, J = 13.0, Ha-1), 1.90 (He-1), 4.03 (dt, Ha-2), 4.15 (m, He-3), 1.75 (Ha-4), 1.90 (He-4), 2.43 (dd, J = 3.5, 13.5, H-5), 5.98 (d, J = 2.5, H-7), 3.12 (m, H-9), 1.75 (Ha-11), 1.86 (He-11), 1.95 (Ha-12), 1.75 (He-12), 2.04 (Ha-15), 1.65 (Hb-15), 1.85 (Ha-16), 1.80 (Hb-16), 2.33 (t, J = 9.6, H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.25 (s, CH_3-21), 3.43 (dd, J = 1.4, 10.7, H-22), 1.33 (Ha-23), 1.65 (Hb-23), 1.52 (dt, J = 3.4, 12.8, Ha-24), 1.80 (Hb-24), 1.23 (s, CH_3-26), 1.24 (s, CH_3-27), Other: β-D-Xylp′: 4.48 (d, J = 7.8, Ha-1), 3.33 (dd, J = 7.8, 9.3, Ha-2), 3.47 (t, J = 9.3, Ha-3), 3.65 (ddd, J = 5.5, 9.2, 10.5, Ha-4), 3.96 (dd, J = 5.5, 11.6, Ha-5), 3.29 (dd, J = 10.5, 11.6, He-5) [2]
^{13}C NMR (125 MHz, D_2O) [2]:

Table 1

C-1	37.2	C-12	31.8	C-23	27.0
2	67.6	13	48.3	24	41.6
3	75.3	14	86.3	25	72.9
4	29.1	15	31.3	26	28.5
5	51.3	16	20.9	27	29.2
6	209.6	17	50.1	Glc′-1	101.8
7	122.1	18	18.0	2	73.9
8	167.9	19	24.0	3	77.0
9	34.8	20	78.1	4	70.5
10	38.9	21	20.3	5	66.3
11	21.0	22	78.3		

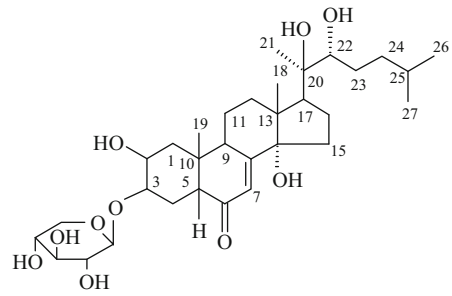
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.6 \times 10^{-6}$ M [1].

References

1. Y. Meng, P. Whiting, V. Sik, H.H. Rees, L. Dinan, Z. Naturforsch. **56 c**, 988 (2001)
2. S.D. Sarker, J.P. Girault, R. Lafont, L. Dinan, Phytochemistry **44**, 513 (1997)

Limnantheoside B

CAS Registry Number: 188358-80-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Limnanthes douglasii* [1]
$C_{32}H_{52}O_{10}$: 596.3560
Mp: gum [1]
UV λ_{max}^{EtOH} nm (log ε): 242 (4.00) [1]
CI-MS m/z: 614 $[M + H + NH_3]^+$, 597 $[M + H]^+$, 579 $[M + H–H_2O]^+$, 561 $[579\text{-}H_2O]^+$, 543, 512, 481, 465 $[M + H–C_5H_8O_4]^+$, 447, 429, 363, 345, 191, 166, 150, 116, 102 [1]
^{1}H NMR (500 MHz, J/Hz, D_2O): 1.46 (t, J = 13.0, Ha-1), 1.90 (He-1), 4.03 (dt, Ha-2), 4.15 (m, He-3), 1.75 (Ha-4), 1.90 (He-4), 2.43 (dd, J = 3.5, 13.5, H-5), 5.98 (d, J = 2.5, H-7), 3.12 (m, H-9), 1.75 (Ha-11), 1.86 (He-11), 1.95 (Ha-12), 1.75 (He-12), 2.05 (Ha-15), 1.65 (Hb-15), 1.85 (Ha-16), 1.80 (Hb-16), 2.33 (t, J = 9.6, H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.23 (s, CH_3-21), 3.45 (dd, J = 1.4, 10.7, H-22), 1.25 (Ha-23), 1.60 (Hb-23), 1.37 (Ha-24), 1.26 (Hb-24), 1.55 (H-25), 1.23 (s, CH_3-26), 0.91 (d, J = 6.8, CH_3-27), Other: β-D-Xylp′: 4.48 (d, J = 7.8, Ha-1), 3.33 (dd, J = 7.8, 9.3, Ha-2), 3.47 (t, J = 9.3, Ha-3), 3.65 (ddd, J = 5.5, 9.2, 10.5, Ha-4), 3.96 (dd, J = 5.5, 11.6, Ha-5), 3.29 (dd, J = 10.5, 11.6, He-5) [1]
^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

C-1	37.2	C-12	31.8	C-23	29.8
2	67.6	13	48.3	24	36.9
3	75.3	14	86.3	25	28.4
4	29.1	15	31.3	26	22.6
5	51.3	16	20.9	27	23.5

(*continued*)

Table 1 (continued)

6		17	50.1	Xyl′-1	101.8
7	122.1	18	18.0	2	73.9
8		19	24.0	3	77.0
9	34.8	20	78.9	4	70.5
10	38.9	21	20.5	5	66.3
11	21.0	22	77.9		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.5 \times 10^{-6}$ M [2].

References

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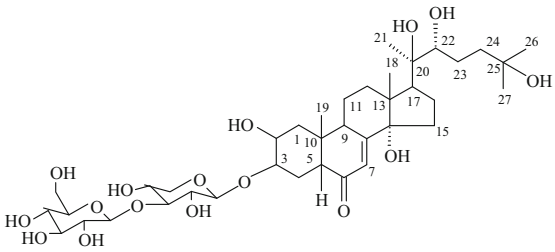
Limnantheoside C

CAS Registry Number: 405291-86-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Limnanthes alba* [1]

$C_{38}H_{62}O_{16}$: 774.4037

Mp: gum [1]

UV λ_{max}^{MeOH} nm (log ε): 243 (4.12) [1]

LSI-MS m/z: 775 $[M + H]^+$ [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.42 (Ha-1), 1.84 (He-1), 3.85 (m, Ha-2), 4.06 (m, He-3), 1.69 (Ha-4), 1.88 (He-4), 2.43 (dd, J = 3.8, 13.0, H-5), 5.82 (d, J = 2.2, H-7), 3.15 (m, H-9), 1.68 (Ha-11), 1.82 (He-11), 2.14 (ddd, J = 5.0, 13.0, 13.0, Ha-12), 1.88 (He-12), 1.96 (Ha-15), 1.59 (Hb-15), 2.00 (Ha-16), 1.73 (Hb-16), 2.39 (m, H-17), 0.89 (s, CH_3-18), 0.97 (s, CH_3-19), 1.20 (s, CH_3-21), 3.33 (H-22), 1.29 (Ha-23), 1.67 (Hb-23), 1.81 (Ha-24), 1.42 (Hb-24), 1.19 (s, CH_3-26), 1.20 (s, CH_3-27), Other: β-D-Glcp′: 4.38 (d, J = 7.3, Ha-1), 3.49 (dd, J = 7.3, 8.9, Ha-2), 3.54 (t, J = 8.9, Ha-3), 3.63 (ddd, J = 5.1, 8.9, 11.0, Ha-4), 3.94 (dd, J = 5.1, 11.5, Ha-5), 3.26 (dd, J = 11.0, 11.5, He-5), β-D-Xylp″: 4.61 (d, J = 7.6, Ha-1), 3.28 (dd, J = 7.6, 9.0, Ha-2), 3.40 (t, J = 9.0, Ha-3), 3.29 (t, J = 9.0, Ha-4), 3.32 (ddd, J = 2.0, 5.8, 9.0, Ha-5), 3.64 (dd, J = 5.8, 11.8, Ha-6), 3.88 (dd, J = 2.0, 11.8, He-6) [1]

^{13}C NMR (100 MHz, CD_3OD) [1]:

Table 1

C-1	37.2	C-11	20.2	C-21	19.6	Xylp′-4	68.5
2	66.6	12	31.1	22	76.8	5	65.2
3	75.1	13		23	25.9	Glc″-1	103.6
4	29.0	14	83.8	24	41.0	2	74.1
5	50.3	15	30.4	25	69.9	3	76.5
6	204.9	16	20.1	26	28.3	4	72.2
7	120.7	17	49.1	27	27.6	5	77.0
8	166.9	18	16.6	Xylp′-1	101.8	6	61.3
9	33.7	19	22.8	2	72.4		
10	37.8	20	76.6	3	85.5		

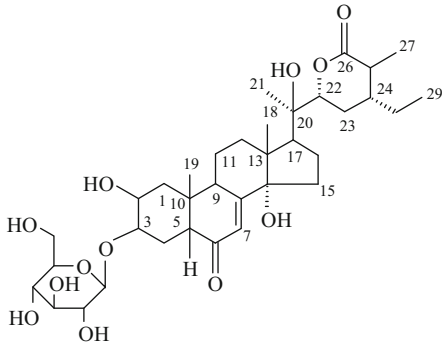
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.3 \times 10^{-6}$ M.

References

1. Y. Meng, P. Whiting, V. Sik, H.H. Rees, L. Dinan, Z. Naturforsch **56 c**, 988 (2001)

Lygodiumsteroside A

CAS Registry Number: 1186470-15-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Lygodium japonicum* [1]

$C_{35}H_{54}O_{12}$: 666.3615

Mp: 245–246°C [1]

IR (KBr) ν_{max} cm^{-1}: 3416, 1730, 1646 [1]

UV λ_{max}^{MeOH} nm: 243 [1]

ESI-MS m/z: 665.6 $[M-H]^-$ [1]

HR-ESI-MS m/z: for $C_{35}H_{54}O_{12}Cl$ $[M + Cl]^+$ calcd. 701.3309, found 701.3309 [1]

^{1}H NMR (600 MHz, J/Hz, C_5D_5N): 1. 72 (t, J = 12.6, Ha-1), 2.05 (m, He-1), 4.06 (br d, J = 11.4, Ha-2), 4.29 (br s, He-3), 1.66 (m, Ha-4), 2.16 (m, He-4), 2.90 (m, H-5), 6.18 (br s, H-7), 3.50 (br t, H-9), 1.64 (Ha-11), 1.77 (He-11), 1.86 (m, Ha-12), 2.57 (m, He-12), 1.86 (m, Ha-15), 2.12 (m, Hb-15), 2.05 (m, Ha-16), 2.39 (m, Hb-16), 2.93 (m, H-17), 1.09 (s, CH_3-18), 0.86 (s, CH_3-19), 1.44 (s, CH_3-21), 4.44 (dd, J = 11.5, 2.5, H-22), 1.41 (m, Ha-23), 2.05 (m, Hb-23), 1.41 (H-24), 2.17 (m, H-25), 1.28 (d, J = 7.2, CH_3-27), 0.67 (t, J = 7.2, CH_3-29), Other: β-D-Glcp′: 4.89 (d, J = 7.8, H-1), 4.01 (t-like, H-2), 4.18 (overlap, H-3), 4.06 (overlap, H-4), 3.90 (t-like, H-5), 4.31 (m, H-6), 4.49 (br d, J = 11.5, H-6′) [1]

^{13}C NMR (150 MHz, C_5D_5N) [1]:

Table 1

C-1	38.0	C-13	47.2	C-25	40.7
2	66.8	14	83.4	26	173.9
3	77.1	15	31.1	27	15.2
4	29.9	16	20.7	28	25.9
5	50.7	17	49.2	29	9.6
6	202.3	18	17.3	Glc′-1	103.5
7	121.1	19	23.4	2	74.0
8	165.4	20	75.1	3	78.0
9	33.5	21	20.7	4	70.9
10	38.4	22	85.3	5	77.8
11	20.3	23	29.0	6	61.9
12	31.2	24	39.5		

References

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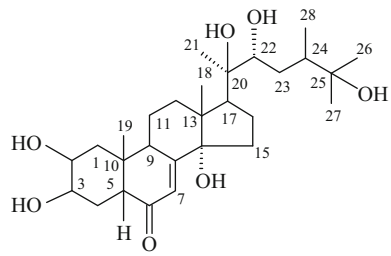
Makisterone A

CAS Registry Number: 20137-14-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga australis* [1], *A. chamapitys* [2], *A. iva* [3, 4], *A. laxmanni* [1], *A. macrosperma* var. *breviflora* [5], *A. multiflora* [6], *Centaurea americana* [7], *Dacridium intermedium* [8], *Diplazium donianum* [9], *Diploclisia glaucescens* [10], *Fibraurea tinctoria* [11], *Ipomoea calonyction* [12], *Leuzea carthamoides* [13], *Lychnis flos-cuculi* [14], *Microsorum maximum, M. membranifolium, M. punctatum* [15], *Microsorum scolopendria* [16], *Palisota schweinfurthii* [17], *Penstemon venustus* [18], *Podocarpus elatus* [19], *P. macrophyllus* [20], *Serratula coronata* [21], *Taxus cuspidata* [22], *Vitex leptobortys* [23]

$C_{28}H_{46}O_7$: 494.3243

Mp: 268–269°C [3], 263–265°C (dec.) [8, 20], 286–287°C [12]

$[\alpha]_D^{20}$ + 83.3° (c 1.0, MeOH) [12], $[\alpha]_D^{20}$ + 60.3° (dioxane) [20]

IR (Nujol) ν_{max} cm^{-1}: 3200–3600, 1650, 1610 [12]

IR (KBr) ν_{max} cm^{-1}: 3500, 1655, 1630 [3], 3420, 1655, 1630 [20]

UV λ_{max}^{MeOH} nm (ε): 243 (18000) [3], 242 (11700) [8], 244 (12400) [12], 243 (12400) [20]

EI-MS m/z: 476 $[M-H_2O]^+$, 458, 440, 365, 345, 327 [3], 494 $[M]^+$(1), 476 (1), 458 (2), 448 (8), 363 (18), 346 (22), 345 (58), 344 (13), 156 (18), 131 (12), 113 (100), 95 (45), 91 (30), 85 (30), 83 (48), 70 (69) [8]

HR-MS m/z: for $C_{28}H_{44}O_6$ $[M-H_2O]^+$ calcd. 476.3137, found 476.3124 [3]

CD (c, 0.041, dioxane): $[\theta]_{385}$ 0, $[\theta]_{339}$ +5.474 × 10^3, $[\theta]_{275–290}$ 0, $[\theta]_{247}$ −11.35 × 10^3, $[\theta]_{230}$ 0 [8]

^{1}H NMR (J/Hz, C_5D_5N): 6.28 (H-7), 1.24 (s, CH_3-18), 1.10 (s, CH_3-19), 1.60 (s, CH_3-21), 1.35 (s, CH_3-26), 1.32 (s, CH_3-27), 1.05 (d, J = 6.0, CH_3-28) [2], 6.20 (d, J = 2.0, H-7), 1.24 (s, CH_3-18), 1.06 (s, CH_3-19), 1.57 (s, CH_3-21), 1.32 (s, CH_3-26), 1.32 (s, CH_3-27), 1.07 (d, J = 7.0, CH_3-28) [12]

^{1}H NMR (500 MHz, J/Hz, Me_2CO-d_6): 3.82 (dt, J = 3.8, 3.8, 11.3, Ha-2), 3.90 (um, He-3), 2.33 (dd, J = 7.1, 10.2, H-5), 5.71 (d, J = 2.6, H-7), 3.16 (ddd, J = 2.6, 7.0, 10.0, H-9), 2.43 (t, J = 9.1, H-17), 0.92 (s, CH_3-18), 0.94 (s, CH_3-19), 1.19 (s, CH_3-21), 3.46 (br d, J < 2.0, 11.0, H-22), 1.15 (s, CH_3-26), 1.11 (s, CH_3-27), 0.92 (d, J = 6.8, CH_3-28) [13]

^{13}C NMR (125.7 MHz, CD_3OD) [13]:

Table 1

C-1	37.4	C-11	21.5	C-21	21.0
2	68.7	12	32.5	22	75.4
3	68.5	13	49.0	23	34.5
4	32.9	14	82.3	24	41.7
5	51.8	15	31.8	25	73.8
6	206.5	16	21.4	26	27.5
7	122.2	17	50.4	27	26.1
8	168.0	18	18.1	28	11.9
9	35.1	19	24.4		
10	39.3	20	78.0		

Pharm./Biol.: *Brine shrimp* lethality assay (LD_{50} = 460 µg/mL) [7], Inhibition of Human CYP3A4- Catalyzed Nifedipine oxidation activity: IC50 > 100 µM (inactive) [11], *Chilo suppressalis* bioassay: strong moulting hormone activity [24], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.3 \times 10^{-8}$ M [25–29].

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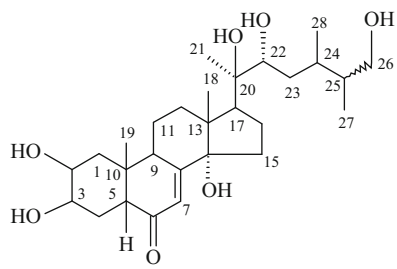
Makisterone B

CAS Registry Number: 20512-31-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Podocarpus macrophyllus* [1, 2]

$C_{28}H_{46}O_7$: 494.3243

Mp: 172–173°C (dec.) [2]

$[\alpha]_D$ + 53.2° (dioxane) [2]

IR (KBr) ν_{max} cm^{-1}: 3400, 1660, 1630 [2]

UV λ_{max}^{MeOH} nm (ε): 243 (11100) [2]

EI-MS m/z: 476 $[M\text{-}H_2O]^+$, 363, 345, 131 (19), 113 (94), 95 (39), 43 (100) [2]

^{1}H NMR (J/Hz, C_5D_5N): 1.16 (s, CH_3-18), 1.04 (s, CH_3-19), 1.54 (s, CH_3-21), 1.00 (d, J = 6.0, CH_2OH-26), 1.00 (d, J = 6.0, CH_3-27), 0.90 (d, J = 6.0, CH_3-29) [2]

Pharm./Biol.: *Chilo suppresalis* dipping assay: strong insect moulting activity [3].

References

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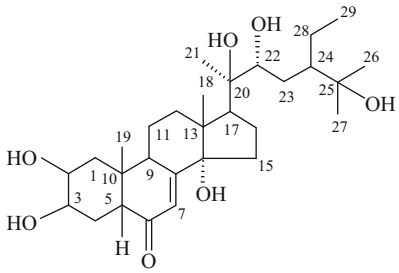
Makisterone C (Lemmasterone, Podecdysone A)

CAS Registry Number: 19974-41-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Diploclisia glaucescens* [1], *Lemmaphyllum microphyllum* [2], *Leuzea carthamoides* [3, 4], *Microsorum membranifolium* [5], *Microsorum scolopendria* [6], *Penstemon venustus* [7], *Podocarpus elatus* [8], *P. macrophyllus* [9], *Serratula coronata* [10], *S. tinctoria* [11], *Sida spinosa* [12]

$C_{29}H_{48}O_7$: 508.3400

Mp: 268–270°C [1], 258–259°C [2], 266–270°C (EtOAc-MeOH) [4], 262–264 (dec.) °C [8], 263–265°C (dec.) [9]

$[\alpha]_D^{25}$ + 54.8° (c 1.3, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3400, 1643 [2], 3410, 1654 [3], 3470, 1650 [8], 3400, 1650, 1630 [9]

UV λ_{max}^{EtOH} nm: 243.4 [1], 244 [2], 242 [4], 243 (ε 14000) [9]

UV λ_{max}^{MeOH} nm: 243 (ε 10900) [9]

EI-MS m/z: 508 $[M]^+$, 490 $[M\text{-}H_2O]^+$, 472 $[M\text{-}2H_2O]^+$, 454 $[M\text{-}3H_2O]^+$, 436 $[M\text{-}4H_2O]^+$, 493 $[M\text{-}CH_3]^+$, 475 $[M\text{-}H_2O\text{–}CH_3]^+$, 457 $[M\text{-}2H_2O\text{-}CH_3]^+$, 439 $[M\text{-}3H_2O\text{–}CH_3]^+$, 363 $[M\text{-}145]^+$, 345 $[M\text{-}145\text{-}H_2O]^+$, 327 $[M\text{-}145\text{-}2H_2O]^+$, 145 $[M\text{-}363]^+$, 127 $[M\text{-}363\text{-}H_2O]^+$, 109 $[M\text{-}363\text{-}2H_2O]^+$ [2]; 481 $[M\text{-}27]^+$ (1), 463 (1), 455 (2), 363 (63), 345 (100), 327 (62), 189 (11), 171 (14), 145 (22) [12]

FAB-MS m/z: 509 $[M + H]^+$, 491, 473, 455 [1]; 531 $[M + Na]^+$ (41), 509 $[M + H]^+$(41), 492 (15), 491 (50), 473 (89), 455 (62), 445 (44), 437 (27), 427 (28), 363 (33), 347 (73), 329 (88), 313 (46), 303 (98), 301 (100) [3]

HR-MS m/z: for $C_{29}H_{49}O_7$ $[M + H]^+$ calcd. 509.3478, found 509.3416 [3]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (dd, Ha-1), 1.43 (dd, He-1), 3.84 (ddd, Ha-2), 3.95 (q, He-3), 1.74 (Ha-4), 1.70 (He-4), 2.38 (dd, H-5), 5.81 (d, H-7), 3.16 (H-9), 1.80 (Ha-11), 1.71 (He-11), 2.13 (dt, Ha-12), 1.88 (He-12), 1.96 (Ha-15), 1.61 (Hb-15), 1.76 (Ha-16), 2.03 (Hb-16), 2.41 (dd, H-17), 0.90 (s, CH_3-18), 0.97 (s, CH_3-19), 1.20 (s, CH_3-21), 3.42 (dd, H-22), 1.55 (Ha-23), 1.40 (Hb-23), 1.15 (Ha-24), 1.22 (s, CH_3-26), 1.11 (s, CH_3-27), 1.58 (Ha-28), 1.48 (Hb-28), 1.02 (t, CH_3-29) [3]

^{1}H NMR (300 MHz, J/Hz, DMSO-d_6): 1.30 (Ha-1), 1.62 (He-1), 3.59 (Ha-2), 3.74 (He-3), 1.50 (Ha-4), 1.64 (He-4), 2.19 (dd, J = 4.0, 13.0, H-5), 5.63 (br s, H-7), 3.02 (t, J = 7.2, H-9), 1.54 (Ha-11), 1.70 (He-11), 2.01 (ddd, J = 5.0, 12.0, 12.0, Ha-12), 1.75 (He-12), 1.90 (Ha-15), 1.50 (Hb-15), 1.80 (Ha-16), 1.65

(Hb-16), 2.22 (dd, J = 3.8, 12.5, H-17), 0.74 (s, CH_3-18), 0.84 (s, CH_3-19), 1.21 (s, CH_3-21), 3.18 (H-22), 1.50 (Ha-23), 1.47 (Hb-23), 1.31 (Ha-24), 1.08 (s, CH_3-26), 1.23 (s, CH_3-27), 1.12 (Ha-28), 1.49 (Hb-28), 0.88 (t, J = 6.7, CH_3-29) [12]

^{13}C NMR (125.7 MHz, CD_3OD) [3]: **^{13}C NMR** (75 MHz, DMSO-d_6) [12]:

Table 1

C-1	37.37	C-16	21.62	C-1	35.2	C-16	20.8
2	68.71	17	50.43	2	66.5	17	48.5
3	68.53	18	18.06	3	66.7	18	16.0
4	32.87	19	24.40	4	31.4	19	23.8
5	51.80	20	78.04	5	50.0	20	75.5
6	206.50	21	20.96	6	202.6	21	17.0
7	122.12	22	77.22	7	120.4	22	74.8
8	168.04	23	33.06	8	165.1	23	28.7
9	35.12	24	50.30	9	33.2	24	37.5
10	39.27	25	74.14	10	36.5	25	73.9
11	21.54	26	29.09	11	20.2	26	28.9
12	32.51	27	25.97	12	30.8	27	31.8
13	49.00	28	25.61	13	46.8	28	20.0
14	85.20	29	14.35	14	82.9	29	19.3
15	31.80			15	30.3		

Pharm./Biol.: *Calliphora* bioassay: moulting hormone activity equal to that 20-hydroxyecdysone [8], *Sarcophaga* test: high moulting hormone activity [2, 13], high accelerating effect on the protein anabolism in mouse liver [13].

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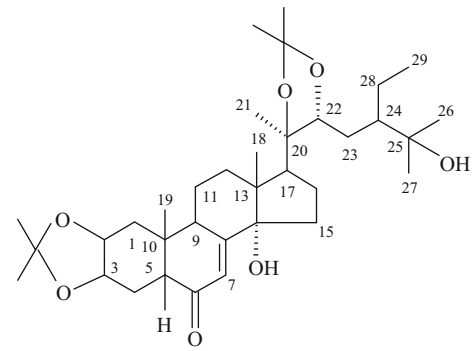
Makisterone C-2,3;20,22-Diacetonide

CAS Registry Number: 1146696-54-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *S. viridiflora* [1]

$C_{35}H_{56}O_7$: 588.4026

$[\alpha]_D^{25}$ + 65° (c 0.005, MeOH) [1]

UV λ_{max}^{MeOH} nm: 240 (log ε 3.4) [1]

ESI-MS m/z: 627 $[M + K]^+$ (42), 612 $[M + H + Na]^+$ (41), 611 $[M + Na]^+$ (100), 588 $[M]^+$ (6.4), 576 $[M + H + Na–2H_2O]^+$ (55), 563 (41), 545 (55), 531 $[M + H\text{-acetone}]^+$ (40), 513 $[M + H–H_2O\text{-acetone}]^+$ (42), 495 $[M + H–2H_2O\text{-acetone}]^+$ (20), 473 $[M + H\text{-2acetone}]^+$ (17), 455 $[M + H–H_2O\text{-2acetone}]^+$ (24), 437 $[M + H–2H_2O\text{-2cetone}]^+$ (25), 419 $[M + H–3H_2O\text{-2acetone}]^+$ (56), 391 (86), 381 (28), 338 (25), 333 (29) [1]

HR-ESI-MS m/z: for $C_{35}H_{56}NaO_7$ $[M + Na]^+$ calcd. 611.3924, found 611.3913 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.99 (d, J = 15.0, Ha-1), 1.23 (t, J = 14.5, He-1), 4.27 (dt, J = 9.4, 5.0, Ha-2), 4.30 (q, J = 4.0, He-3), 1.95–2.01 (m, Ha-4), 1.95–2.01 (m, He-4), 2.245 (dd, J = 9.3, 8.2, H-5), 5.80 (d, J = 2.5, H-7), 2.935 (ddd, J = 11.7, 7.0, 2.5, H-9), 1.74–1.81 (m, Ha-11), 1.65–1.70 (m,

He-11), 2.105 (dt, J = 13.0, 4.9, Ha-12), 1.81–1.89 (m, He-12), 1.96–2.02 (m, Ha-15), 1.58–1.67 (m, Hb-15), 1.83–1.90 (m, Ha-16), 2.03–2.10 (m, Hb-16), 2.304 (t, J = 8.9, H-17), 0.825 (s, CH_3-18), 0.96 (s, CH_3-19), 1.173 (s, CH_3-21), 3.834 (d, J = 10.0, H-22), 1.16–1.25 (m, Ha-23), 1.71–1.79 (m, Hb-23), 1.45 (ddd, J = 12.5, 6.6, 3.0, Ha-24), 1.16 (s, CH_3-26), 1.18 (s, CH_3-27), 1.18–1.24 (m, Ha-28), 1.63–1.72 (m, Hb-28), 1.006 (s, CH_3-29), Other: 1.32 and 1.47 (s, 2,3-iPr), 1.325 and 1.39 (s, 20,22-iPr) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

C-1	38.9	C-13	49.0	C-25	74.4
2	73.8	14	85.4	26	26.8
3	73.3	15	31.8	27	27.9
4	27.8	16	22.7	28	25.3
5	52.6	17	50.4	29	14.9
6	205.8	18	17.8	2,3-iPr	26.8
7	122.0	19	24.2		29.0
8	167.0	20	86.1		109.6
9	35.9	21	22.6	20,22-iPr	27.2
10	39.0	22	81.5		29.5
11	21.8	23	30.9		108.1
12	32.5	24	50.0		

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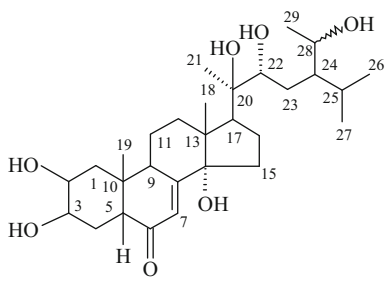
Makisterone D

CAS Registry Number: 20137-11-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Diplazium donianum* [1], *Podocarpus macrophyllus* [2, 3]

$C_{29}H_{48}O_7$: 508.3400

Mp: 244–246°C [1]

$[\alpha]_D$ + 42° (dioxane) [3]

IR (KBr) ν_{max} cm^{-1}: 3380, 1650 [1], 3400, 1650, 1630 [3]

UV λ_{max}^{MeOH} nm: 244 [3]

EI-MS m/z: 472, 454, 439, 436, 363, 189, 171, 153, 145, 127, 109, 84, 83 [1], 490 $[M\text{-}H_2O]^+$, 363, 345, 145 (22), 127 (100) [3]

^{1}H NMR (J/Hz, C_5D_5N): 1.18 (s, CH_3-18), 1.05 (s, CH_3-19), 1.57 (s, CH_3-21), 0.95 (d, CH_3-26), 1.12 (d, CH_3-27), 1.38 (d, CH_3-29) [1]

^{1}H NMR (J/Hz, C_5D_5N): 1.20 (s, CH_3-18), 1.06 (s, CH_3-19), 1.57 (s, CH_3-21), 0.87 (d, J = 6.0, CH_3-26), 0.87 (d, J = 6.0, CH_3-27), 1.30 (d, CH_3-29) [3]

Pharm./Biol.: *Chilo suppresalis* dipping assay: strong insect moulting activity [4].

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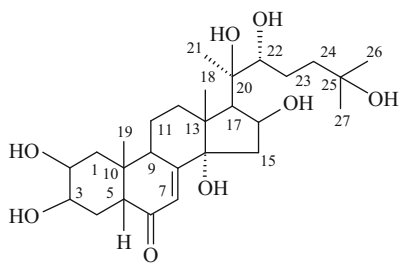
Malacosterone

CAS Registry Number: 100665-32-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Tapinella panuoides* [1]

$C_{27}H_{44}O_8$: 496.3036

IR (KBr) ν_{max} cm^{-1}: 3397, 1653 [1]

CI-MS m/z: 497 $[M + H]^+$, 479, 461, 443, 425, 407, 379, 363, 361, 345, 343 [2]

FAB-MS m/z: 519 $[M + Na]^+$ (47), 497 $[M + H]^+$ (51), 479 $[M + H–H_2O]^+$ (20), 461 $[M + H–2H_2O]^+$ (65), 443 $[M + H–3H_2O]^+$ (64), 340 (100) [1]

HR-MS m/z: for $C_{27}H_{45}O_8$ $[M + H]^+$ calcd. 497.3114, found 497.2990 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (dd, J = 4.5, 13.5, Ha-1), 1.43 (dd, J = 12.3, 13.0, He-1), 3.82 (ddd, J = 3.5, 4.0, 12.0, Ha-2), 3.94 (q, J = 3.0, He-3), 1.72 (Ha-4), 1.68 (He-4), 2.40 (dd, J = 4.8, 12.6, H-5), 5.81 (d, J = 2.0, H-7), 3.16 (ddd, J = 2.5, 7.0, 10.5, H-9), 1.70 (Ha-11), 1.82 (He-11), 2.14 (dt, J = 5.2, 12.5, 12.5, Ha-12), 1.93 (ddd, J = 2.5, 4.5, 12.8, He-12), 2.25 (dd, J = 7.6, 13.6, Ha-15), 2.08 (dd, J = 4.7, 13.6, Hb-15), 4.68 (dt, J = 4.7, 7.6, 7.6, Ha-16), 2.44 (d, J = 7.6, H-17), 1.136 (s, CH_3-18), 0.990 (s, CH_3-19), 1.197 (s, CH_3-21), 3.88 (dd, J = 1.5, 10.6, H-22), 1.67 (Ha-23), 1.36 (Hb-23), 1.86 (ddd, J = 5.0, 11.5, 13.3, Ha-24), 1.50 (ddd, J = 4.0, 11.5, 13.3, Hb-24), 1.197 (s, CH_3-26), 1.213 (s, CH_3-27) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

C-1	37.32	C-10	39.29	C-19	24.42
2	68.70	11	21.39	20	80.82
3	68.50	12	32.42	21	20.64
4	32.86	13		22	77.79
5	51.81	14	83.27	23	27.77
6	206.36	15	44.95	24	42.57
7	122.09	16	73.34	25	71.29
8	167.00	17	51.66	26	29.79
9	34.90	18	18.41	27	28.89

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 9.0 \times 10^{-6}$ M [3–5].

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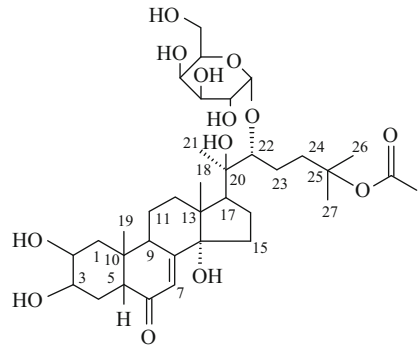
Melandrioside A

CAS Registry Number: 148297-90-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Melandrium turkestanicum* [1]

$C_{35}H_{56}O_{13}$: 684.3720

Mp: 204–206°C (EtOAc–MeOH) [1]

$[\alpha]_D^{20}$ + 92.3 ± 2° (c 0.17, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3400–3450, 1720, 1670, 1270 [1]

EI-MS m/z: 588 $[M\text{-}CH_3COOH–2H_2O]^+$ (0.7), 573 (0.4), 570 (0.8), 46 (1.5), 444 (18), 426 (80), 411 (26), 408 (60), 393 (27), 363 (18), 345 (100), 328 (98), 327 (99), 301 (40), 300 (40), 145 (30), 145 (32), 125 (32), 99 (32), 81 (32), 69 (32) [1]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 3.99–4.10 (m, H-2), 3.99–4.10 (m, H-3), 6.04 (br s, H-7), 3.47 (m, H-9), 1.07 (s, CH_3-18), 0.91 (s, CH_3-19), 1.51 (s, CH_3-21), 3.58 (m, H-22), 1.40 (s, CH_3-26), 1.47 (s, CH_3-27), Other: 1.84 (s, CH_3COO-22), β-D-Galp′: 5.46 (d, J = 3.2, H-1) [1].

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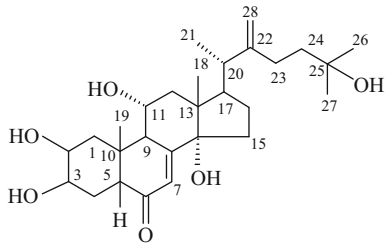
22-Methylene-2β,3β,11α,14α,25-Pentahydroxy-5β-Cholesta-7-en-6-one



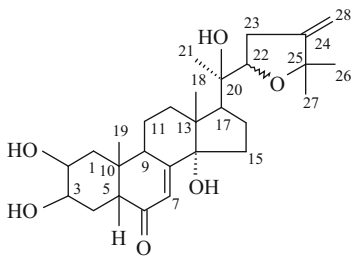
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Serratula wolffii* [1]
$C_{28}H_{44}O_6$: 476.3137

References

1. E. Liktor-Busa, A. Simon, M. Bathori, in *55th International Congress and Annual Meeting of the Society for Medicinal Plant Research*, Graz, 2007, p. 364, 936

24-Methyleneshidasterone

CAS Registry Number: 1009011-94-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Serratula wolffii* [1]
$C_{28}H_{42}O_6$: 474.2981
$[\alpha]_D^{28}$ + 3° (c 0.05, MeOH) [1]
UV λ_{max}^{MeOH} nm (log ε): 241.8 (3.7) [1]
ESI-MS m/z: 497 $[M + Na]^+$ (10), 475 $[M + H]^+$ (100), 457 $[M + H–H_2O]^+$ (72), 439 $[M + H–2H_2O]^+$ (5.7), 421 $[M + H + 3H_2O]^+$ (3), 364 (2) [1]
HR-ESI-MS m/z: for $C_{28}H_{42}O_6$ $[M]^+$ calcd. 474.2970, found 474.2975 [1]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.43 (dt, J = 12.5, 13.1, Ha-1), 1.795 (He-1), 3.84 (ddd, J = 3.3, 4.3, 12.1, Ha-2), 3.95 (q, J = 2.9, He-3), 1.72 (Ha-4), 1.76 (He-4), 2.38 (dt, J = 4.7, 8.1, H-5), 5.81 (d, J = 2.7, H-7), 3.15 (ddd, J = 2.7, 7.1, 11.3, H-9), 1.67 (Ha-11), 1.80 (He-11), 2.165 (td, J = 4.8, 13.3, Ha-12), 1.84 (He-12), 1.62 (Ha-15), 1.97 (Hb-15), 1.83 (Ha-16), 2.00 (Hb-16), 2.42 (dd, J = 8.2, 9.5, H-17), 0.84 (s, CH_3-18), 0.96 (s, CH_3-19), 1.21 (s, CH_3-21), 3.91 (t, J = 8.1, H-22), 2.545 (dt, J = 2.2, 8.2, Ha-23), 2.545 (dt, J = 2.2, 8.2, Hb-23), 1.28 (s, CH_3-26), 1.33 (s, CH_3-27), 4.805 (t, J = 2.3, Ha-28), 4.895 (t, J = 2.2, Hb-28) [1]
^{13}C NMR (125 MHz, CD_3OD) [1]:

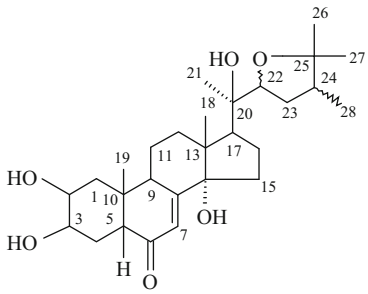
Table 1

C-1	37.5	C-11	21.6	C-21	20.7
2	68.9	12	32.45	22	82.4
3	68.7	13	48.4	23	35.6
4	33.2	14	85.4	24	158.3
5	51.9	15	31.8	25	83.2
6	206.6	16	22.0	26	27.9
7	122.3	17	52.0	27	29.7
8	168.1	18	18.35	28	104.1
9	35.3	19	24.5		
10	39.4	20	76.8		

References

1. A. Simon, G. Toth, E. Luktor-Busa, Z. Kele, M. Takacs, A. Gergely, M. Bathori, Steroids **72**, 751 (2007)

24-Methylshidasterone



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Vitex canescens* [1]

$C_{28}H_{44}O_6$: 476.3138

Mp: 241–243°C [1]

IR (KBr) ν_{max} cm^{-1}: 3415, 1656 [1]

EI-MS m/z: 458 $[M\text{-}H_2O]^+$, 440 (22), 422 (1), 363 (8), 345 (58), 327 (46), 309 (12), 301 (27), 283, 157 (12), 113 (37) [1]

ES-MS m/z: 499 $[M + H + Na]^+$ [1]

^{1}H NMR (J/Hz, C_5D_5N): 4.18 (br t, Ha-2), 4.26 (br s, He-3), 3.03 (dd, J = 3.5, 13.1, H-5), 6.22 (d, J = 2.1, H-7), 3.61 (m, H-9), 2.82 (H-17), 1.07 (s, CH_3-18), 0.99 (s, CH_3-19), 1.39 (s, CH_3-21), 4.09 (dd, J = 5.1, 8.9, H-22), 1.09 (s, CH_3-26), 1.20 (s, CH_3-27), 0.80 (d, J = 6.8, CH_3-28) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

C-1	38.00	C-11	21.70	C-21	21.10
2	68.16	12	31.82	22	81.60
3	68.24	13	47.77	23	35.50
4	32.56	14	84.24	24	42.96
5	51.47	15	31.80	25	82.50
6	203.67	16	21.70	26	21.00
7	121.76	17	50.80	27	27.40
8	166.28	18	18.00	28	15.50
9	34.50	19	24.50		
10	38.76	20	76.29		

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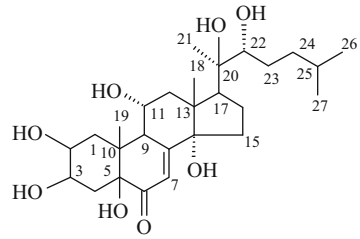
Muristerone A

CAS Registry Number: 38778-30-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ipomoea calonyction* [1–3]

$C_{27}H_{44}O_8$: 496.3036

Mp: 238–241°C [1], 238–244°C (MeOH) [2, 3]

$[\alpha]_D^{20}$ + 49.6° (c 1.0, pyridine) [1–3]

IR (KBr) ν_{max} cm^{-1}: 3100–3600, 1660, 1630 [2, 3]

UV λ_{max}^{MeOH} nm (ε): 326 (8900) [2, 3]

FAB-MS m/z: 497 $[M + H]^+$ [2]

HR-MS m/z: for $C_{27}H_{44}O_8$ $[M]^+$ calcd. 496.3034, found 496.3033, for $C_{27}H_{42}O_7$ calcd. 478.2933, found 478.2930, for $C_{27}H_{40}O_6$ calcd. 460.2824, found 460.2811, for $C_{27}H_{38}O_5$ calcd. 442.2718, found 442.2727, for $C_{27}H_{36}O_4$ calcd. 424.2613, found 424.2624, for $C_{27}H_{34}O_3$ calcd. 406.2508, found 406.2542 [3]

^{1}H NMR (J/Hz, C_5D_5N): 6.28 (d, J = 2.5, H-7), 1.24 (s, CH_3-18), 1.38 (s, CH_3-19), 1.53 (s, CH_3-21), 0.82 (d, J = 6.0, CH_3-26), 0.82 (d, J = 6.0, CH_3-27) [2]

^{13}C NMR (C_5D_5N) [3]:

Table 1

C-1	36.2	C-10	45.5	C-19	18.8
2	68.2	11	69.6	20	76.8
3	69.9	12	44.0	21	21.4
4	35.9	13	48.2	22	76.8
5	80.0	14	84.2	23	30.1
6	201.1	15	31.7	24	37.0
7	120.3	16	21.4	25	28.2
8	165.0	17	49.4	26	22.4
9	46.2	18	17.4	27	23.4

Pharm./Biol.: very high moulting activity [1], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 2.2 \times 10^{-8}$ M [4–7].

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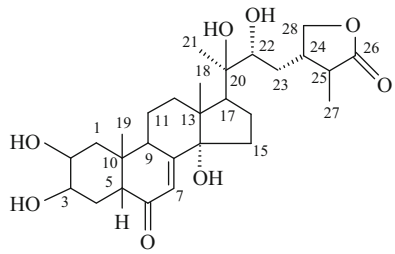
29-Norcyasterone

CAS Registry Number: 79495-93-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* [1]

$C_{28}H_{42}O_8$: 506.2879

Mp: 152–155°C (MeOH) [1]

$[\alpha]_D^{20}$ + 32.4° (c 6.25, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 1750, 1650 [1]

UV λ_{max}^{MeOH} nm (ε): 241 (9800) [1]

EI-MS m/z: 488 $[M\text{-}18]^+$, 363, 345, 327, 309, 187, 169, 143 [1]

CD(c, 0.36, dioxane): $[\theta]_{340}$ +4.9 × 10^3 [1]

^{1}H NMR (J/Hz, $CDCl_3$): 6.25 (d, J = 2.0, H-7), 1.20 (s, CH_3-18), 1.04 (s, CH_3-19), 1.55 (s, CH_3-21), 1.18 (d, J = 7.0, CH_3-27) [1]

^{13}C NMR ($CDCl_3$) [1]:

Table 1

C-1	38.0 (t)	C-11	21.6	C-21	21.4
2	68.2 (d)	12	31.9	22	76.2 (d)
3	68.2 (d)	13	48.3 (s)	23	34.8 (t)
4	32.6	14	84.3 (s)	24	40.5 (d)
5	51.5 (d)	15	32.1	25	43.5 (d)
6	203.9 (s)	16	21.7	26	181.1 (s)
7	121.9 (d)	17	50.3 (d)	27	14.6 (q)
8	166.2 (s)	18	18.0 (q)	28	73.1 (t)
9	34.6 (d)	19	24.6 (q)		
10	38.8 (s)	20	76.9 (s)		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.2 \times 10^{-8}$ M [2, 3].

References

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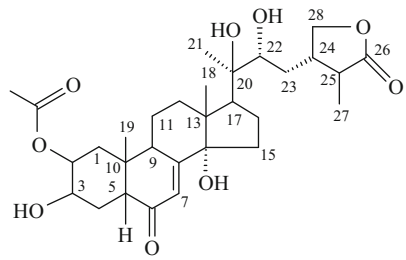
2. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
3. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

29-Norcyasterone-2-Acetate

CAS Registry Number: 97210-19-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* [1, 2]

$C_{30}H_{44}O_9$: 548.2985

EI-MS m/z: 530 $[M\text{-}H_2O]^+$ [1]

References

1. F. Camps, J. Coll, A. Cortel, E. Molins, C. Miravittles, J. Chem. Res. (S) **1**, 14 (1985)
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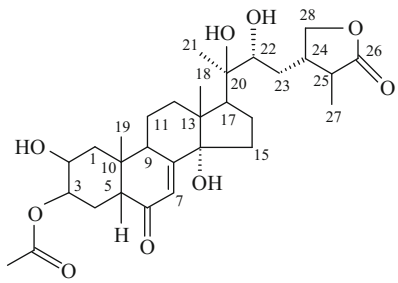
29-Norcyasterone-3-Acetate

CAS Registry Number: 97210-20-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *atropurpurea* [1]

$C_{30}H_{44}O_9$: 548.2985

TSP-MS m/z: 566 $[M + NH_4]^+$ (100), 549 $[M + H]^+$ (41), 548 $[M]^+$ (19), 531 $[M + H–H_2O]^+$ (61), 506 $[M + NH_4–CH_3COOH]^+$ (4), 489 $[M + H–CH_3COOH]^+$ (3) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.28 (br m, Ha-2), 5.49 (br m, He-3), 2.67 (dd, J = 4.2, 13.5, H-5), 6.26 (d, J = 1.8, H-7), 3.59 (br t, H-9), 2.87 (br t, J = 9.0, H-17), 1.24 (s, CH_3-18), 1.08 (s, CH_3-19), 1.57 (s, CH_3-21), 3.89 (br d, H-22), 2.22 (dq, J = 6.9, 10.8, H-25), 1.16 (d, J = 6.9, CH_3-27), 4.65 (dd, J = 7.6, 9.2, Ha-28), 3.96 (dd, J = 8.8, 10.4, Hb-28), 1.96 (s, CH_3COO-3) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	38.70	C-11	21.07	C-21	21.26
2	66.07	12	31.78	22	75.97
3	71.26	13	48.14	23	34.75
4	29.65	14	84.05	24	40.68
5	51.93	15	31.94	25	43.32
6	202.15	16	21.35	26	179.78
7	121.55	17	50.11	27	14.44
8	166.28	18	17.88	28	72.89
9	34.40	19	24.26	CH_3COO	21.07
10	38.57	20	76.64	CH_3COO	170.56

References

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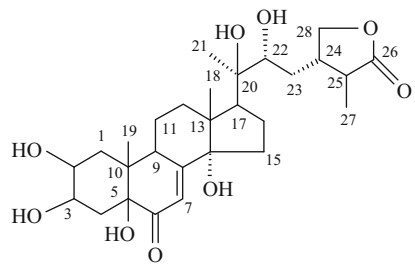
29-Norsengosterone

CAS Registry Number: 79495-94-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* [1]

$C_{28}H_{42}O_9$: 522.2828

Mp: amorphous [1]

$[\alpha]_D^{20}$ + 51.0° (c 4.7, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 1755, 1670 [1]

UV λ_{max}^{MeOH} nm (ε): 238 (9000) [1]

EI-MS m/z: 504 $[M\text{-}H_2O]^+$, 361, 343, 325, 187, 169, 143 [1]

CD (c 0.35, dioxane): $[\theta]_{330}$ +6.5 × 10^3 [1]

^{1}H NMR (J/Hz, $CDCl_3$): 6.25 (d, J = 2.0, H-7), 1.13 (s, CH_3-18), 1.13 (s, CH_3-19), 1.53 (s, CH_3-21), 1.18 (d, J = 7.0, CH_3-27) [1]

^{13}C NMR ($CDCl_3$) [1]:

Table 1

C-1	34.7 (t)	C-11	22.0 (t)	C-21	21.3 (q)
2	67.9 (d)	12	31.7 (t)	22	76.0 (d)
3	69.8 (d)	13	48.2 (s)	23	34.7 (t)
4	35.9 (t)	14	84.0 (s)	24	40.7 (d)
5	79.8 (s)	15	32.1 (t)	25	43.3 (d)
6	201.0 (s)	16	21.3 (t)	26	179.8 (s)
7	120.0 (d)	17	50.0 (d)	27	14.5 (q)
8	166.7 (s)	18	17.9 (q)	28	72.9 (t)
9	38.2 (d)	19	17.1 (q)		
10	44.8 (s)	20	76.7 (s)		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: EC_{50} = 1.3 × 10^{-7} M [2, 3].

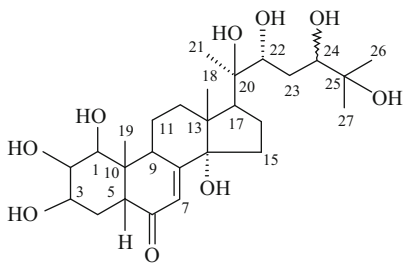
References

1. F. Camps, J. Coll, A. Cortel, Chem. Lett. **11**, 1313 (1982)

2. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
3. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

Nusilsterone

CAS Registry Number: 102099-20-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Silene nutans* [1]
$C_{27}H_{44}O_9$: 512.2985
Mp: 218–219°C (CH_3OH-acetone) [1]
$[\alpha]_D^{20}$ + 111.2 ± 2° (c 0.37, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3350–3450, 1660 [1]
UV λ_{max}^{EtOH} nm (log ε): 244 (4.09) [1]
EI-MS m/z: 512 $[M]^+$(0), 495 $[M + H–H_2O]^+$(1), 476 (2), 458 (10), 440 (4), 425 (6), 391 (3), 379 (4), 369 (2), 368 (5), 367 (2), 361 (15), 360 (11), 344 (25), 343 (24), 326 (35), 325 (27), 316 (25), 301 (17), 300 (23), 299 (15), 283 (21), 281 (21), 115 (60), 97 (100) [1]
CD (c, 0.06, dioxane): Δε = +1.59 (331 nm), Δε = −3.38 (251 nm) [1]
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.10 (m, H-1), 4.10 (m, H-2), 4.10 (m, H-3), 6.12 (br s, H-7), 3.51 (m, H-9), 0.91 (s, CH_3-18), 1.32 (s, CH_3-19), 1.42 (s, CH_3-21), 3.69–3.74 (m, H-22), 3.69–3.74 (m, H-24), 0.98 (s, CH_3-26), 1.04 (s, CH_3-27) [1]
Pharm./Biol.: *Galleria mellonella* bioassay: EC_{50} = 12.5 μg/g, *Sarcophaga bullata* bioassay: EC_{50} = 52.0 μg/g [2].

References

1. U.A. Baltaev, Y.V. Rashkes, N.K. Abubakirov, Chem. Nat. Comp. **21**, 489 (1985)
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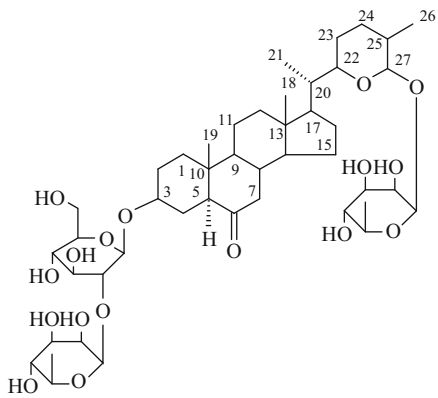
Osladin

CAS Registry Number: 33650-66-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Polypodium vulgare* [1]
$C_{45}H_{76}O_{17}$: 888.5082
Mp: 198–199°C (MeOH), aglycone: 193–195°C (MeOH) [1]
IR (Nujol) ν_{max} cm^{-1}:3400, 1704 [1]
IR ($CDCl_3$) ν_{max} cm^{-1} (aglycone): 3600, 1697 [1]
EI-MS m/z (aglycone): 432 $[M]^+$ (1.8), 414 $[M\text{-}H_2O]^+$ (61), 345 (26), 317 (63), 299 (38), 287 (84), 126 (77), 115 (56), 97 (100) [1]
^{1}H NMR (100 MHz, J/Hz, DMSO-d_6, aglycone): 0.64 (s, $2CH_3$), 0.71 (d, J = 6.0, CH_3CH), 0.81 (d, J = 6.0, CH_3CH), 3.33 (m, 2CH-O), 6.10 (d, J = 6.3, 1H, 1OH), 4.49 (d, J = 4.6, 1H, 1OH) [1].

References

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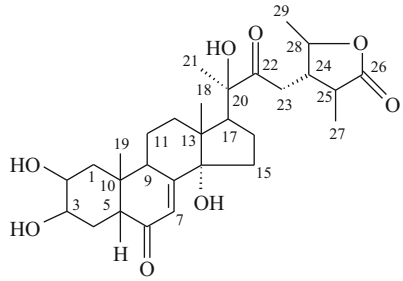
22-Oxocyasterone (22-Dehydrocyasterone)

CAS Registry Number: 145075-78-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga iva* [1], *A. nipponensis* [2]

$C_{29}H_{42}O_8$: 518.2879

IR (KBr) ν_{max} cm^{-1}: 1750, 1702, 1652 [1]

CI-MS m/z: 536 $[M + H + NH_3]^+$, 519 $[M + H]^+$, 501 $[M + H\text{-}H_2O]^+$ [1]

^{1}H NMR (J/Hz, CD_3OD): 3.82 (m, H-2), 3.94 (m, H-3), 5.80 (d, J = 2.5, H-7), 3.16 (m, H-9), 2.64 (t, J = 7.9, H-17), 0.87 (s, CH_3-18), 0.96 (s, CH_3-19), 1.39 (s, CH_3-21), 2.90 (dd, J = 6.0, 18.0, Ha-23), 2.98 (dd, J = 5.6, 18.0, Hb-23), 2.50 (m, H-25), 1.19 (d, J = 7.0, CH_3-26), 4.22 (dq, J = 6.0, 9.0, H-28), 1.36 (d, J = 6.0, CH_3-29) [1]

^{1}H NMR (J/Hz, D_2O): 1.40 (Ha-1), 1.85 (He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.36 (H-5), 5.96 (d, J = 2.5, H-7), 3.12 (m, H-9), 1.75 (Ha-11), 1.85 (He-11), 2.54 (H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.49 (s, CH_3-21), 2.95 (Ha-23), 2.95 (Hb-23), 2.35 (H-24), 2.60 (m, H-25), 1.20 (d, J = 7.0, CH_3-26), 4.39 (dq, J = 6.0, 9.0, H-28), 1.42 (d, J = 6.0, CH_3-29) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.16 (dm, J = 14.4, Ha-2), 4.23 (He-3), 3.01 (dd, J = 3.6, 13.0, H-5), 6.24 (d, J = 2.1, H-7), 3.58 (ddd, J = 2.0, 7.0, 10.0, H-9), 2.66 (ddd, J = 5.0, 12.5, 12.5, H-12), 1.12 (s, CH_3-18), 1.04 (s, CH_3-19), 1.67 (s, CH_3-21), 1.26 (d, J = 6.6, CH_3-27), 4.23 (dq, J = 6.3, 8.1, H-28), 1.32 (d, J = 6.0, CH_3-29) [2]

^{13}C NMR (75 MHz, C_5D_5N) [2]:

Table 1

C-1	37.97 (t)	C-11	21.02 (t)	C-21	25.55 (q)
2	68.08 (d)	12	31.93 (t)	22	215.00 (s)
3	68.04 (d)	13	48.16 (s)	23	39.08 (t)
4	32.42 (t)	14	84.00 (s)	24	46.06 (d)
5	51.39 (d)	15	31.81 (t)	25	42.12 (d)
6	203.34 (s)	16	21.58 (t)	26	178.53 (s)
7	121.90 (d)	17	51.67 (d)	27	14.39 (q)
8	165.37 (s)	18	17.32 (q)	28	79.79 (d)
9	34.42 (d)	19	24.41 (q)	29	9.89 (q)
10	38.71 (s)	20	81.33 (s)		

References

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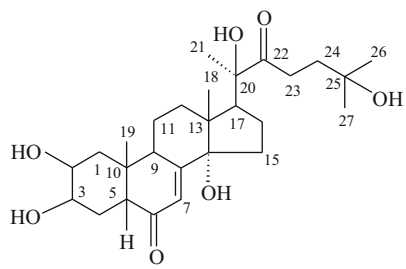
22-Oxo-20-Hydroxyecdysone

CAS Registry Number: 19974-12-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1], *Serratula tinctoria* [2]

$C_{27}H_{42}O_7$: 478.2930

Mp: 207–209°C (MeOH) [3], 209–210°C [4]

IR (KBr) ν_{max} cm^{-1}: 3402, 1702, 1653 [1], 1700, 1650 [3]
UV λ_{max}^{EtOH} nm (ε): 242 (11900) [4]
FAB-MS m/z: 501 $[M + Na]^+$ (6), 479 $[M + H]^+$ (32), 461 (100), 443 (38), 425 (10), 413 (5), 411 (4), 405 (6), 363 (18), 355 (6), 345 (6), 329 (12), 327 (6), 303 (11), 301 (12), 250 (57) [1]
FAB-MS (glycerol) m/z: 501 $[M + Na]^+$ (20), 479 $[M + H]^+$ (31), 461 (100), 443 (35), 425 (28), 363 (5), 348 (39), 329 (35), 303 (45) [3]
HR-MS m/z: for $C_{27}H_{43}O_7$ $[M + H]^+$ calcd. 479.3009, found 479.2937 [1]
CD (c, MeOH): $\Delta\varepsilon = +2.25$ (218 nm), $\Delta\varepsilon = -2.63$ (257 nm), $\Delta\varepsilon = -0.98$ sh (285 nm), $\Delta\varepsilon = +1.01$ (328 nm) [2]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 3.84 (ddd, Ha-2), 3.95 (bq, He-3), 1.75 (Ha-4), 1.70 (He-4), 2.38 (dd, H-5), 5.81 (d, H-7), 3.15 (ddd, H-9), 1.78 (Ha-11), 1.68 (He-11), 2.12 (dt, Ha-12), 1.84 (He-12), 1.95 (Ha-15), 1.61 (Hb-15), 1.71 (Ha-16), 1.92 (Hb-16), 2.34 (dd, H-17), 0.86 (s, CH_3-18), 0.97 (s, CH_3-19), 1.40 (s, CH_3-21), 1.20 (s, CH_3-26), 1.20 (s, CH_3-27) [1]
^{1}H NMR (250 MHz, J/Hz, D_2O): 3.99 (m, H-2), 4.07 (m, H-3), 2.36 (t-like, H-5), 5.97 (d, J = 2.5, H-7), 3.12 (m, H-9), 2.59 (m, H-17), 0.87 (s, CH_3-18), 1.02 (s, CH_3-19), 1.51 (s, CH_3-21), 2.80 (m, Ha-23), 2.80 (m, Hb-23), 1.76 (Ha-24), 1.76 (Hb-24), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27) [2]
^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

C-1	37.37	C-10	39.28	C-19	24.39
2	68.70	11	21.51	20	82.02
3	68.51	12	32.48	21	25.37
4	32.74	13	49.00	22	217.29
5	51.80	14	85.14	23	32.86
6	206.36	15	31.81	24	38.14
7	122.19	16	21.69	25	70.68
8	167.58	17	51.64	26	29.21
9	35.11	18	17.91	27	29.21

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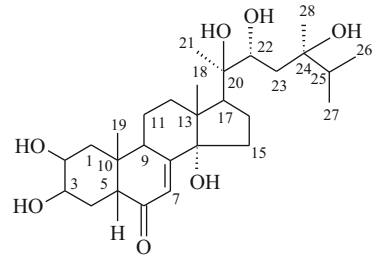
Panuosterone

CAS Registry Number: 220623-94-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Tapinella panuoides* [1, 2]
$C_{28}H_{46}O_7$: 494.3243
Mp: 207–214°C (Me_2CO) [2]
IR (KBr) ν_{max} cm^{-1}: 3416, 1653 [2]
FAB-MS m/z: 517 $[M + Na]^+$ (100), 495 $[M + H]^+$ (94), 477 $[M + H–H_2O]^+$ (85), 459 $[M + H–2H_2O]^+$ (54), 441 $[M + H–3H_2O]^+$ (35) [2]
HR-MS m/z: for $C_{28}H_{47}O_7$ $[M + H]^+$ calcd. 495.3320, found 495.3312 [2]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (dd, J = 13.2, 4.0, Ha-1), 1.43 (dd, J = 13.2, 12.4, He-1), 3.83 (ddd, J = 12.4, 4.0, 3.4, Ha-2), 3.95 (q, J = 2.8, He-3), 1.75 (Ha-4), 1.69 (dt, He-4), 2.38 (dd, J = 13.0, 4.5, H-5), 5.81 (d, J = 2.6, H-7), 3.15 (ddd, J = 10.5, 7.0, 2.6, H-9), 1.71 (Ha-11), 1.79 (He-11), 2.11 (Ha-12), 1.87 (He-12), 1.95 (Ha-15), 1.59 (Hb-15), 2.02 (Ha-16), 1.79 (Hb-16), 2.26 (dd, J = 10.0, 8.5, H-17), 0.896 (s, CH_3-18), 0.968 (s, CH_3-19), 1.204 (s, CH_3-21), 3.78 (dd, J = 11.4, 1.7, H-22), 1.73 (Ha-23), 1.44 (dd, J = 14.7, 10.6, Hb-23), 1.90 (h, J = 6.5, H-25), 0.980 (d, J = 6.5, CH_3-26), 0.911 (d, J = 6.5, CH_3-27), 1.079 (s, CH_3-28) [2]
^{13}C NMR (125.7 MHz, CD_3OD) [2]:

Table 1

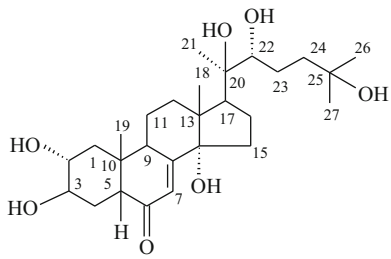
C-1	37.38	C-11	21.54	C-21	20.69
2	68.72	12	32.44	22	74.06
3	68.52	13		23	41.18
4	32.86	14	85.40	24	76.26
5	51.80	15	31.83	25	37.28
6	205.42	16	21.44	26	18.82
7	122.30	17	50.19	27	17.30
8	167.60	18	17.98	28	22.16
9	34.90	19	24.40		
10	39.30	20	77.81		

References

1. K. Vokas, M. Budesinsky, J. Harmatha, in *XIth Ecdysone Workshop*, Ceske Budejovice, Abstracts, 1994, p. 119
2. K. Vokas, M. Budesinsky, J. Harmatha, J. Kohoutova, Phytochemistry **49**, 2109 (1998)

Paristerone (2-Epiecdysterone)

CAS Registry Number: 84580-28-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Paris polyphylla* [1]

$C_{27}H_{44}O_8$: 496.3036

Mp: 216–220°C (dec.) (MeOH) [1]

$[\alpha]_D^{25}$ + 41.9° (c 0.5, pyridine) [1]

IR (KBr) ν_{max} cm^{-1}: 3300, 1650, 1435, 1380, 1260, 1150, 1060, 1030, 940, 920, 900, 888 [1]

UV λ_{max}^{MeOH} nm (ε): 240 (10314) [1]

EI-MS m/z:462, 444, 426, 411 (5), 363 (33), 345 (62), 327 (23), 320 (4), 309 (6), 301 (8), 300 (5), 285 (5), 269 (12), 250 (9), 225 (3), 213 (4), 191 (8), 173 (12), 161 (6), 143 (10), 117 (6), 99 (40), 81 (27), 69 (28), 58 (100) [1]

HR-MS m/z: for $C_{27}H_{38}O_4$ calcd. 426.2770, found 426.2788; for $C_{21}H_{31}O_5$ calcd. 363.2171, found 363.2166; for $C_{21}H_{29}O_4$ calcd. 345.2066, found 345.2052; for $C_{21}H_{27}O_3$ calcd. 327.1960, found 327.1962 [1]

FD-MS m/z: 480.4 $[M]^+$ (34) [1]

CD (c, dioxane): $[\theta]_{343}$ +5.07 × 10^3, $[\theta]_{246}$ −16.49 × 10^3 [1]

CD (c, MeOH): $[\theta]_{332}$ +6.82 × 10^3, $[\theta]_{252}$ −17.06 × 10^3 [1]

^{1}H NMR (DMSO-d_6): 3.75 (br s, He-2), 3.75 (br s, He-3), 5.65 (br s, H-7), 4.60 (OH-14), 0.77 (s, CH_3-18), 0.84 (s, CH_3-19), 1.10 (s, CH_3-21), 3.20 (br s, H-22), 1.10 (s, CH_3-26), 1.10 (s, CH_3-27), 3.32 (all other OH) [1]

^{13}C NMR (DMSO-d_6) [1]:

Table 1

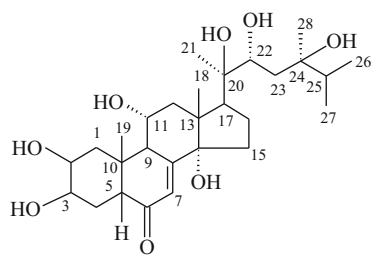
C-1	37.6	C-10	38.5	C-19	26.1
2	66.8	11	20.3	20	75.8
3	68.8	12	30.9	21	20.9
4	33.2	13	46.9	22	76.2
5	50.1	14	83.1	23	29.0
6	202.7	15	31.5	24	41.3
7	120.5	16	23.8	25	75.8
8	165.2	17	48.8	26	29.8
9	36.7	18	17.1	27	29.8

References

1. S.B. Singh, R.S. Thakur, Tetrahedron **38**, 2189 (1982)

Paxillosterone

CAS Registry Number: 190519-36-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Paxillus atrotomentosus* [1, 2]
$C_{28}H_{46}O_8$: 510.3192
Mp: amorphous [2]
IR (KBr) ν_{max} cm^{-1}: 3420, 1650 [2]
UV λ_{max}^{EtOH} nm (log ε): 243 (4.07) [2]
EI-MS m/z: 474 (8), 456 (39), 438 (41), 420 (31), 413 (54), 361 (28), 343 (57), 325 (28), 299 (21), 267 (32), 213 (21), 185 (18), 171 (23), 143 (17), 95 (24), 71 (44), 69 (41), 55 (36), 43 (100) [2]
FAB-MS m/z: 533 $[M + Na]^+$ (3), 511 $[M + H]^+$ (96), 493 $[M + H–H_2O]^+$ (100), 475 $[M + H–2H_2O]^+$ (55), 457 $[M + H–3H_2O]^+$ (39), 441 (15), 439 (15), 391 (13), 373 (28), 345 (29), 327 (19), 317 (24), 299 (29), 266 (19), 249 (27), 225 (24), 213 (23), 189 (23), 178 (28), 151 (64), 139 (41) [2]
HR-MS m/z: for $C_{28}H_{46}O_8$ $[M + Na]^+$ calcd. 533.3090, found 533.3201 [2], for $C_{28}H_{47}O_8$ $[M + H]^+$ calcd. 511.3271, found 511.3135 [2]
^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.37 (dd, J = 12.5, 11.8, Ha-1), 2.58 (dd, J = 12.5, 4.0, He-1), 4.00 (ddd, J = 11.8, 4.0, 2.6, Ha-2), 3.95 (q, J = 2.6, He-3), 1.78 (ddd, J = 14.0, 12.8, 2.6, Ha-4), 1.68 (He-4), 2.33 (dd, J = 12.8, 4.0, H-5), 5.80 (dd, J = 2.7, 0.7, H-7), 3.13 (dd, J = 8.9, 2.7, Ha-9), 4.09 (ddd, br, J = 10.3, 8.9, 6.3, He-11), 2.19 (dd, J = 12.5, 10.3, Ha-12), 2.14 (dd, J = 12.5, 6.3, He-12), 1.95 (m, Ha-15), 1.56 (m, Hb-15), 2.01 (m, Ha-16), 1.82 (m, Hb-16), 2.28 (dd, J = 9.9, 8.4, H-17), 0.879 (s, CH_3-18), 1.057 (s, CH_3-19), 1.226 (s, CH_3-21), 3.76 (dd, J = 10.5, 1.7, H-22), 1.72 (dd, J = 14.7, 1.7, Ha-23), 1.44 (dd, J = 14.7, 10.5, Hb-23), 1.89 (h, J = 6.8, H-25), 0.980 (d, J = 6.8, CH_3-26), 0.912 (d, J = 6.8, CH_3-27), 1.081 (s, CH_3-28) [2]
^{13}C NMR (125.7 MHz, CD_3OD) [2]:

Table 1

C-1	39.06	C-11	69.46	C-21	20.66
2	68.92	12	43.68	22	74.00
3	68.55	13		23	41.20
4	33.26	14	85.04	24	76.25
5	51.76	15	31.90	25	37.32
6	206.58	16	21.46	26	17.32
7	122.88	17	49.97	27	18.85
8	165.41	18	18.85	28	22.11
9	42.93	19	24.64		
10	39.93	20	77.72		

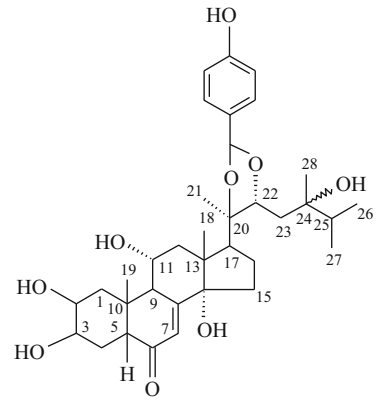
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.2 \times 10^{-7}$ M [3].

References

1. K. Vokas, M. Budesinsky, J. Harmatha, in *Xth Ecdysone Workshop*, Liverpool, Abstracts, 1992, p. 125
2. K. Vokas, M. Budesinsky, J. Harmatha, J. Kohoutova, Phytochemistry **49**, 2109 (1998)
3. J. Harmatha, L. Dinan, Arch. Insect Biochem. Physiol. **35**, 219 (1997)

Paxillosterone 20,22-P-Hydroxybenzylidene Acetal

CAS Registry Number: 190513-10-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Paxillus atrotomentosus* [1]
$C_{35}H_{50}O_9$: 614.3454
IR (KBr) ν_{max} cm^{-1}: 3409, 1657, 1617, 1518, 1102 [1]
EI-MS m/z: 456 (1), 438 (3), 423 (2), 420 (1), 413 (3), 404 (2), 395 (3), 354 (7), 342 (10), 337 (6), 326 (14), 299 (21), 281 (10), 157 (26), 139 (19), 121 (96), 107 (30), 87 (70), 69 (68), 55 (68), 43 (100) [1]
FAB-MS m/z: 637 $[M + Na]^+$ (3), 615 $[M + H]^+$ (2), 597 (2), 475 (7), 457 (5), 439 (3), 422 (8), 400 (20), 391 (4), 383 (2), 355 (4), 345 (2), 327 (3), 312 (6),

299 (4), 284 (4), 263 (7), 250 (7), 188 (17), 121 (39), 109 (61), 92 (36), 83 (42), 69 (72), 55 (100) [1]

HR-MS m/z: for $C_{35}H_{51}O_9$ $[M + H]^+$ calcd. 615.7439, found 615.7342 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.38 (dd, J = 12.3, 13.0, Ha-1), 2.59 (dd, J = 4.2, 12.8, He-1), 4.01 (ddd, J = 3.3, 4.0, 11.7, Ha-2), 3.96 (q, J = 2.8, He-3), 1.79 (dt, J = 2.5, 13.2, 14.2, Ha-4), 1.69 (dt, 3.5, 4.0, 14.2, He-4), 2.34 (dd, J = 3.8, 13.2, H-5), 5.82 (dd, J = 0.8, 2.7, H-7), 3.15 (dd, J = 2.7, 9.0, H-9), 4.10 (ddd, J = 6.0, 8.7, 10.7, He-11), 2.22 (dd, J = 10.8, 12.2, Ha-12), 2.14 (dd, J = 6.0, 12.0, He-12), 2.05 (Ha-15), 1.63 (m, Hb-15), 2.05 (Ha-16), 2.05 (Hb-16), 2.42 (dd, J = 8.5, 9.0, H-17), 0.871 (s, CH_3-18), 1.051 (s, CH_3-19), 1.280 (s, CH_3-21), 4.18 (d, J = 9.4, H-22), 1.80 (dd, J = 9.4, 14.8, Ha-23), 1.56 (bd, J = 14.8, Hb-23), 1.74 (h, J = 6.8, H-25), 0.968 (d, J = 6.8, CH_3-26), 0.934 (d, J = 6.8, CH_3-27), 1.135 (s, CH_3-28), Other: 5.73s, 6.77 s, 7.29 m (O–CH(O)–C_6H_4–OH) [1]

^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

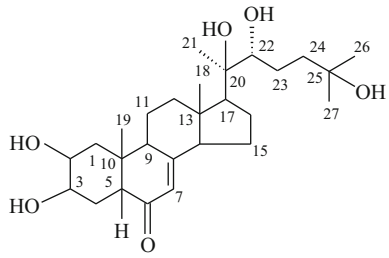
C-1	39.09	C-11	69.44	C-21	23.52
2	68.96	12	43.43	22	81.30
3	68.58	13		23	39.38
4	33.31	14	85.04	24	75.23
5	52.79	15	31.84	25	39.55
6	206.71	16	22.67	26	18.17
7	122.89	17	50.72	27	17.52
8	165.32	18	18.54	28	22.13
9	42.92	19	24.62	O-CH(O)-C_6H_5-OH	105.26, 131.22, 129.45 (2), 115.86 (2), 159.39
10	39.88	20	85.73		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 3.0 \times 10^{-7}$ M [2].

References

1. K. Vokas, M. Budesinsky, J. Harmatha, J. Pis, Tetrahedron **54**, 1657 (1998)
2. J. Harmatha, L. Dinan, Arch. Insect Biochem. Physiol. **35**, 219 (1997)

(20R,22R)-2β,3β,20,22,25-Pentahydroxy-5β-Cholesta-7-en-6-one



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula wolffii* [1]

$C_{27}H_{44}O_6$: 464.3138

References

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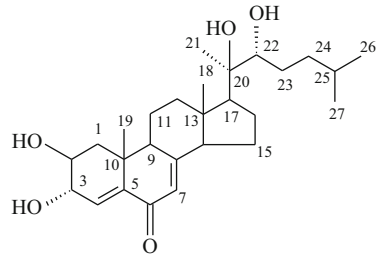
Pinnasterol

CAS Registry Number: 80981-63-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

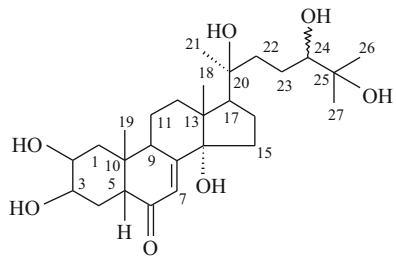
Biological sources: *Laurencia pinnata* [1, 2]
$C_{27}H_{42}O_5$: 446.3032
Mp: 198–201°C [1]
$[\alpha]_D$ + 37° (c, MeOH) [1]
EI-MS m/z: 446 $[M]^+$ [1].

References

1. A. Fukuzawa, Y. Kumagai, T. Masamune, A. Furusaki, C. Katayama, T. Masamune, Tetrah. Lett. **22**, 4085 (1981)
2. A. Fukuzawa, M. Miyamoto, Y. Kumagai, T. Masamune, Phytochemistry **25**, 1305 (1986)

Pinnatasterone (24β-Hydroxy-22-deoxy-20-Hydroxyecdysone)

CAS Registry Number: 146959-88-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Lychnis miqueliana* [1, 2], *P. polyphylla* [3], *Vitex pinnata* [4], *V. scabra* [5]
$C_{27}H_{44}O_7$: 480.3087
Mp: 198–200°C [4]
$[\alpha]_D^{25}$ + 41.2° (c 0.199, MeOH) [4]
IR (KBr) ν_{max} cm^{-1}: 3400, 1640 [4]
UV λ_{max}^{EtOH} nm (log ε): 242 (4.02) [4]
CI-MS m/z: 481 $[M + H]^+$ (7), 463 $[M + H–H_2O]^+$ (45), 445 $[M + H–2H_2O]^+$ (82), 427 $[M + H–3H_2O]^+$ (81), 143 $[C_8H_{13}O_3–H_2O]^+$ (100) [4]
EI-MS m/z: 444 $[M\text{-}2H_2O]^+$ (2), 426 (1), 385 (2), 363 (1), 327 (3), 309 (1), 301 (5), 283 (1), 161 (4), 143 (100), 125 (22), 117 (3), 107 (10), 99 (3), 89 (2), 81 (7), 71 (20), 59 (13) [4]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.15 (m, Ha-2), 4.23 (br s, He-3), 2.96 (dd, J = 13, 4, H-5), 6.19 (d, J = 2.5, H-7), 3.56 (m, Ha-9), 2.85 (t, J = 9.0, H-17), 1.09 (s, CH_3-18), 1.00 (s, CH_3-19), 1.55 (s, CH_3-21), 3.74 (br d, J = 8.5, H-24), 1.43 (s, CH_3-26), 1.47 (s, CH_3-27) [5]
^{13}C NMR (100 MHz, C_5D_5N) [5]:

Table 1

C-1	37.6	C-10	38.8	C-19	24.3
2	68.0	11	20.9	20	74.2
3	67.9	12	31.7	21	27.0
4	32.3	13	47.4	22	42.3
5	51.2	14	84.3	23	26.6
6	203.5	15	31.4	24	79.8
7	121.5	16	21.9	25	72.7
8	166.3	17	53.6	26	25.9
9	34.2	18	17.8	27	25.8

Pharm./Biol.: *Musca* bioassay: $EC_{50} = 6.9 \times 10^{-4}$ M [5].

References

1. M. Kozuka, M. Takasaki, T. Konoshima, T. Shingu, M. Saitoh, Y. Asaka, G. de Boer, I. Kubo, in *16th International Symposium on the Chemistry of Natural Products (IUPAC)*, Kyoto, 1988
2. S. Imai, T. Toyosato, M. Sakai, Y. Sato, S. Fujioka, E. Murata, M. Goto, Chem. Pharm. Bull. **17**, 340 (1969)
3. V.T.B. Nguyen, N. Darbour, Ch. Bayet, A. Doreau, I. Raad, B.H. Phung, C. Dumontet, A. Di Pietro, M.-G. Dijoux-Franca, D. Guilet, Fitoterapia **80**, 39 (2009)
4. A. Suksamrarn, C. Sommechai, Phytochemistry **32**, 303 (1993)
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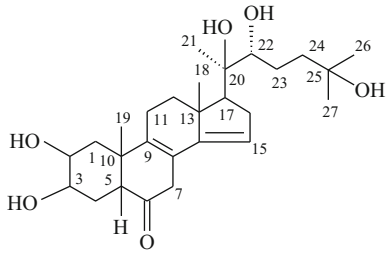
Podecdysone B

CAS Registry Number: 22612-27-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Pfaffia iresinoides* [1], *Podocarpus elatus* [2]

$C_{27}H_{42}O_6$: 462.2981

Mp: 122–124°C [1], 125–127°C [2]

$[\alpha]_D^{15}$ −15.7° (c 1.1, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3400, 1710, 1650 [1], 3490, 1705, 1650 [2]

UV λ_{max}^{EtOH} nm: 244 (log ε 4.14) [1], 244 (ε 13200) [2]

EI-MS m/z: 444 $[M\text{-}H_2O]^+$, 344, 327, 300, 99, 81 [2]

FAB-MS m/z: 463 $[M + H]^+$ [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 3.92 (br dt, J = 3.0, 11.4, Ha-2), 4.46 (br s, He-3), 3.04 (dd, J = 4.0, 12.4, H-5), 2.90 (br d, J = 21.0, Ha-7), 3.44 (br d, J = 21.0, Hb-7), 5.43 (br s, H-15), 3.01 (br dd, J = 10.6, 16.0, H-16), 1.35 (s, CH_3-18), 1.07 (s, CH_3-19), 1.55 (s, CH_3-21), 3.86 (br d, J = 8.2, H-22), 1.43 (s, CH_3-26), 1.44 (s, CH_3-27) [1]

^{1}H NMR (C_5D_5N): 1.35 (CH_3-18), 1.08 (CH_3-19), 1.55 (CH_3-21), 1.43 (CH_3-26), 1.43 (CH_3-27) [2]

^{1}H NMR (CD_3OD): 5.38 (H-15), 1.04 (CH_3-18), 0.98 (CH_3-19), 1.23 (CH_3-21), 1.17 (CH_3-26), 1.17 (CH_3-27) [2]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.6	C-10	43.6	C-19	29.6
2	69.6	11	23.0	20	76.2
3	68.3	12	37.5	21	20.8
4	32.9	13	46.6	22	77.7
5	53.6	14	148.9	23	27.4
6	212.4	15	119.5	24	42.7
7	39.4	16	31.5	25	69.7
8	122.9	17	57.0	26	30.0
9	136.4	18	18.7	27	30.7

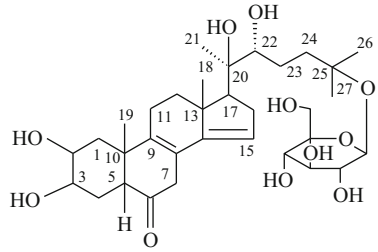
Pharm./Biol.: *Calliphora* bioassay: shows about one fifth of the activity of the 20-hydroxyecdysone [2], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.2 \times 10^{-5}$ M [3].

References

1. N. Nishimoto, Y. Shiobara, S.S. Inoue, M. Fujino, T. Takemoto, C.L. Yeoh, F. De Oliveira, G. Akisue, M.K. Akisue, G. Hashimoto, Phytochemistry **27**, 1665 (1988)
2. M.N. Galbraith, D.H.S. Horn, E.J. Middleton, R.J. Hackey, Chem. Comm. **8**, 402 (1969)
3. J. Harmatha, L. Dinan, R. Lafont, Insect Biochem. Mol. Biol. **32**, 181 (2002)

Podecdysone B-25-β-D-Glucoside

CAS Registry Number: 116424-82-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Pfaffia iresinoides* [1]

$C_{33}H_{52}O_{11}$: 624.3509

$[\alpha]_D^{15}$ −18.9° (c 1.1, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3400, 1710, 1650 [1]

UV λ_{max}^{EtOH} nm (log ε): 244 (4.12) [1]

FAB-MS m/z: 625 $[M + H]^+$ [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.47 (br s, H-3), 3.05 (dd, J = 12.4, 4.0, H-5), 2.89, 3.40 (br d,

J = 21.0, H-7), 5.44 (br s, H-15), 3.02 (br dd, J = 16.0, 10.4, H-16), 2.89 (t, J = 9.0, H-17), 1.34 (s, CH_3-18), 1.06 (s, CH_3-19), 1.54 (s, CH_3-21), 3.84 (br d, J = 7.8, H-22), 1.42 (s, CH_3-26), 1.47 (s, CH_3-27), Other: β-D-Glcp′: 5.02 (d, J = 7.4, H-1) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.5	C-12	37.4	C-23	26.6
2	69.6	13	46.7	24	40.0
3	68.3	14	148.9	25	77.4
4	32.9	15	119.6	26	27.5
5	53.6	16	31.5	27	27.6
6	212.4	17	56.9	Glc′-1	98.9
7	39.4	18	18.7	2	75.4
8	122.8	19	29.5	3	78.8
9	136.3	20	76.3	4	72.1
10	43.6	21	20.8	5	78.6
11	23.0	22	77.7	6	63.5

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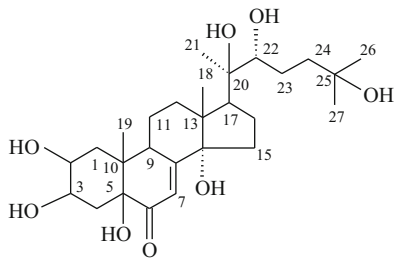
Polypodine B

CAS Registry Number: 18069-14-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Achyranthes bidentata* [1], *Ajuga incisa* [2, 3], *A. nipponensis* [2, 4, 5], *A. reptans* [6], *Asparagus falcatus, A. laricinus, A. scandens* [7], *Atriplex nummularia* [8], *Axyris amaranthoides* [9], *Blandfordia graudiflora, B. punicea* [10], *Briza maxima* [11], *Chenopodium album* L. [12, 13], *Chenopodium bonus-henricus L* [13, 14], *Coronaria flos-cuculi* [15], *Cyanotis longifolia* [16], *Dacrydium intermedium* [17, 19], *Dianthus hoeltzeri* [20], *Eriophyton wallchii* [21], *Gomphrena haageana* [22], *Helleborus atrorubens, H. bocconei, H. cyclophyllus, H. dumentorum, H. dumentorum* ssp. *atrorubens, H. guttatus, H. multifidus, H. multifidus* ssp. *serbicus, H. orientalis, H. viridis* ssp. *occidentalis* [23], *Kochia scoparia* [24], *Lamium album* [25], *Lloydia serotina* [26], *Lychnis arkwrigtii, L. chalcedonica, L. cognate* [27], *L. flos-cuculi* [28], *L. fulgens* [27, 29], *L. haageana* [27], *L. miqueliana* [4, 30], *L. sibirica, L. villosula, L. wilfordii* [27], *Melandrium turkestanicum* [31], *Ourisia macrocarpa, O. macrophylla* [32], *Paris quadrifolia* [33], *P. tetraphulla* [4], *Phymatodes novaezelandiae* [34], *Polypodium vulgare* [35, 36], *Rhagodia baccata* [37], *Rhaponticum carthamoides* [38–40], *Serratula coronata* [41], *S. inermis* [42, 43], *S. tinctoria* [44, 45], *S. wolffi* [46], *Silene altaica* [47], *S. antirrhina* [48], *S. brahuica* [49, 50], *S. brachypoda* [51], *S. campanulata, S. caramanica* [52], *S. catholica* [47, 53], *S. caucasica* [52], *S. chlorifolia* [51, 53, 54], *S. ciliata* [51, 54], *S. cretica* [13, 55], *S. damboldtiana* [52, 54], *S. disticha* [13, 55], *S. echinata* [51], *S. fridvaldszkyana* [56], *S. italica* [13, 51, 53, 57], *S. linicola* [13, 55, 58], *S. mellifera* [56], *S. nutans* [13, 59, 60], *S. paradoxa, S. parnassica, S. portensis* [51, 54], *S. pseudotites* [53], *S. repens* [61], *S. roemeri* [52], *S. schmuckeri* [56], *S. sendtneri* [47, 54], *S. tomentella* [62], *S. viridiflora* [13, 63], *Spinacia oleracea* [14], *Trillium erectum* [64], *Vitex megapotamica* [65, 66], *V. scabra* [67]

$C_{27}H_{44}O_8$: 496.3036

Mp: 251–252°C (acetone) [20], 254–257°C [35], 256–257°C [41], 252–254°C [68], 253–256°C [69]

$[\alpha]_D^{20}$ + 92.4 ± 2° (c 0.56, MeOH) [20], $[\alpha]_D^{15}$ + 59.4° (c 0.9, MeOH) [41]

IR (KBr) ν_{max} cm^{-1}: 3400, 1685 [20], 3340, 1687, 1657, 1636 [35], 3380, 1685 [68]

UV λ_{max}^{MeOH} nm: 242 [8], 317 (log ε 2.21), 243 (log ε 4.07) [35]

UV λ_{max}^{EtOH} nm: 241 [69]

EI-MS m/z: 478, 460, 442, 424, 361, 360, 344, 343, 99, 81 [35]

^{1}H NMR (400 MHz, J/Hz, CD_3OD): 1.43 (Ha-1), 1.78 (He-1), 3.95 (Ha-2), 3.99 (He-3), 1.67 (Ha-4), 1.77 (He-4), 5.85 (d, J = 2.7, H-7), 3.13 (m, H-9), 1.67 (Ha-11), 1.78 (He-11), 2.13 (ddd, J = 13.0, 13.5, Ha-12), 1.86 (He-12), 2.00 (Ha-15), 1.64 (Hb-15), 1.98 (Ha-16), 1.77 (Hb-16), 2.39 (m, H-17), 0.90 (s, CH_3-18), 0.92 (s, CH_3-19), 1.20 (s, CH_3-21), 3.33 (H-22), 1.29 (Ha-23), 1.65 (Hb-23), 1.75 (Ha-24), 1.45 (Hb-24), 1.19 (s, CH_3-26), 1.19 (s, CH_3-27) [8]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.26 (br dt, J = 4.0, 11.4, Ha-2), 4.15 (br s, He-3), 6.25 (d, J = 2.2, H-7), 3.62 (br t, J = 8.6, H-9), 2.54 (dt, J = 4.6, 12.6, H-12), 2.43 (q, J = 10.2, H-16), 2.96 (t, J = 9.0, H-17), 1.19 (s, CH_3-18), 1.13 (s, CH_3-19), 1.57 (s, CH_3-21), 3.84 (br d, J = 9.2, H-22), 1.35 (s, CH_3-26), 1.35 (s, CH_3-27) [68]

^{1}H NMR (400 MHz, J/Hz, CD_3OD): 1.68 (Ha-1), 1.78 (He-1), 3.94 (Ha-2), 3.99 (He-3), 1.75 (Ha-4), 2.08 (He-4), 5.85 (d, J = 2.5, H-7), 3.19 (m, H-9), 1.70 (Ha-11), 1.80 (He-11), 2.13 (Ha-12), 1.88 (He-12), 2.00 (Ha-15), 1.60 (Hb-15), 2.00 (Ha-16), 1.75 (Hb-16), 2.39 (m, H-17), 0.89 (s, CH_3-18), 0.92 (s, CH_3-19), 1.20 (s, CH_3-21), 3.33 (dd, J = 2.0, 11.0, H-22), 1.28 (Ha-23), 1.66 (Hb-23), 1.75-1.80 (Ha-24), 1.45 (Hb-24), 1.19 (s, CH_3-26), 1.19 (s, CH_3-27) [69]

^{13}C NMR (125.76 MHz, C_5D_5N) [41]: **^{13}C NMR** (100 MHz, C_5D_5N) [68]:

Table 1

C-1	34.12 (t)	C-15	31.72 (t)	C-1	34.9	C-15	31.8
2	68.37 (d)	16	21.43 (t)	2	68.1	16	21.4
3	70.22 (d)	17	50.41 (d)	3	69.9	17	50.1
4	36.11 (t)	18	16.96 (q)	4	36.1	18	18.0
5	80.35 (s)	19	18.08 (q)	5	79.9	19	17.3
6	202.50 (s)	20	77.97 (s)	6	201.0	20	76.9
7	120.62 (d)	21	21.03 (q)	7	119.9	21	21.7
8	167.53 (s)	22	78.44 (d)	8	167.0	22	77.7
9	38.97 (d)	23	27.31 (t)	9	38.4	23	27.6
10	45.46 (s)	24	42.37 (t)	10	44.8	24	42.3
11	22.48 (t)	25	71.38 (s)	11	22.1	25	69.7
12	32.57 (t)	26	28.94 (q)	12	32.2	26	30.1
13		27	29.72 (q)	13	48.2	27	30.2
14	85.09 (s)			14	84.1		

Pharm./Biol.: *Drosophila melanogaster in vitro* bioassay: active [46], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 3.4 \times 10^{-9}$ M [8], $EC_{50} = 1.0 \times 10^{-9}$ M [41, 70–72], *Galleria mellonella* bioassay: $ED_{50} = 7.8$ μg/g, *Sarcophaga bullata* bioassay: $ED_{50} = 7.8$ μg/g, *Dermestes vulpinus* bioassay: $ED_{50} = 29.0$ μg/g [73], cytotoxic active for C6 rat glioma cells [74].

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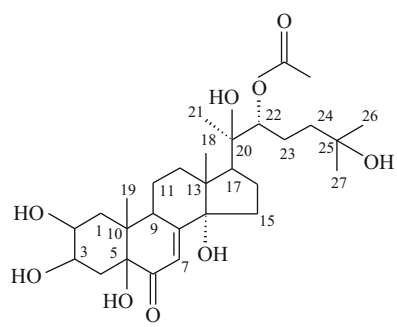
Polypodine B-22-Acetate

CAS Registry Number: 133066-62-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Melandrium turkestanicum* [1], *Serratula coronata* [2]
$C_{29}H_{46}O_9$: 538.3141
Mp: 150–152°C (MeOH–H_2O) [1]
$[\alpha]_D^{20}$ + 120 ± 2° (c 0.30, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}:3400–3500, 1735, 1685, 1260 [1]
EI-MS m/z: 520 $[M\text{-}H_2O]^+$ (0.3), 502 (0.7), 484 (1), 460 (18), 442 (100), 427 (18), 424 (14), 409 (9), 391 (4.5), 379 (1), 361 (4), 343 (5.9), 325 (5), 266 (18), 265 (18), 203 (8), 185 (11), 153 (51), 152 (50), 99 (22), 81 (25), 69 (41) [1]
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.10 (m, H-2), 4.10 (m, H-3), 6.25 (br s, H-7), 3.62 (m, H-9), 1.16 (s, CH_3-18), 1.16 (s, CH_3-19), 1.65 (d, CH_3-21), 5.49 (m, H-22), 1.35 (s, CH_3-26), 1.35 (s, CH_3-27), 2.04 (s, CH_3COO-22) [1]
^{1}H NMR (500 MHz, J/Hz, D_2O): 1.77 (Ha-1), 1.80 (He-1), 4.13 (m, Ha-2), 4.12 (m, He-3), 2.05 (m, Ha-4), 1.87 (m, He-4), 6.00 (d, J = 2.5, H-7), 3.16 (m, H-9), 1.76 (Ha-11), 1.87 (He-11), 1.76 (Ha-12), 1.96 (He-12), 1.65 (Ha-15), 2.05 (Hb-15), 1.86 (Ha-16), 1.92 (Hb-16), 2.31 (t, J = 9.5, H-17), 0.87 (s, CH_3-18), 0.94 (s, CH_3-19), 1.34 (s, CH_3-21), 4.85 (dd, J = 10.0, 2.0, H-22), 1.55 (Ha-23), 1.76 (Hb-23), 1.53 (Ha-24), 1.46 (Hb-24), 1.215 (s, CH_3-26), 1.218 (s, CH_3-27), 2.17 (s, CH_3COO-22) [2]
^{13}C NMR (125 MHz, D_2O) [2]:

Table 1

C-1	33.4 (t)	C-11	22.2 (d)	C-21	21.3 (q)
2	68.0 (d)	12	32.3 (t)	22	81.0 (d)
3	69.3 (d)	13	48.5 (s)	23	26.2 (t)
4	36.1 (t)	14	86.2 (s)	24	41.1 (t)
5	81.0 (s)	15	31.6 (t)	25	72.8 (s)
6		16	21.4 (t)	26	28.7 (q)
7	120.8 (d)	17	50.2 (d)	27	28.7 (q)
8		18	18.2 (q)	CH_3COO	21.8 (q)
9	38.7 (d)	19	16.8 (q)	CH_3COO	176.0 (s)
10	45.9 (s)	20	78.4 (s)		

Pharm./Biol.: *Drosophila melanogaster* B_{II} cell bioassay: $EC_{50} = 9.0 \times 10^{-8}$ M [2].

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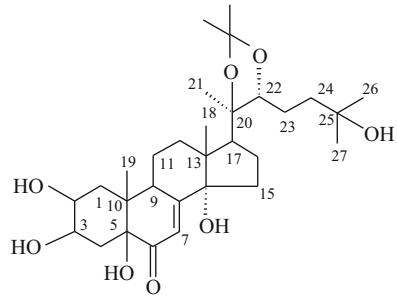
Polypodine B-20,22-Acetonide

CAS Registry Number: 159858-85-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Leuzea carthamoides* [1], *Stachyurus himalaicus* var. *himalaicus* [2]
$C_{30}H_{48}O_8$: 536.3349
IR (KBr) ν_{max} cm^{-1}: 3599, 3439, 1673, 1171, 1061 [1]
EI-MS m/z: 503 (1), 485 (1), 461 (1), 443 (2), 425 (2), 379 (20), 361 (2) [1]
FAB-MS m/z: 559 $[M + Na]^+$ (40), 537 $[M + H]^+$ (60), 520 (10), 479 (5), 461 (7), 443 (2), 425 (8) [1]
^{1}H NMR (500 MHz, J/Hz, Me_2CO-d_6): 3.82 (m, Ha-2), 3.82 (m, He-3), 5.87 (d, J = 2.5, H-7), 3.24 (ddd, J = 2.5, 7.0, 12.0, H-9), 2.37 (dd, J = 8.5, 9.0, H-17), 0.84 (s, CH_3-18), 0.87 (s, CH_3-19), 1.18 (s, CH_3-21), 3.68 (dd, J = 5.5, 7.0, H-22), 1.18 (s, CH_3-26), 1.17 (s, CH_3-27), Other: 1.30 and 1.36 (s, 20,22-iPr) [1]
^{13}C NMR (125.7 MHz, CD_3OD) [1]:

Table 1

C-1	36.2	C-11	22.5	C-21	22.6
2	70.2	12	32.4	22	83.3
3	68.4	13	48.5	23	24.7

(*continued*)

Table 1 (continued)

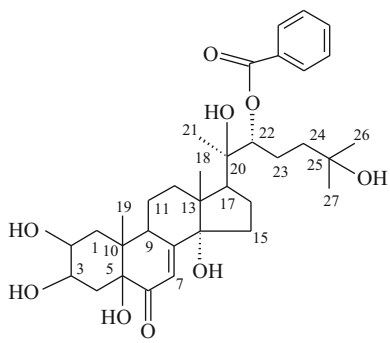
4	34.2	14	85.1	24	42.2
5	80.3	15	31.7	25	71.1
6	202.4	16	22.4	26	29.5
7	120.6	17	50.4	27	29.3
8	167.2	18	17.7	20,22-iPr	108.0, 29.0, 27.2
9	39.0	19	17.0		
10	45.4	20	85.8		

References

1. J. Pis, M. Budesinsky, K. Vokas, V. Laudova, J. Harmatha, Phytochemistry **37**, 707 (1994)
2. Y.S. Wang, J.H. Yang, S.D. Luo, H.B. Zhang, L. Li, Molecules **11**, 536 (2006)

Polypodine B-22-Benzoate

CAS Registry Number: 213321-82-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum carthamoides* [1]

$C_{34}H_{48}O_9$: 600.3298

Mp: 196–198°C (MeOH–H_2O) [1]

IR (KBr) ν_{max} cm^{-1}:3432, 1710, 1654, 1610, 1587, 1281, 714 [1]

EI-MS m/z: 442 $[M\text{-}C_6H_5COOH\text{–}2H_2O]^+$ (47), 429 (99), 409 (57), 391 (29), 373 (29), 361 (100), 343 (47), 325 (47), 299 (57), 298 (56), 265 (45), 229 (57), 122 $[C_7H_8O_2]^+$(95), 105 $[C_7H_5O]^+$ (71), 81 (23), 77 $[C_6H_5]^+$ (71) [1]

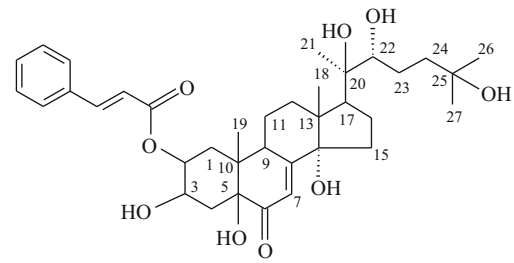
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.15 (m, H-2), 4.15 (m, H-3), 6.17 (s, H-7), 3.50 (m, H-9), 1.07 (s, CH_3-18), 1.00 (s, CH_3-19), 1.65 (s, CH_3-21), 5.70 (d, J = 7.5, H-22), 1.17 (s, CH_3-26), 1.17 (s, CH_3-27), Other: Ar: 7.35 (m, 3H), 8.24 (dd, J = 7.5, 1.0, 2H) [1].

References

1. Z.T. Sadikov, N.Sh. Ramazanov, Z. Saatov, Khim. Prir. Soedin. 851 (1997). [in Russian]

Polypodine B-2-Cinnamate

CAS Registry Number: 38147-16-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Dacrydium intermedium* [1, 2]

$C_{36}H_{50}O_9$: 626.3454

Mp: 268–270°C [1, 2]

IR (KBr) ν_{max} cm^{-1}: 3400, 1700, 1670, 1640 [2]

UV λ_{max}^{EtOH} nm: 276 (ε 21500), 248 (sh.), 223 (ε 19990), 217 (ε 20000) [2]

EI-MS m/z: 608 $[M\text{-}H_2O]^+$, 590 $[M\text{-}2H_2O]^+$, 572 $[M\text{-}3H_2O]^+$, 510 [M-116 (side chain)]$^+$, 442 [M-148 (cinnamic acid) – 36]$^+$, 361 [M-148-117]$^+$, 148 (cinnamic acid), 147 (base peak) (cinnamoyl-oxy), 131 (cinnamoyl) [2]

HR-MS m/z: for $C_{36}H_{44}O_6$ $[M\text{-}3H_2O]^+$ calcd. 572 [2]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 5.55 (m, Ha-2), 4.34 (m, He-3), 6.25 (H-7), 1.19 (s, CH_3-18), 1.19 (s, CH_3-19), 1.55 (s, CH_3-21), 1.38 (s, CH_3-26),

1.38 (s, CH_3-27), Other: 7.38 (Ar), 6.71 (d, J = 16.0, vinylic), 7.97 (d, J = 16.0, vinylic) [2]

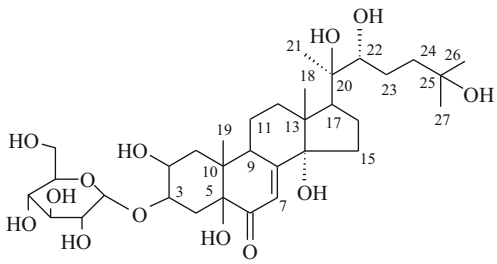
Pharm./Biol.: *Musca* bioassay: 1/10th the moulting hormone activity of 20-hydroxyecdysone [1].

References

1. G.B. Russel, D.H.S. Horn, E.J. Middleton, J. Chem. Soc. Chem. Comm. **2**, 71 (1971)
2. G.B. Russel, P.G. Fenemore, D.H.S. Horn, E.J. Middleton, Aust. J. Chem. **25**, 1935 (1972)

Polypodine B-3-β-Glucoside

CAS Registry Number: 109771-10-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Helleborus odorus, Helleborus purpurascens* [1]

$C_{33}H_{54}O_{13}$: 658.3564

PD-MS (plasma desorption 252Cf): 705 $[M + H + 2Na]^+$, 704 $[M + 2Na]^+$, 682 $[M + H + Na]^+$, 681 $[M + Na]^+$, 357 $[M + Na]^+$-glucose–H_2O [1]

^{1}H NMR (400 MHz, J/Hz, DMSO-d_6): 4.00 (He-3), 5.65 (H-7), 4.09 (OH-14), 0.75 (s, CH_3-18), 0.85 (s, CH_3-19), 1.05 (s, CH_3-21), 1.05 (s, CH_3-26), 1.07 (s, CH_3-27), Other: β-D-Glcp′: 4.34-4.41 (H-1 and OH-6), 3.13 (H-3), 2.96 (H-4), 3.45 (H-6), 4.67-4.93 (OH-2, 3 and 4) [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 6.27 (H-7), 1.17 (s, CH_3-18), 1.12 (s, CH_3-19), 1.56 (s, CH_3-21), 1.38 (s, CH_3-26), 1.38 (s, CH_3-27) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

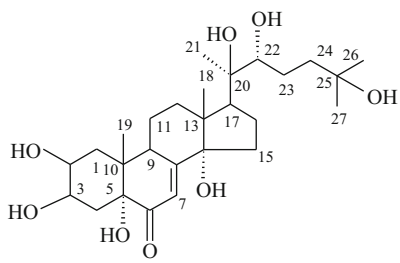
C-1	38.7	C-12	32.0	C-23	27.5
2	64.8	13	48.1	24	42.6
3	75.7	14	84.3	25	69.7
4	32.7	15	31.7	26	30.0
5	79.6	16	21.5	27	30.1
6	203.0	17	50.1	Glc′-1	102.0
7	121.8	18	17.8	2	75.5
8	166.0	19	24.2	3	78.4
9	38.4	20	77.0	4	71.8
10	44.9	21	21.7	5	78.6
11	21.9	22	77.6	6	62.8

References

1. B. Kissmer, M. Wichtl, Arch. Pharm. (Weinheim) **320**, 541 (1987)

5α-Polypodine B

CAS Registry Number: 109786-20-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Helleborus odorus, Helleborus purpurascens* [1]

$C_{27}H_{44}O_8$: 496.3036

PD-MS (plasma desorption 252Cf): 520 $(M + H + Na)^+$, 519 $(M + Na)^+$, 153, 131, 117, 111, 99, 92, 81 [1]

^{1}H NMR (400 MHz, J/Hz, DMSO-d_6): 5.66 (d, J = 2.0, H-7), 4.10 (OH-14), 0.75 (s, CH_3-18), 0.77 (s, CH_3-19), 1.03 (s, CH_3-21), 1.04 (s, CH_3-26), 1.05 (s, CH_3-27) [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 6.23 (H-7), 1.21 (s, CH_3-18), 1.07 (s, CH_3-19), 1.58 (s, CH_3-21), 1.37 (s, CH_3-26), 1.37 (s, CH_3-27) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

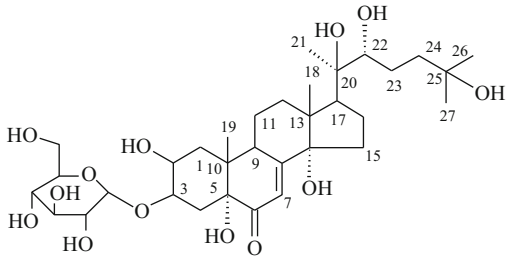
C-1	35.8	C-10	44.6	C-19	16.9
2	67.7	11	21.8	20	76.8
3	69.6	12	31.3	21	21.1
4	34.4	13	47.9	22	77.4
5	79.6	14	83.9	23	27.2
6	200.9	15	31.8	24	42.3
7	119.7	16	21.4	25	69.6
8	166.7	17	49.8	26	29.6
9	38.1	18	17.6	27	29.8

References

1. B. Kissmer, M. Wichtl, Arch. Pharm. (Weinheim) **320**, 541 (1987)

5α-Polypodine B-3-Glucoside

CAS Registry Number: 109771-10-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Helleborus odorus, Helleborus purpurascens* [1]
$C_{33}H_{54}O_{13}$: 658.3564
Mp: 162°C [1]
IR (KBr) ν_{max} cm^{-1}: 16540, 1630 [1]
UV λ_{max}^{EtOH} nm: 242 [1]
PD-MS (plasma desorption 252Cf): 705 $[M + H + 2Na]^+$, 704 $[M + 2Na]^+$, 682 $[M + H + Na]^+$, 681 $[M + Na]^+$, 357 $[M + Na]^+$-glucose–H_2O [1]

^{1}H NMR (400 MHz, J/Hz, DMSO-d_6): 4.00 (He-3), 5.63 (d, J = 2.0, H-7), 4.09 (OH-14), 0.75 (s, CH_3-18), 0.80 (s, CH_3-19), 1.05 (s, CH_3-21), 1.05 (s, CH_3-26), 1.07 (s, CH_3-27), Other: β-D-Glcp′: 4.34–4.41 (H-1 and OH-6), 3.13 (H-3), 2.96 (H-4), 3.45 (H-6), 4.67–4.93 (OH-2,3 and 4) [1]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 6.27 (H-7), 1.17 (s, CH_3-18), 1.01 (s, CH_3-19), 1.55 (s, CH_3-21), 1.38 (s, CH_3-26), 1.38 (s, CH_3-27) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

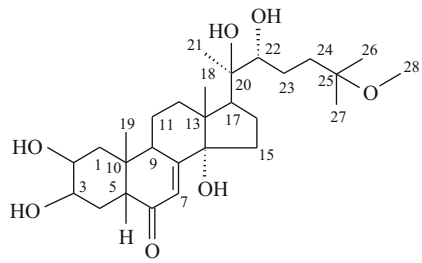
C-1	38.7	C-12	32.0	C-23	27.5
2	66.8	13	48.1	24	42.6
3	75.7	14	84.1	25	69.7
4	35.5	15	31.6	26	30.0
5	79.6	16	21.4	27	30.1
6	200.6	17	50.0	Glc′-1	102.6
7	120.2	18	17.8	2	75.4
8	166.5	19	17.0	3	78.4
9	38.4	20	76.9	4	71.8
10	44.9	21	21.7	5	78.6
11	21.9	22	77.6	6	62.8

References

1. B. Kissmer, M. Wichtl, Arch. Pharm. (Weinheim) **320**, 541 (1987)

Polypodoaurein

CAS Registry Number: 52677-91-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

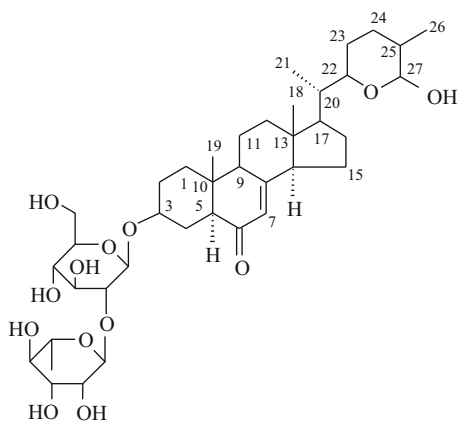
Biological sources: *Polypodium aureum* [1]
$C_{28}H_{46}O_7$: 494.3244
Mp: 251–253°C (MeOH) [1]
UV λ_{max}^{EtOH} nm (log ε): 244 (4.0) [1]
EI-MS m/z: 476 $[M\text{-}H_2O]^+$ (0.08), 458 (0.8), 440 (3.8), 426 (4.3), 363 (42), 345 (75), 327 (50), 301 (19), 300 (20), 285 (20), 269 (30), 267 (22), 213 (17), 113 (91), 99 (67), 95 (81), 81 (100) [1]
Pharm./Biol.: *Calliphora erythrocephala*: polypodoaurein was injected (1 mg/larvae), this causes a 90% puparation in the *Calliphora* test. Polypodoaurein was shown ecdysterone-type activity [1].

References

1. J. Jizba, L. Dolejs, V. Herout, Phytochemistry **13**, 1915 (1974)

Polypodosaponin

CAS Registry Number: 33285-16-4



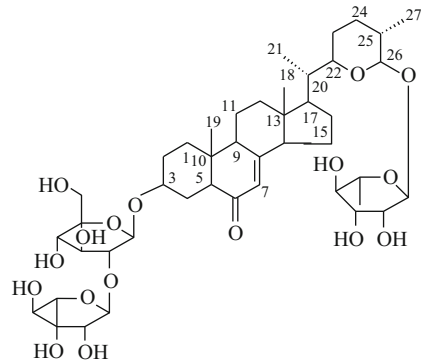
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Polypodium vulgare* [1]
$C_{39}H_{62}O_{13}$: 738.4190

References

1. J. Jizba, L. Dolejs, V. Herout, F. Sorm, H.W. Fehlhaber, G. Snatzke, R. Tschesche, G. Wulff, Chem. Berichte. **104**, 837 (1971) [Chem. Abst. 71. 77147j (1971)]

Polypodoside A

CAS Registry Number: 119784-25-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Polypodium glycyrrhiza* [1]
$C_{45}H_{72}O_{17}$: 884.4770
Mp: 198–200°C (MeOH) [1]
$[\alpha]_D$ −37° (c 0.3, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3435, 1667, 1460, 1453, 1225, 1036 [1]
UV λ_{max}^{EtOH} nm (log ε): 244 (4.03) [1]
EI-MS m/z: 884 $[M]^+$, 430 [aglycone]$^+$ (1), 412 [aglycone-H_2O]$^+$ (23), 395 (32), 379 (5), 342 (5), 285 (9), 261 (8), 147 (12), 128 (17), 97 (37), 43 (100) [1]
FAB-MS m/z: 907 $[M + Na]^+$, 885 $[M + H]^+$, 739, 721, 577, 559, 431, 413, 395, 309 [1]
HR-MS m/z: for $C_{45}H_{73}O_{17}$ $[M + H]^+$ calcd. 885.4848, found 885.4843; for $C_{33}H_{53}O_8$ calcd. 577.3740, found 577.3723 [1]
Table 1
^{1}H NMR (360 MHz, J/Hz, C_5D_5N): 3.84 (m, H-3), 5.84 (br s, H-7), 6.26 (br s, H-9), 1.74 (d, J = 6.0, H-14), 5.61 (br s, H-16), 0.48, (s, CH_3-18), 0.86 (s, CH_3-19), 1.01 (d, J = 6.0, CH_3-21), 3.46 (m, H-22), 4.45 (d, J = 8.0, H-26), 0.91 (d, J = 6.0, CH_3-27), Other: β-D-Glcp′: 5.02 (d, J = 6.6, H-1),

α-L-Rhap″: 6.26 (br s, H-1), 1.71 (d, J = 6.0, CH_3), α-L-Rhap‴: 5.61 (br s, H-1), 1.66 (d, J = 6.0, CH_3) [1]

^{13}C NMR (90.8 MHz, C_5D_5N) [1]:

Table 1

C-1	36.86 (t)	C-16	26.83 (t)	4	71.87 (d)
2	29.22 (t)	17	52.88 (d)	5	78.11 (d)
3	76.31 (d)	18	12.09 (q)	6	62.74 (t)
4	26.98 (t)	19	13.10 (q)	Rha′-1	102.17 (d)
5	53.13 (d)	20	40.38 (d)	2	72.78 (d)
6	198.69 (s)	21	13.85 (q)	3	72.50 (d)
7	123.21 (d)	22	78.30 (d)	4	73.95 (d)
8	163.02 (s)	23	23.98 (t)	5	69.49 (d)
9	49.91 (d)	24	31.49 (t)	6	18.75 (q)
10	38.39 (s)	25	36.45 (d)	Rha″-1	102.03 (d)
11	21.89 (t)	26	107.32 (d)	2	72.78 (d)
12	38.85 (t)	27	16.68 (q)	3	72.14 (d)
13	44.69 (s)	Glc′-1	99.53 (d)	4	74.12 (d)
14	55.05 (d)	2	79.47 (d)	5	70.48 (d)
15	22.90 (t)	3	78.30 (d)	6	18.44 (q)

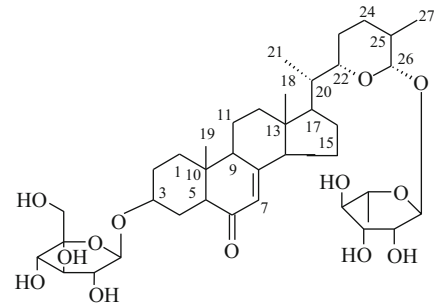
Pharm./Biol.: At the dose 0.31–5.0 mg/ml not to be mutagenic for *Salmonella typhimurium* strain TM 677. Polyposida A evaluated for acute toxity with male *Swiss-Webster* mice at dose levels of 2 g/kg body wt [1].

References

1. J. Kim, J.M. Pezzuto, D.D. Soejarto, F.A. Lang, D.A. Kinghorn, J. Nat. Prod. **51**, 1166 (1988)

Polypodoside B

CAS Registry Number: 120015-16-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polypodium glycyrrhiza* [1]

$C_{39}H_{62}O_{13}$: 738.4190

Mp: 207–209°C (MeOH) [1]

$[\alpha]_D$−27° (c 0.1, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3420, 1666, 1382, 1225, 1142, 1094, 1062, 1031, 984 [1]

UV λ_{max} nm (log ε): 244 (4.08) [1]

EI-MS m/z: 738 $[M]^+$ (missing), 574 $[M\text{-}162]^+$ (26), 430 $[aglycone]^+$ (11), 413 $[aglycone\text{-}OH]^+$ (49), 395 (94), 97 (100) [1]

FAB-MS (DTE/DTT) m/z: 761 $[M + Na]^+$ [1]

FAB-MS (LiI/3-NBA) m/z: 745 $[M + Li]^+$ [1]

HR-MS m/z: for $C_{39}H_{62}O_{13}Li$, calcd. 745.4359, found 745.4320 [1]

^{1}H NMR (360 MHz, J/Hz, C_5D_5N): 5.85 (br s, H-7), 0.49 (s, CH_3-18), 0.74 (s, CH_3-19), 1.02 (d, J = 6.0, CH_3-21), 3.46 (m, H-22), 4.47 (d, J = 8.0, H-26), 0.91 (d, J = 6.0, CH_3-27), Other: β-D-Glcp′: 5.05 (d, J = 7.6, H-1), α-L-Rhap″: 5.64 (br s, H-1), 1.68 (d, J = 6.0, 2H) [1]

Table 1

C-1	38.28 (t)	C-11	21.88 (t)	C-21	13.84 (q)	Glc′-4	71.69 (d)
2	29.32 (t)	12	38.83 (t)	22	78.10 (d)	5	78.35 (d)
3	76.89 (d)	13	44.68 (s)	23	23.99 (t)	6	62.88 (t)
4	27.30 (t)	14	55.03 (d)	24	31.47 (t)	Rha′-1	101.87 (d)
5	53.18 (d)	15	22.85 (t)	25	36.40 (d)	2	72.70 (d)
6	198.72 (s)	16	26.95 (t)	26	107.25 (d)	3	72.04 (d)
7	123.19 (d)	17	52.85 (d)	27	16.65 (q)	4	73.87 (d)
8	162.99 (s)	18	12.12 (q)	Glc′-1	102.19 (d)	5	70.36 (d)
9	49.92 (d)	19	13.02 (q)	2	75.24 (d)	6	18.37 (q)
10	36.79 (s)	20	40.35 (d)	3	78.44 (d)		

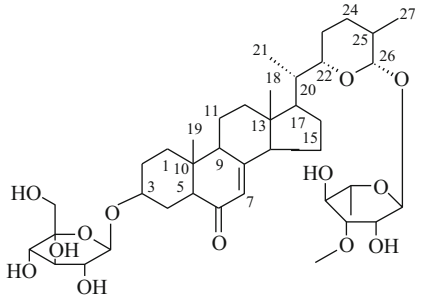
^{13}C NMR (90.8 MHz, C_5D_5N) [1]:

References

1. J. Kim, A.D. Kinghorn, Phytochemistry **28**, 1225 (1989)

Polypodoside C

CAS Registry Number: 120015-17-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polypodium glycyrrhiza* [1]

$C_{40}H_{64}O_{13}$: 752.4347

Mp: 200–202°C (MeOH) [1]

$[\alpha]_D$−26.3° (c 0.3, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3450, 1659, 1384, 1143, 1102, 1074, 1058, 1048, 1033, 987 [1]

UV λ_{max} nm (log ε): 244 (4.16) [1]

EI-MS m/z: 752 $[M]^+$ (missing), 430 $[aglycone]^+$ (23), 413 $[aglycone\text{-}OH]^+$ (63), 395 (40), 43 (100) [1]

FAB-MS (3-NBA) m/z: 775 $[M + Li]^+$, 753 $[M + H]^+$ [1]

HR-MS m/z: for $C_{40}H_{65}O_{13}$, calcd. 753.4425, found 753.4437 [1]

^{1}H NMR (360 MHz, J/Hz, C_5D_5N): 5.86 (br s, H-7), 0.50 (s, CH_3-18), 0.74 (s, CH_3-19), 1.05 (d, J = 6.0, CH_3-21), 3.49 (m, H-22), 4.50 (d, J = 8.0, H-26), 0.99 (d, J = 6.0, CH_3-27), Other: β-D-Glcp′: 5.07 (d, J = 7.0, H-1), α-L-Rhap-3-Me″: 5.65 (br s, H-1), 1.67 (d, J = 6.0, 2H), 3.56 (s, OCH_3) [1] Table 1

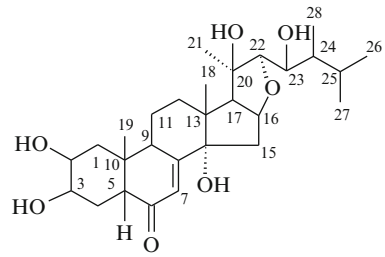
^{13}C NMR (90.8 MHz, C_5D_5N) [1]:

References

1. J. Kim, A.D. Kinghorn, Phytochemistry **28**, 1225 (1989)

Polyporoid A

CAS Registry Number: 1042362-43-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polyporus umbellatus* [1]

$C_{28}H_{44}O_7$: 492.3087

Mp: amorphous [1]

$[\alpha]_D^{25}$ + 10.1° (c 0.05; MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3396, 2961, 2873, 1644, 1623, 1562, 1413, 1384, 1054 [1]

UV λ_{max}^{MeOH} nm (log ε): 240 (1.2) [1]

FAB-MS m/z: 493.31601 $[M + H]^+$ [1]

Table 1

C-1	36.78 (t)	11	21.87 (t)	C-21	13.85 (q)	Glc′-4	71.67 (d)
2	29.31 (t)	12	38.81 (t)	22	78.15 (d)	5	78.43 (d)
3	76.83 (d)	13	44.67 (s)	23	23.95 (t)	6	62.88 (d)
4	27.30 (t)	14	55.02 (d)	24	31.48 (t)	Rha-3-Me″-1	101.74 (d)
5	53.15 (d)	15	22.85 (t)	25	36.42 (d)	2	70.38 (d)
6	198.78 (s)	16	26.97 (t)	26	107.19 (d)	3	82.62 (d)
7	123.21 (d)	17	52.82 (d)	27	16.72 (q)	4	72.14 (d)
8	163.04 (s)	18	12.11 (q)	Glc′-1	102.17 (d)	5	67.85 (d)
9	49.90 (d)	19	13.02 (q)	2	75.26 (d)	6	18.37 (q)
10	38.28 (s)	20	40.36 (d)	3	78.48 (d)	O-Me	57.07 (q)

HR-FAB-MS m/z: for $C_{28}H_{45}O_7$ $[M + H]^+$ calcd. 493.31653, found 493.31601 [1]

^{1}H NMR (J/Hz, CD_3OD): 1.79 (m, Ha-1), 1.42 (m, He-1), 3.81 (dt, J = 4.1, 11.9, Ha-2), 3.93 (br s, He-3), 1.70 (m, H-4), 2.38 (dd, J = 5.0, 12.7, H-5), 5.76 (d, J = 2.4, H-7), 3.15 (m, H-9), 1.82 (m, Ha-11), 1.76 (m, He-11), 2.12 (m, Ha-12), 1.80 (m, He-12), 2.14 (dd, J = 7.4, 13.3, Ha-15), 2.08 (dd, J = 4.8, 13.3, Hb-15), 4.65 (m, H-16), 2.54 (d, J = 7.4, H-17), 1.18 (s, CH_3-18), 0.99 (s, CH_3-19), 1.43 (s, CH_3-21), 3.94 (d, J = 9.4, Hb-22), 3.78 (dd, J = 1.9, 9.4, H-23), 1.40 (m, H-24), 1.81 (m, H-25), 0.95 (d, J = 6.7, CH_3-26), 0.92 (d, J = 6.7, CH_3-27), 0.87 (d, J = 7.0, CH_3-28) [1]

^{13}C NMR (CD_3OD) [1]:

Table 1

C-1	37.3	C-11	21.6	C-21	26.6
2	68.6	12	31.2	22	84.7
3	68.5	13	47.8	23	72.8
4	32.8	14	86.2	24	42.5
5	51.9	15	43.0	25	31.3
6	205.6	16	83.0	26	24.4
7	122.0	17	63.6	27	21.1
8	167.1	18	18.5	28	10.0
9	34.7	19	24.4		
10	39.4	20	80.9		

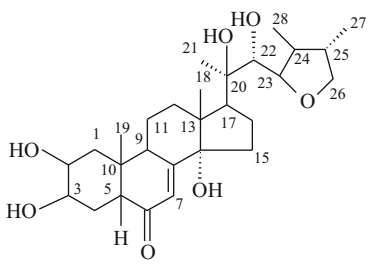
Pharm./Biol.: TPA-induced inflammation test: ID_{50} = 0.531 μM/ear [1].

References

1. Y. Sun, K. Yasukawa, Bioorg. Med. Chem. Lett. **18**, 3417 (2008)

Polyporoid B

CAS Registry Number: 1042362-45-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polyporus umbellatus* [1]

$C_{28}H_{44}O_7$: 492.3087

Mp: amorphous [1]

$[\alpha]_D^{25}$ + 24.0° (c 0.10; MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3400, 2960, 2870, 1648, 1620, 1565, 1418, 1385, 1062 [1]

UV λ_{max}^{MeOH} nm (log ε): 241 (1.6) [1]

FAB-MS m/z: 493.31601 $[M + H]^+$ [1]

HR-FAB-MS m/z: for $C_{28}H_{45}O_7$ $[M + H]^+$ calcd. 493.31653, found 493.31668 [1]

^{1}H NMR (J/Hz, CD_3OD): 1.77 (m, Ha-1), 1.42 (t, J = 13.4, He-1), 3.85 (dt, J = 3.6, 11.3, Ha-2), 3.94 (br s, He-3), 1.72 (m, H-4), 2.37 (dd, J = 4.4, 12.7, H-5), 5.80 (d, J = 2.4, H-7), 3.15 (m, H-9), 1.80 (m, Ha-11), 1.68 (m, He-11), 2.12 (m, Ha-12), 1.88 (m, He-12), 1.96 (m, Ha-15), 1.59 (m, Hb-15), 1.88 (m, Ha-16), 1.68 (m, He-16), 2.78 (t, J = 8.0, H-17), 0.87 (s, CH_3-18), 0.96 (s, CH_3-19), 1.26 (s, CH_3-21), 3.32 (d, J = 5.1, Hb-22), 3.52 (t, J = 5.1, H-23), 1.70 (m, H-24), 1.75 (m, H-25), 3.89 (t, J = 7.9, Ha-26), 3.35 (t, J = 7.6, Hb-26), 1.02 (d, J = 6.5, CH_3-27), 1.14 (d, J = 6.2, CH_3-28) [1]

^{13}C NMR (CD_3OD) [1]:

Table 1

C-1	37.4	C-11	21.5	C-21	23.2
2	68.7	12	32.3	22	80.2
3	68.5	13	49.0	23	87.8
4	32.9	14	85.2	24	47.9
5	51.8	15	31.8	25	43.7
6	206.6	16	22.1	26	75.4
7	121.9	17	50.2	27	15.5
8	168.5	18	18.4	28	18.2
9	35.1	19	24.4		
10	39.2	20	78.2		

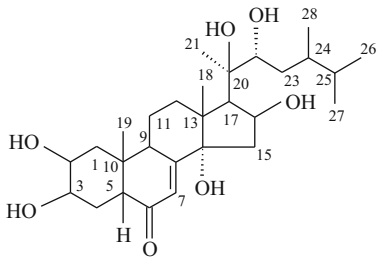
Pharm./Biol.: TPA-induced inflammation test: ID_{50} = 0.682 μM/ear [1].

References

1. Y. Sun, K. Yasukawa, Bioorg. Med. Chem. Lett. **18**, 3417 (2008)

Polyporoid C

CAS Registry Number: 1042362-47-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Polyporus umbellatus* [1]
$C_{28}H_{46}O_7$: 494.3243
Mp: amorphous [1]
$[\alpha]_D^{25}$ + 20.5° (c 0.10; MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3398, 2959, 2872, 1645, 1621, 1561, 1415, 1382, 1057 [1]
UV λ_{max}^{MeOH} nm (log ε): 243 (0.6) [1]
FAB-MS m/z: 495.33269 $[M + H]^+$ [1]
HR-FAB-MS m/z: for $C_{28}H_{47}O_7$ $[M + H]^+$ calcd. 495.33218, found 495.33269 [1]
^{1}H NMR (J/Hz, CD_3OD): 1.77 (dd, J = 4.3, 13.2, Ha-1), 1.43 (t, J = 13.2, He-1), 3.82 (dt, J = 4.0, 11.3, Ha-2), 3.94 (br s, He-3), 1.70 (m, H-4), 2.38 (dd, J = 5.0, 12.4, H-5), 5.79 (d, J = 2.4, H-7), 3.16 (m, Ha-9), 1.80 (m, Ha-11), 1.72 (m, He-11), 2.12 (m, Ha-12), 1.93 (m, He-12), 2.25 (dd, J = 7.6, 13.6, Ha-15), 2.05 (dd, J = 4.8, 13.6, Hb-15), 4.65 (m, H-16), 2.43 (d, J = 7.6, H-17), 1.13 (s, CH_3-18), 0.98 (s, CH_3-19), 1.17 (s, CH_3-21), 4.02 (dd, J = 1.4, 10.3, Hb-22), 1.53 (m, H-23), 1.74 (m, H-24), 1.85 (m, H-25), 0.80 (d, J = 6.9, CH_3-26), 0.86 (d, J = 6.8, CH_3-27), 0.94 (d, J = 6.9, CH_3-28) [1]
^{13}C NMR (CD_3OD) [1]:

Table 1

C-1	37.3	C-11	21.4	C-21	20.4
2	68.7	12	32.4	22	74.9
3	68.5	13	49.0	23	38.0
4	32.8	14	83.1	24	36.9
5	51.8	15	44.9	25	30.4
6	206.3	16	73.5	26	16.3
7	122.0	17	51.4	27	15.7
8	167.0	18	18.9	28	21.6
9	34.9	19	24.4		
10	39.2	20	80.9		

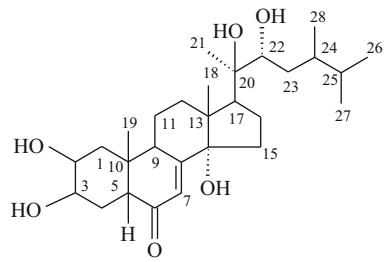
Pharm./Biol.: TPA-induced inflammation test: ID_{50} = 0.184 μM/ear [1].

References

1. Y. Sun, K. Yasukawa, Bioorg. Med. Chem. Lett. **18**, 3417 (2008)

Polyporusterone A

CAS Registry Number: 141360-88-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Polyporus umbellatus* [1, 2]
$C_{28}H_{46}O_6$: 478.3294
Mp: 261.5°C (MeOH) [1]
$[\alpha]_D^{20}$ + 52.9° (c 0.61, EtOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3300, 1650 [1]
UV λ_{max}^{MeOH} nm (log ε): 241 (4.03) [1]
FD-MS m/z: 501 $[M + Na]^+$, 479 $[M + H]^+$, 478 $[M]^+$, 363 $[M\text{-}C_7H_{15}O]^+$, 115 $[C_7H_{15}O]^+$ [1]
^{1}H NMR (270 MHz, J/Hz, C_5D_5N): 4.18 (br d, J = 11.2, Ha-2), 4.24 (br s, He-3), 6.28 (d, J = 2.5, H-7), 3.61 (m, H-9), 2.94 (dd, J = 9.0, 9.4, H-17), 1.25 (s, CH_3-18), 1.09 (s, CH_3-19), 1.59 (s, CH_3-21), 3.93 (br d, J = 9.5, H-22), 1.88 (m, H-24), 1.45 (septed, J = 6.2, H-25), 0.88 (d, J = 6.1, CH_3-26), 0.87 (d, J = 6.4, CH_3-27), 0.76 (d, J = 6.8, CH_3-28) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-11	21.1	C-21	21.3
2	67.8	12	21.4	22	74.3
3	67.8	13	47.9	23	37.1
4	32.3	14	83.7	24	36.0
5	51.2	15	31.9	25	29.6
6	202.4	16	31.6	26	16.1
7	121.1	17	49.7	27	15.8
8	165.3	18	17.8	28	21.2
9	34.4	19	24.4		
10	38.5	20	76.5		

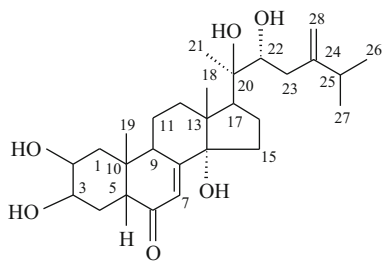
Pharm./Biol.: Cytotoxic activity: Inhibited the proliferation of leukemia *L-1210* cells [1], TPA-induced inflammation test: $ID_{50} = 0.141$ μM/ear [2].

References

1. T. Ohsawa, M. Yukawa, C. Takao, M. Murayama, H. Bando, Chem. Pharm. Bull. **40**, 143 (1992)
2. Y. Sun, K. Yasukawa, Bioorg. Med. Chem. Lett. **18**, 3417 (2008)

Polyporusterone B

CAS Registry Number: 141360-89-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polyporus umbellatus* [1, 2]

$C_{28}H_{44}O_6$: 476.3138

Mp: 250°C (MeOH) [1]

$[\alpha]_D^{20}$ + 56.1° (c 0.46, EtOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3300, 1650, 803 [1]

UV λ_{max}^{MeOH} nm (log ε): 241 (4.05) [1]

FD-MS m/z: 499 $[M + Na]^+$, 477 $[M + H]^+$, 476 $[M]^+$, 363 $[M\text{-}C_7H_{13}O]^+$, 113 $[C_7H_{13}O]^+$ [1]

^{1}H NMR (270 MHz, J/Hz, C_5D_5N): 4.20 (dt, J = 4.0, 11.4, Ha-2), 4.25 (m, He-3), 6.28 (d, J = 2.5, H-7), 3.61 (m, H-9), 2.96 (dd, J = 8.8, 9.4, H-17), 1.24 (s, CH_3-18), 1.09 (s, CH_3-19), 1.60 (s, CH_3-21), 4.05 (dd, J = 1.0, 10.0, H-22), 2.62 (br d, J = 14.5, Ha-23), 2.30 (dd, J = 10.0, 14.5, Hb-23), 1.88 (m, H-24), 2.42 (septed, J = 6.8, H-25), 1.05 (d, J = 6.8, CH_3-26), 1.03 (d, J = 6.8, CH_3-27), 5.10 (br s, H-28), 4.96 (br s, H′-28) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.0	C-11	21.1	C-21	21.5
2	68.1	12	21.5	22	75.4
3	68.1	13	48.1	23	38.3
4	32.5	14	84.2	24	154.4
5	51.4	15	32.0	25	33.7
6	203.5	16	31.7	26	22.1
7	121.7	17	50.0	27	21.8
8	166.1	18	17.9	28	108.7
9	34.5	19	24.5		
10	38.7	20	76.7		

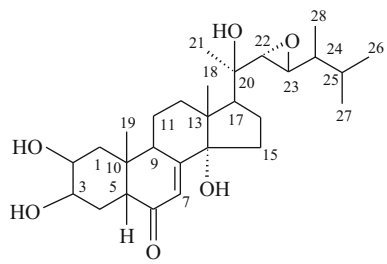
Pharm./Biol.: Cytotoxic activity: Inhibited the proliferation of leukemia *L-1210* cells [1], TPA-induced inflammation test: $ID_{50} = 0.289$ μM/ear [2].

References

1. T. Ohsawa, M. Yukawa, C. Takao, M. Murayama, H. Bando, Chem. Pharm. Bull. **40**, 143 (1992)
2. Y. Sun, K. Yasukawa, Bioorg. Med. Chem. Lett. **18**, 3417 (2008)

Polyporusterone C

CAS Registry Number: 141360-90-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Polyporus umbellatus* [1, 2]
$C_{28}H_{44}O_6$: 476.3138
Mp: 250°C (MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3350, 1645, 907, 880 [1]
FD-MS m/z: 499 $[M + Na]^+$, 477 $[M + H]^+$, 476 $[M]^+$, 319 $[M\text{-}C_9H_{17}O_2]^+$, 157 $[C_9H_{17}O_2]^+$, 113 $[C_7H_{13}O]^+$ [1]
^{1}H NMR (270 MHz, J/Hz, C_5D_5N): 4.20 (dt, J = 3.2, 10.2, Ha-2), 4.28 (m, He-3), 6.24 (d, J = 2.2, H-7), 3.62 (m, H-9), 1.16 (s, CH_3-18), 1.09 (s, CH_3-19), 1.54 (s, CH_3-21), 3.04 (d, J = 2.4, H-22), 2.97 (dd, J = 2.4, 7.6, H-23), 1.19 (dq, J = 6.8, 7.6, H-24), 1.61 (septed, J = 6.8, H-25), 1.01 (d, J = 6.8, CH_3-26), 0.95 (d, J = 6.8, CH_3-27), 0.91 (d, J = 6.8, CH_3-28) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.0	C-11	21.1	C-21	24.3
2	68.1	12	21.8	22	66.2
3	68.1	13	47.9	23	58.1
4	32.5	14	84.0	24	42.1
5	51.4	15	31.8	25	31.5
6	203.4	16	31.7	26	19.7
7	121.7	17	54.0	27	20.5
8	165.9	18	17.7	28	13.9
9	34.5	19	24.4		
10	38.7	20	72.0		

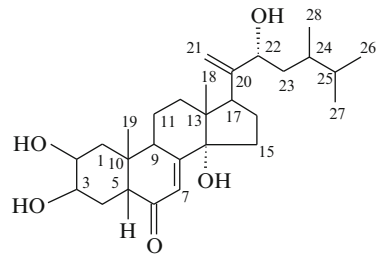
Pharm./Biol.: Cytotoxic activity: Inhibited the proliferation of leukemia *L-1210* cells [1], TPA-induced inflammation test: ID_{50} = 0.117 μM/ear [2].

References

1. T. Ohsawa, M. Yukawa, C. Takao, M. Murayama, H. Bando, Chem. Pharm. Bull. **40**, 143 (1992)
2. Y. Sun, K. Yasukawa, Bioorg. Med. Chem. Lett. **18**, 3417 (2008)

Polyporusterone D

CAS Registry Number: 141360-91-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Polyporus umbellatus* [1]
$C_{28}H_{44}O_5$: 460.3188
IR (KBr) ν_{max} cm^{-1}: 3350, 1650, 803 [1]
UV λ_{max}^{MeOH} nm (log ε): 241 (4.01) [1]
EI-MS m/z: 460 $[M]^+$, 432, 249 [1]
^{1}H NMR (270 MHz, J/Hz, C_5D_5N): 4.14 (br d, J = 10.9, Ha-2), 4.23 (br s, He-3), 6.27 (d, J = 2.3, H-7), 3.60 (m, H-9), 3.82 (m, H-17), 0.84 (s, CH_3-18), 1.05 (s, CH_3-19), 5.49 (br s, H-21), 5.13 (br s, H′-21), 4.49 (t, J = 6.6, H-22), 1.83 (m, H-24), 1.46 (septed, J = 6.5, H-25), 0.94 (d, J = 6.6, CH_3-26), 0.88 (d, J = 6.6, CH_3-27), 0.83 (d, J = 8.3, CH_3-28) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.1	C-11	21.2	C-21	111.6
2	68.2	12	28.0	22	74.3
3	68.2	13	48.4	23	41.4
4	32.6	14	84.1	24	35.7
5	51.6	15	32.3	25	30.0
6	203.6	16	31.8	26	17.6
7	121.6	17	46.8	27	17.7
8	165.9	18	16.1	28	20.6
9	34.6	19	24.5		
10	38.8	20	154.1		

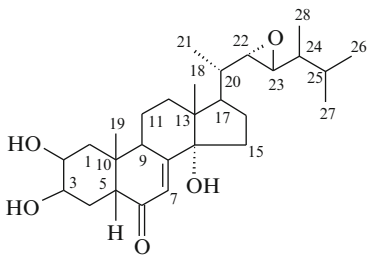
Pharm./Biol.: Cytotoxic activity: Inhibited the proliferation of leukemia *L-1210* cells [1].

References

1. T. Ohsawa, M. Yukawa, C. Takao, M. Murayama, H. Bando, Chem. Pharm. Bull. **40**, 143 (1992)

Polyporusterone E

CAS Registry Number: 141360-92-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polyporus umbellatus* [1]

$C_{28}H_{44}O_5$: 460.3188

Mp: 232°C (MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3296, 1644, 907, 880 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (4.02) [1]

EI-MS m/z: 460 $[M]^+$, 432, 345, 301, 290, 249 [1]

^{1}H NMR (270 MHz, J/Hz, C_5D_5N): 4.18 (br d, J = 10.2, Ha-2), 4.26 (br s, He-3), 6.23 (d, J = 2.2, H-7), 3.59 (m, H-9), 0.72 (s, CH_3-18), 1.09 (s, CH_3-19), 0.94 (d, J = 7.9, CH_3-21), 2.67 (d, J = 6.9, H-22), 2.54 (dd, J = 2.4, 6.9, H-23), 1.26 (m, H-24), 1.45 (septed, J = 6.2, H-25), 1.07 (d, J = 6.9, CH_3-26), 1.01 (d, J = 6.6, CH_3-27), 0.92 (d, J = 6.9, CH_3-28) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.0	C-11	21.0	C-21	20.5
2	68.0	12	26.0	22	64.0
3	68.0	13	47.5	23	59.9
4	32.5	14	83.6	24	42.4
5	51.4	15	32.0	25	31.3
6	203.4	16	32.0	26	15.9
7	121.6	17	50.9	27	16.5
8	165.4	18	15.9	28	13.8
9	34.6	19	24.4		
10	38.7	20	36.0		

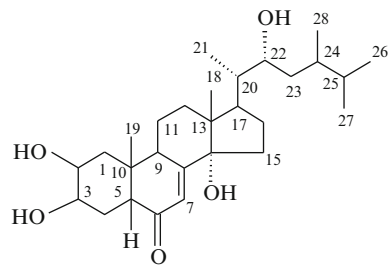
Pharm./Biol.: Cytotoxic activity: Inhibited the proliferation of leukemia *L-1210* cells [1].

References

1. T. Ohsawa, M. Yukawa, C. Takao, M. Murayama, H. Bando, Chem. Pharm. Bull. **40**, 143 (1992)

Polyporusterone F

CAS Registry Number: 141360-93-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polyporus umbellatus* [1]

$C_{28}H_{46}O_5$: 462.3345

Mp: 251°C (MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3338, 1649 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (4.02) [1]

EI-MS m/z: 462 $[M]^+$, 434, 250, 249 [1]

^{1}H NMR (270 MHz, J/Hz, C_5D_5N): 4.11 (br d, J = 10.5, Ha-2), 4.21 (br s, He-3), 6.24 (d, J = 2.5, H-7), 3.57 (m, H-9), 0.73 (s, CH_3-18), 1.09 (s, CH_3-19), 1.28 (d, J = 6.9, CH_3-21), 4.11 (m, H-22), 1.58 (septed, J = 6.5, H-25), 0.90 (d, J = 6.9, CH_3-26), 0.88 (d, J = 6.9, CH_3-27), 0.73 (d, J = 6.8, CH_3-28) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.1	C-11	21.3	C-21	13.6
2	68.2	12	26.9	22	70.9
3	68.2	13	48.3	23	35.3
4	32.6	14	83.9	24	35.8
5	51.5	15	32.1	25	29.8
6	203.7	16	31.6	26	16.3
7	121.7	17	47.7	27	16.0
8	165.9	18	16.0	28	21.6
9	34.7	19	24.6		
10	38.8	20	43.5		

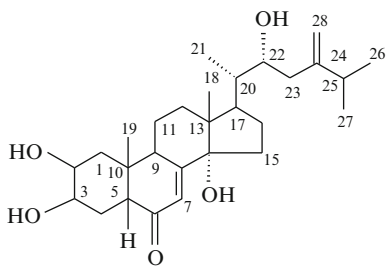
Pharm./Biol.: Cytotoxic activity: Inhibited the proliferation of leukemia *L-1210* cells [1].

References

1. T. Ohsawa, M. Yukawa, C. Takao, M. Murayama, H. Bando, Chem. Pharm. Bull. **40**, 143 (1992)

Polyporusterone G

CAS Registry Number: 141360-94-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polyporus umbellatus* [1]

$C_{28}H_{44}O_5$: 460.3188

IR (KBr) ν_{max} cm^{-1}: 3340, 1650, 803 [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (4.02) [1]

EI-MS m/z: 460 $[M]^+$, 432, 249, 247 [1]

^{1}H NMR (270 MHz, J/Hz, C_5D_5N): 4.11 (br d, J = 10.5, Ha-2), 4.21 (br s, He-3), 6.24 (d, J = 2.5, H-7), 3.57 (m, H-9), 0.72 (s, CH_3-18), 1.09 (s, CH_3-19), 1.28 (d, J = 6.9, CH_3-21), 4.11 (m, H-22), 2.48 (septed, J = 6.8, H-25), 1.06 (d, J = 6.9, CH_3-26), 1.01 (d, J = 6.9, CH_3-27), 5.11 (br s, H-28), 4.99 (br s, H′-28) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.1	C-11	21.3	C-21	13.6
2	68.2	12	26.9	22	71.7
3	68.2	13	48.4	23	36.5
4	32.6	14	83.9	24	154.9
5	51.5	15	32.1	25	33.9
6	203.7	16	31.6	26	22.3
7	121.7	17	47.7	27	22.1
8	165.7	18	16.0	28	108.7
9	34.7	19	24.6		
10	38.8	20	43.0		

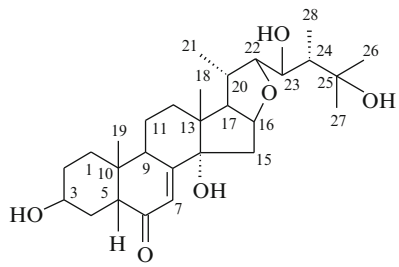
Pharm./Biol.: Cytotoxic activity: Inhibited the proliferation of leukemia *L-1210* cells [1], TPA-induced inflammation test: ID_{50} = 0.207 μM/ear [2].

References

1. T. Ohsawa, M. Yukawa, C. Takao, M. Murayama, H. Bando, Chem. Pharm. Bull. **40**, 143 (1992)
2. Y. Sun, K. Yasukawa, Bioorg. Med. Chem. Lett. **18**, 3417 (2008)

Polyporusterone H (16,22-Epoxy-3β,14α,23β,25-Tetrahydroxyergost-7-en-6-one)

CAS Registry Number: 1021913-46-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Polyporus umbellatus* [1]
$C_{28}H_{44}O_6$: 476.3138
Mp: amorphous (MeOH) [1]
$[\alpha]_D^{20}$ + 65.7° (c 0.39, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3350, 1650 [1]
UV λ_{max}^{MeOH} nm (log ε): 242 (4.01) [1]
EI-MS m/z: 458 $[M\text{-}H_2O]^+$ (8), 440 (10), 425 (4), 359 $[M\text{-}C_6H_{13}O_2]^+$ (39), 342 (63), 341 $[M\text{-}C_6H_{13}O_2\text{-}H_2O]^+$ (100), 300 (12), 285 (71), 286 (66), 263 (20), 95 (66), 79 (25) [1]
HR-FAB-MS m/z: for $C_{28}H_{44}O_6Na$ $[M + Na]^+$ calcd. 499.3030, found 499.3030 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.13 (br s, He-3), 2.97 (m, H-5), 6.18 (br s, H-7), 3.54 (br s, H-9), 5.29 (m, H-16), 2.85 (d, J = 8.0, H-17), 0.97 (s, CH_3-18), 1.04 (s, CH_3-19), 2.70 (m, H-20), 1.39 (d, J = 7.1, CH_3-21), 4.44 (dd, J = 5.6, 9.2, H-22), 4.69 (br d, J = 9.1, H-23), 2.21 (m, H-24), 1.47 (s, CH_3-26), 1.56 (s, CH_3-27), 1.45 (d, J = 7.0, CH_3-28) [1]
^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

C-1	36.5	C-11	22.0	C-21	17.0
2	29.6	12	32.9	22	84.1
3	63.8	13	49.1	23	69.8
4	34.2	14	84.9	24	43.1
5	51.6	15	41.0	25	73.3
6	202.9	16	82.8	26	29.5
7	120.9	17	61.4	27	28.9
8	165.1	18	17.8	28	7.8
9	35.2	19	24.0		
10	37.0	20	37.0		

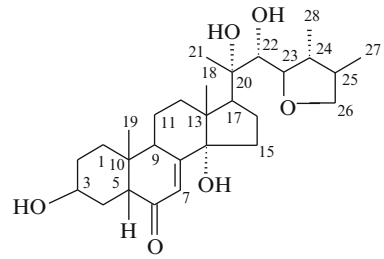
Pharm./Biol.: Cytotoxic active [1].

References

1. W.W. Zhou, W.H. Lin, S.X. Guo, Chem. Pharm. Bull. **55**, 1148 (2007)

Polyporusterone I (23,26-Epoxy-3β,14α,21α,22α-Tetrahydroxyergost-7-en-6-one)

CAS Registry Number: 1021913-47-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Polyporus umbellatus* [1]
$C_{28}H_{44}O_6$: 476.3138
Mp: amorphous (MeOH) [1]
$[\alpha]_D^{20}$ + 58.9° (c 0.41, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3350, 1650 [1]
UV λ_{max}^{MeOH} nm (log ε): 242 (3.98) [1]
EI-MS m/z: 476 $[M]^+$ (2), 458 (11), 440 (8), 422 (3), 407 (1), 347 (57), 329 (71), 311 (34), 295 (6), 287 (18), 269 (21), 99 (100), 81 (12) [1]
FAB-HR-MS m/z: for $C_{28}H_{44}O_6Na$ $[M + Na]^+$ calcd. 499.3030, found 499.3033 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.12 (br s, He-3), 2.98 (m, H-5), 6.26 (br s, H-7), 3.56 (br s, H-9), 2.47 (m, Ha-16), 2.30 (m, Hb-16), 3.46 (d, J = 9.1, H-17), 1.23 (s, CH_3-18), 1.05 (s, CH_3-19), 1.70 (s, CH_3-21), 3.89 (m, H-22), 3.89 (m, H-23), 1.94 (m, H-24), 1.70 (m, H-25), 3.89 (m, Ha-26), 3.38 (t, J = 8.4, Hb-26), 0.87 (d, J = 6.6, CH_3-27), 1.27 (d, J = 6.5, CH_3-28) [1]
^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

C-1	36.8	C-11	21.5	C-21	22.9
2	29.2	12	32.1	22	79.3
3	64.0	13	48.0	23	86.9

(*continued*)

Table 1 (continued)

4	34.2	14	84.1	24	46.9
5	51.6	15	31.5	25	42.5
6	203.9	16	21.8	26	74.3
7	121.1	17	49.8	27	15.3
8	166.6	18	18.0	28	18.0
9	33.5	19	24.2		
10	37.2	20	76.7		

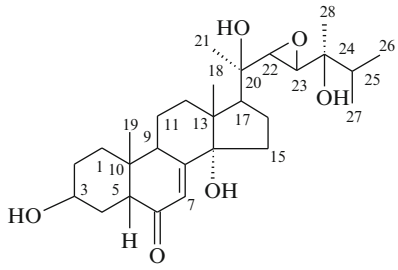
Pharm./Biol.: Cytotoxic active [1].

References

1. W.W. Zhou, W.H. Lin, S.X. Guo, Chem. Pharm. Bull. **55**, 1148 (2007)

Polyporusterone J (22,23-Epoxy-3β,14α,20β,24β-Tetrahydroxy-7-en-6-one)

CAS Registry Number: 141454-09-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Polyporus umbellatus* [1]

$C_{28}H_{44}O_6$: 476.3138

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.15 (br s, He-3), 2.97 (m, H-5), 6.21 (br s, H-7), 3.54 (br s, H-9), 2.43 (m, Ha-16), 2.33 (m, Hb-16), 3.05 (d, J = 9.3, H-17), 1.14 (s, CH_3-18), 1.04 (s, CH_3-19), 1.59 (s, CH_3-21), 3.64 (d, J = 1.9, H-22), 3.31 (d, J = 1.9, H-23), 1.92 (m, H-25), 1.16 (d, J = 6.8, CH_3-26), 1.16 (d, J = 6.8, H-27), 1.38 (s, CH_3-28) [1]

^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

C-1	36.4	C-11	21.8	C-21	24.1
2	29.7	12	31.8	22	62.4
3	63.8	13	48.1	23	60.0
4	34.3	14	83.9	24	71.2
5	51.6	15	31.3	25	36.8
6	203.2	16	21.7	26	17.4
7	121.3	17	51.6	27	17.5
8	166.1	18	17.5	28	22.3
9	34.5	19	24.1		
10	38.3	20	71.8		

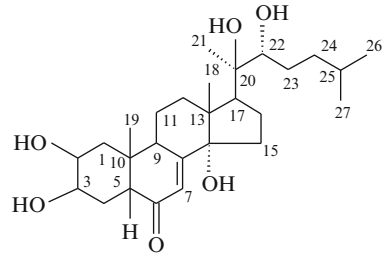
Pharm./Biol.: Cytotoxic active [1].

References

1. W.W. Zhou, W.H. Lin, S.X. Guo, Chem. Pharm. Bull. **55**, 1148 (2007)

Ponasterone A

CAS Registry Number: 13408-56-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Acrostichum aureum* [1], *Athyrium nipponicum, Blechnum amabile* [2, 3], *B. minus* [4], *B. nipponicum* [2, 3], *B. pennamarina* [4], *Cheilantes seiberi* [1], *Dacridium pierrei* [5], *Dryopteris thelypteris, Gleichenia glauca* [6], *Hicriopteris glauca* [2], *Limnanthes douglasii* [7], *Matteuccia struthiopteris* [8], *Onoclea sensibilis, Osmunda asiatica, O. japonica* [2], *Podocarpus chinensis* [9, 10], *P. dispermus* [1], *P. gracilior* [11], *P. macrophyllus* [9, 10], *P. nakaii*

[12], *P. nerifolius* [1], *P. selowii* [13], *Pteridium aquilinum, Pteridium aquilinum* var. *latiusculum* [2, 14, 15], *Schizea dichotoma* [1], *Struthiopteris nipponica* [16], *Tapinella panuoides* [17], *Taxis breviflora* [18], *T. cuspidate* [10], *Woodwardia japonica, W. orietalis var. formosana, W. takeoi, W. unigemmata* [19]

$C_{27}H_{44}O_6$: 464.3137

Mp: 259–260°C (decomp.) [12], 258–260°C (decomp.) [14], 277–278°C (EtOAc–MeOH) [15], 201–203°C (MeOH) [17], 251–255°C (decomp.) [20], 256–258°C (EtOAc–MeOH) [21]

$[\alpha]_D^{15}$ + 90° (c, MeOH) [12]

IR (KBr) ν_{max} cm^{-1}: 3420, 1643 [12], 3400, 1645 [14], 3350, 1640 [15], 3554, 3394, 1646, 1050 [17], 1650 [20]

UV λ_{max}^{MeOH} nm: 244 (ε 12400), 326 (ε 130) [12], 243 [22]

UV λ_{max}^{EtOH} nm: 244 (ε 12000) [14], 242 (ε 12000) [20]

EI-MS m/z: 446 $[M\text{-}H_2O]^+$, 428 $[M\text{-}2H_2O]^+$, 410 $[M\text{-}3H_2O]^+$, 395 $[M\text{-}3H_2O\text{–}CH_3]^+$, 345 $[M\text{-}C_6H_{13}O\text{–}H_2O]^+$, 328, 300 [22]

FAB-MS m/z: 487 $[M + Na]^+$ (33), 465 $[M + H]^+$ (97), 447 $[M + H\text{-}H_2O]^+$ (73), 429 $[M + H\text{-}2H_2O]^+$ (25), 303 (100) [17]

HR-MS m/z: for $C_{27}H_{45}O_6$ $[M + H]^+$ calcd. 465.3220, found 465.3221 [17]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.43 (dd, J = 12.4, 13.2, Ha-1), 1.79 (dd, J = 4.5, 13.2, He-1), 3.84 (ddd, J = 3.3, 4.2, 12.0, Ha-2), 3.95 (q, J = 2.7, He-3), 1.74 (Ha-4), 1.70 (He-4), 2.38 (dd, J = 4.6, 12.8, H-5), 5.81 (d, J = 2.0, H-7), 3.15 (ddd, J = 2.6, 7.0, 10.5, H-9), 1.70 (Ha-11), 1.81 (He-11), 2.12 (dt, J = 5.0, 13.0, 13.0, Ha-12), 1.88 (ddd, J = 2.0, 4.0, 12.8, He-12), 1.96 (Ha-15), 1.59 (Hb-15), 1.99 (Ha-16), 1.70 (Hb-16), 2.37 (t, J = 8.8, H-17), 0.89 (s, CH_3-18), 0.967 (s, CH_3-19), 1.175 (s, CH_3-21), 3.33 (dd, J = 1.7, 10.0, H-22), 1.47 (Ha-23), 1.23 (Hb-23), 1.46 (Ha-24), 1.21 (Hb-24), 1.56 (H-25), 0.924 (d, J = 6.5, CH_3-26), 0.915 (d, J = 6.5, CH_3-27) [17]

^{1}H NMR (J/Hz, C_5D_5N): 6.21 (H-7), 1.19 (s, CH_3-18), 1.05 (s, CH_3-19), 1.53 (s, CH_3-21), 0.83 (d, J = 6.0, CH_3-26), 0.83 (d, J = 6.0, CH_3-27) [20]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.16 (m, Ha-2), 4.23 (br s, He-3), 3.02 (dd, J = 3.8, 13.2, H-5), 6.26 (d, J = 2.4, H-7), 3.60 (m, H-9), 2.93 (t, J = 9.1, H-17), 1.23 (s, CH_3-18), 1.07 (s, CH_3-19), 1.57 (s, CH_3-21), 3.80 (br d, J = 10.4, H-22), 0.81 (d, J = 6.1, CH_3-26), 0.83 (d, J = 6.1, CH_3-27) [21]

^{13}C NMR (125.7 MHz, CD_3OD) [17]: **^{13}C NMR** (C_5D_5N) [23]:

Table 1

C-1	37.37	C-15	31.77	C-1	37.9	C-15	31.9
2	68.73	16	21.51	2	68.0	16	21.4
3	68.51	17	50.48	3	68.0	17	50.0
4	32.88	18	18.02	4	32.4	18	17.9
5	51.80	19	24.39	5	51.3	19	24.4
6	206.50	20	77.86	6	203.5	20	76.7
7	122.14	21	20.98	7	121.7	21	21.1
8	168.00	22	77.99	8	166.0	22	76.7
9	35.11	23	37.66	9	34.4	23	30.2
10	39.26	24	30.48	10	38.7	24	37.1
11	21.51	25	29.23	11	21.4	25	28.1
12	32.53	26	22.74	12	31.8	26	22.3
13		27	23.41	13	48.1	27	23.3
14	85.25			14	84.1		

Pharm./Biol.: *Chilo suppressalis* bioassay: strong moulting activity [9], *Samia cyanthia* bioassay: high active, *Calliphora* bioassay: high active [12], *Musca domestica* bioassay: exert positive moulting hormone activity [22, 24], *Bombyx mori* bioassay: showed very high activity [24], *Galleria mellonella* bioassay: ED_{50} = 12.5 μg/g, *Sarcophaga bullata* bioassay: ED_{50} = 7.3 μg/g, *Dermestes vulpinus* bioassay: ED_{50} = 17.0 μg/g [25], *Drosophila melanogaster* B_{II} bioassay: EC_{50} = 3.1 × 10^{-10} M [26–28].

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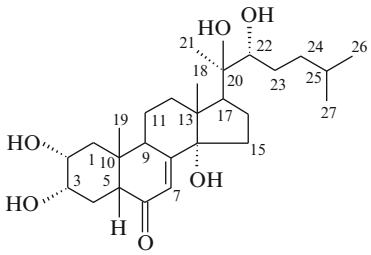
Ponasterone B

CAS Registry Number: 19338-77-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Podocarpus nakaii* [1]

$C_{27}H_{44}O_6$: 464.3137

IR (KBr) ν_{max} cm^{-1}: 3400, 1660, 1630 [1]

UV λ_{max}^{MeOH} nm: 320, 244 [1]

^{1}H NMR (J/Hz, C_5D_5N): 1.17 (s, CH_3-18), 1.11 (s, CH_3-19), 1.54 (s, CH_3-21), 0.82 (d, J = 6.0, CH_3-26), 0.82 (d, J = 6.0, CH_3-27) [1]

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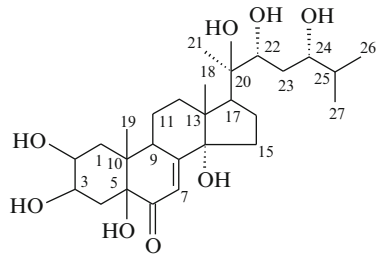
Ponasterone C

CAS Registry Number: 26191-89-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Blandfordia punicea* [1], *Dacrydium intermedium* [2], *Podocarpus nakaii* [3]

$C_{27}H_{44}O_8$: 496.3036

Mp: 271–273°C (MeOH–EtOAc) [2], 270–272°C (dec.) [3]

IR (KBr) ν_{max} cm^{-1}: 3375, 1668, 1626 [3]

UV λ_{max}^{EtOH} nm (ε): 244 (11000), 326 (100) [3]

EI-MS m/z: 478 $[M\text{-}H_2O]^+$, 460 $[M\text{-}2H_2O]^+$, 379, 361, 343, 325, 117, 99, 81 [4]

CD (c, dioxane): Δε = +3.00 (324 nm), Δε = −5.44 (251 nm) [4]

^{1}H NMR (J/Hz, C_5D_5N): 4.12 (H-2), 4.03 (H-3), 6.26 (H-7), 1.19 (s, CH_3-18), 1.13 (s, CH_3-19), 1.57 (s, CH_3-21), 1.02 (d, J = 6.0, CH_3-26), 1.02 (d, J = 6.0, CH_3-27) [2]

^{1}H NMR (J/Hz, C_5D_5N): 1.17 (s, CH_3-18), 1.12 (s, CH_3-19), 1.54 (s, CH_3-21), 1.00 (d, J = 6.0, CH_3-26), 1.00 (d, J = 6.0, CH_3-27) [3]

^{13}C NMR (C_5D_5N) [5]:

Table 1

C-1	34.6	C-10	44.6	C-19	17.0
2	67.8	11	21.3	20	76.8
3	69.7	12	31.5	21	21.5
4	35.9	13	48.0	22	76.7
5	79.7	14	83.9	23	35.6
6	200.8	15	32.0	24	77.5
7	119.8	16	22.0	25	34.0
8	166.8	17	49.8	26	19.5
9	38.2	18	17.8	27	17.0

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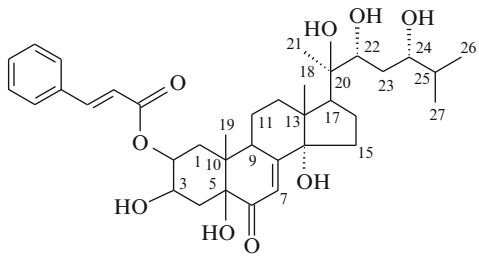
Ponasterone C-2-Cinnamate

CAS Registry Number: 38147-17-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Dacrydium intermedium* [1]

$C_{36}H_{50}O_9$: 626.3454

IR (KBr) ν_{max} cm^{-1}: 3380, 1700, 1670, 1640 [1]

UV λ_{max}^{EtOH} nm: 276 (ε 19200), 250 (sh.), 224 (ε 18500), 218 (ε 19200) [1]

EI-MS m/z: 608 $[M\text{-}H_2O]^+$, 590 $[M\text{-}2H_2O]^+$, 572 $[M\text{-}3H_2O]^+$, 510 [M-116 (side chain)]$^+$, 442 [M-148 (cinnamic acid) - 36]$^+$, 361 [M-148-117]$^+$, 148 (cinnamic acid), 147 (base peak) (cinnamoyl-oxy), 131 (cinnamoyl) [1]

HR-MS m/z: for $C_{36}H_{44}O_6$ $[M\text{-}3H_2O]^+$ calcd. 572 [1]

^{1}H NMR (100 MHz, J/Hz, $CDCl_3$): 5.16 (m, Ha-2), 4.18 (m, He-3), 5.96 (H-7), 0.87 (s, CH_3-18), 0.92 (s, CH_3-19), 1.22 (s, CH_3-21), 0.92 (s, CH_3-26), 0.92 (s, CH_3-27), Other: 7.37 (Ar), 6.50 (d, J = 16.0, vinylic), 7.70 (d, J = 16.0, vinylic) [1].

References

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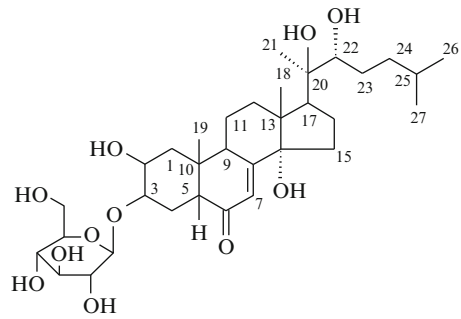
Ponasteroside A

CAS Registry Number: 20117-33-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Pteridium aquilinum* var. *latiusculum* [1], *Lygodium japonicum* [2]

$C_{33}H_{54}O_{11}$: 626.3666

Mp: 278–279.5°C [1], 278–279°C [2]

$[\alpha]_D$ + 28.5° (pyridine) [1]
IR (KBr) ν_{max} cm^{-1}: 3430, 1650 [1]
UV λ_{max}^{EtOH} nm: 245 [1]
EI-MS m/z: 626 $[M]^+$ [1]
CD (c, dioxane): $[\theta]_{339}$ +45 × 10^3 [1]
^{1}H NMR (J/Hz, C_5D_5N): 6.18 (d, H-7), 1.17 (s, CH_3-18), 0.88 (s, CH_3-19), 1.54 (s, CH_3-21), 0.84 (d, CH_3-26), 0.84 (d, CH_3-27) [1]
^{1}H NMR (600 MHz, J/Hz, C_5D_5N): 1. 76 (m, Ha-1), 2.10 (m, He-1), 4.10 (br d, J = 11.4, Ha-2), 4.30 (overlap, He-3), 1.73 (m, Ha-4), 2.20 (m, He-4), 2.93 (m, H-5), 6.23 (d, J = 1.8, H-7), 3.55 (t, J = 8.4, H-9), 1.65 (m, Ha-11), 1.83 (m, He-11), 2.02 (m, Ha-12), 2.58 (dt, J = 4.2, 12.6, He-12), 1.92 (m, Ha-15), 2.15 (m, Hb-15), 2.08 (m, Ha-16), 2.44 (m, Hb-16), 2.91 (m, H-17), 1.19 (s, CH_3-18), 0.87 (s, CH_3-19), 1.58 (s, CH_3-21), 3.81 (br d, J = 10.8, H-22), 1.47 (m, H-23), 1.40 (m, Ha-24), 1.70 (m, Hb-24), 1.54 (m, H-25), 0.81 (d, J = 6.0, CH_3-26), 0.82 (d, J = 6.0, CH_3-27), Other: β-D-Glcp′: 4.90 (d, J = 7.8, H-1), 4.03 (m, H-2), 4.20 (m, H-3), 4.18 (m, H-4), 3.93 (m, H-5), 4.32 (m, H-6), 4.53 (br d, J = 10.2, H-6′) [2]
^{13}C NMR (150 MHz, C_5D_5N) [2]:

Table 1

C-1	38.7	C-12	32.0	C-23	28.2
2	67.5	13	48.1	24	37.2
3	76.8	14	84.2	25	30.6
4	30.3	15	31.8	26	23.4
5	51.4	16	21.5	27	22.4
6	203.1	17	50.1	Glc′-1	104.2
7	121.7	18	17.9	2	74.7
8	166.4	19	24.1	3	78.7
9	34.3	20	77.7	4	71.6
10	39.0	21	21.6	5	78.5
11	21.1	22	76.8	6	62.6

Pharm./Biol.: *Sarcophaga* test: high insect moulting hormone activity; high stimulating effect on protein synthesis in mouse [1].

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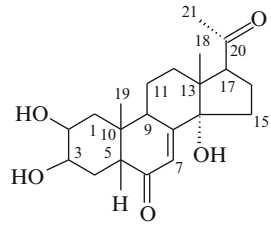
Poststerone

CAS Registry Number: 10162-99-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Cyanotus longifolia* [1], *Cyathula capitata* [2], *Leuzea carthamoides* [3], *Lychnis flos-cuculi* [4], *Microsorum scolopendria* [5], *Serratula tinctoria* [6], *Silene otites* [7]
$C_{21}H_{30}O_5$: 362.2093
Mp: 234–236°C (incorr.) (MeOH) [2], 232–235°C [8]
IR (KBr) ν_{max} cm^{-1}: 3425, 1710, 1645 [2], 3400, 1711, 1644 [3], 1700, 1647 [8]
UV λ_{max}^{EtOH} nm (ε): 240 (12400) [8]
EI-MS m/z: 362 $[M]^+$, 344 $[M\text{-}H_2O]^+$, 326 $[M\text{-}2H_2O]^+$, 301 $[M\text{-}H_2O\text{–}CH_3CO]^+$, 283 $[M\text{-}2H_2O\text{–}CH_3CO]^+$ [8]
FAB-MS m/z: 363 $[M + H]^+$ (100), 345 (38), 331 (12), 329 (7), 327 (7), 303 (12), 301 (10), 269 (10), 239 (10), 227 (12), 215 (17), 199 (15), 173 (26), 159 (25), 147 (27), 131 (25), 121 (36), 101 (62) [3]
HR-MS m/z: for $C_{21}H_{31}O_5$ $[M + H]^+$ calcd. 363.2172, found 363.2165 [3]
^{1}H NMR (J/Hz, D_2O): 1.40 (t, J = 13.0, Ha-1), 1.89 (He-1), 4.00 (m, Ha-2), 4.09 (m, He-3), 1.76 (Ha-4), 1.76 (He-4), 2.36 (t, H-5), 5.99 (d, J = 2.5, H-7), 3.15 (m, H-9), 1.72 (Ha-11), 1.96 (He-12), 1.91 (Ha-12), 2.18 (He-12), 2.12 (Ha-15), 1.76 (Hb-15), 1.91 (Ha-16), 2.22 (Hb-16), 3.34 (dd, J = 9.5, 7.8, H-17), 0.64 (s, CH_3-18), 1.00 (s, CH_3-19), 2.26 (s, CH_3-21) [1]
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.09 (m, H-2), 4.15 (m, H-3), 2.90 (dd, J = 4.0, 12.0, H-5), 6.09 (d, J = 2.0, H-7), 3.46 (m, H-9), 3.52 (dd, J = 8.0, 8.0, H-17), 0.68 (s, CH_3-18), 1.00 (s, CH_3-19), 2.12 (s, CH_3-21) [2]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.80 (dd, Ha-1), 1.44 (He-1), 3.84 (ddd, Ha-2), 3.96 (br q, He-3), 1.75 (Ha-4), 1.70 (He-4), 2.39 (dd, H-5), 5.82 (d, H-7), 3.19 (ddd, H-9), 1.88 (Ha-11), 1.68 (He-11), 2.33 (dt, Ha-12), 1.82 (He-12), 2.00 (Ha-15), 1.68 (Hb-15), 2.25 (Ha-16), 1.88 (Hb-16), 3.33 (dd, H-17), 0.62 (s, CH_3-18), 0.96 (s, CH_3-19) [3]

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.45 (dd, J = 12.0, 13.0, Ha-1), 1.80 (He-1), 3.85 (ddd, J = 3.0, 4.0, 11.5, Ha-2), 3.96 (q, J = 2.7, He-3), 1.72 (Ha-4), 1.78 (He-4), 2.40 (H-5), 5.82 (d, J = 2.5, H-7), 3.20 (ddd, J = 2.5, 7.0, 11.0, H-9), 1.70 (Ha-11), 1.90 (He-11), 2.05 (dt, Ha-12), 1.65 (He-12), 2.00 (Ha-15), 1.65 (Hb-15), 1.90 (Ha-16), 2.25 (Hb-16), 3.34 (t, J = 8.5, H-17), 0.63 (s, CH_3-18), 0.97 (s, CH_3-19), 2.16 (s, CH_3-21) [6]

^{13}C NMR (D_2O) [1]: **^{13}C NMR** (125.7 MHz, CD_3OD) [3]:

Table 1

C-1	37.7	C-12	32.3	C-1	37.37	C-12	32.09
2	69.7	13	50.8	2	68.70	13	49.00
3	69.6	14	87.8	3	68.48	14	85.00
4	33.7	15	33.2	4	32.86	15	31.07
5	53.2	16	23.1	5	51.80	16	22.18
6	210.7	17	61.5	6	206.26	17	60.16
7	123.8	18	19.0	7	122.52	18	17.50
8	168.9	19	25.5	8	166.53	19	24.40
9	36.2	20	219.4	9	35.15	20	212.49
10	40.5	21	33.7	10	39.24	21	31.51
11	22.9			11	21.60		

^{13}C NMR (25 MHz, C_5D_5N) [9]:

Table 2

C-1	37.8	C-12	31.8
2	67.9	13	48.1
3	67.9	14	83.9
4	32.2	15	30.4
5	51.2	16	21.9
6	203.1	17	59.4
7	122.0	18	17.1
8	164.3	19	24.3
9	34.4	20	209.0
10	38.6	21	31.2
11	21.0		

Pharm./Biol.: *Samia cynthia* bioassay: initiated adult development at four times the dose required for α-ecdysone [2, 8], *Calliphora* bioassay: inactive [2, 8], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 2.0 \times 10^{-5}$ M [10–12].

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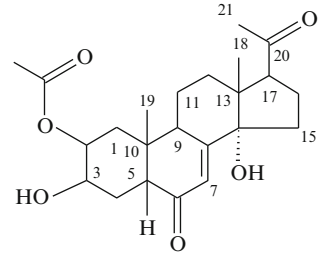
Poststerone-2-Acetate

CAS Registry Number: 19318-05-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyanotus longifolia* [1]

$C_{23}H_{32}O_6$: 404.2198

CI-MS m/z: 422 $[M + NH_4]^+$, 405 $[M + H]^+$, 344 $[M + NH_4–CH_3COOH–H_2O]^+$ [1]

^{1}H NMR (J/Hz, D_2O): 1.56 (t, J = 13.1, Ha-1), 1.99 (He-1), 5.10 (m, Ha-2), 4.24 (m, He-3), 1.80 (Ha-4), 1.84 (He-4), 2.44 (dd, J = 13.8, 4.4, H-5), 6.02 (d, J = 2.2, H-7), 3.22 (m, H-9), 1.73 (Ha-11), 1.96 (He-12), 1.92 (Ha-12), 2.20 (He-12), 2.12 (Ha-15), 1.76 (Hb-15), 1.91 (Ha-16), 2.22 (Hb-16), 3.34 (t, J = 8.5, H-17), 0.64 (s, CH_3-18), 1.03 (s, CH_3-19), 2.26 (s, CH_3-21), 2.13 (s, CH_3COO-2) [1]

^{13}C NMR (D_2O) [1]:

Table 1

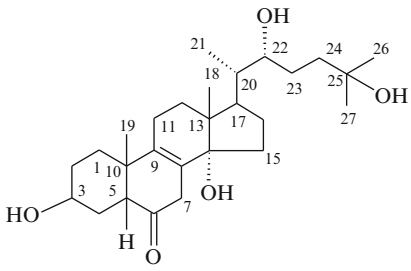
C-1	35.1	C-9	36.1	C-17	61.7
2	74.1	10	40.0	18	19.0
3	67.6	11	22.6	19	25.4
4	33.6	12	31.9	20	221.4
5	52.8	13	50.2	21	33.7
6	n.d.	14	86.9	CH_3COO	23.2
7	123.9	15	33.2	CH_3COO	175.7
8	n.d.	16	23.2		

References

1. S. Crouzet, A. Maria, L. Dinan, R. Lafont, J.P. Girault, Arch. Insect Biochem. Physiol. **72**, 194 (2009)

Praemixisterone

CAS Registry Number: 74396-17-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene praemixta* [1]

$C_{27}H_{44}O_5$: 448.3188

Mp: 110–112°C (EtOH–H_2O) [1], 109–110°C (EtOH–H_2O) [2]

$[\alpha]_D^{24}$ 0 ± 4° (c 0.85, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3415, 1710 [1], 3510, 1708, 1631 [2]

UV λ_{max}^{EtOH} nm (log ε): 202 (3.35) [1]

EI-MS m/z: 448 $[M]^+$ (1), 430 (11), 415 (4), 412 (7), 397 (5), 394 (3), 379 (2), 361 (10), 343 (6), 332 (5), 314 (5), 303 (4), 299 (4), 285 (7), 284 (4), 277 (33), 234 (18), 233 (14), 215 (16), 99 (100), 81 (37) [1], 448 $[M]^+$ (1), 430 $[M\text{-}H_2O]^+$ (30), 415 $[M\text{-}H_2O–CH_3]^+$ (12), 412 (21), 397 (13), 394 (6), 379 (1), 361 (31), 343 (18), 332 (15), 314 (14), 303 (12), 299 (11), 285 (20), 284 (12), 277 (100) [2]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.09 (m, H-3), 0.81 (s, CH_3-18), 0.98 (s, CH_3-19), 1.09 (s, CH_3-21), 3.72 (H-22), 1.30 (s, CH_3-26), 1.30 (s, CH_3-27) [1]

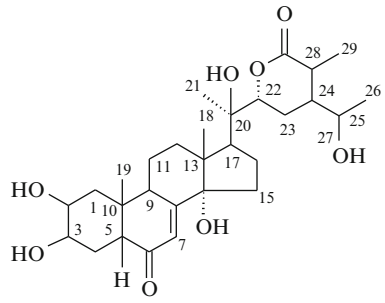
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.12 (m, H-3), 2.24–2.46 (H-5), 2.24–2.46 (H-7), 0.80 (s, CH_3-18), 0.97 (s, CH_3-19), 1.07 (d, J = 6.0, CH_3-21), 3.74 (m, H-22), 1.29 (s, CH_3-26), 1.29 (s, CH_3-27) [2]

References

1. Z. Saatov, B.Z. Usmanov, N.K. Abubakirov, Chem. Nat. Comp. **15**, 703 (1979)
2. G.M. Segal, J.S. Sydykov, N.V. Torgov, Izvestie AN USSR **2**, 317 (1982) [in Russian]

Precyasterone

CAS Registry Number: 27335-85-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Cyathula capitata* [1]

$C_{29}H_{44}O_8$: 520.3036

$[\alpha]_D^{20}$ + 39° (c, MeOH) [1]

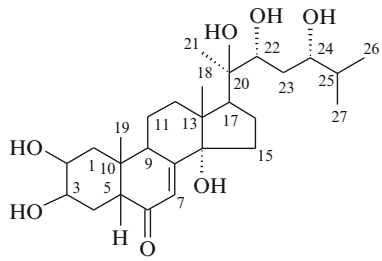
IR (KBr) ν_{max} cm^{-1}: 1710, 1650 [1]
UV λ_{max}^{EtOH} nm: 244 [1]
EI-MS m/z: 502 $[M\text{-}H_2O]^+$, 363, 345, 327, 157, 139, 121 [1]
^{1}H NMR (J/Hz, C_5D_5N): 6.16 (d, H-7), 1.11 (s, CH_3-18), 1.05 (s, CH_3-19), 1.44 (s, CH_3-21), 1.35 (d, CH_3-27), 1.24 (d, CH_3-29) [1]

References

1. H. Hikino, K. Nomoto, R. Ino, T. Takemoto, Chem. Pharm. Bull. **18**, 1078 (1970)

Pterosterone

CAS Registry Number: 18089-44-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Acrostichum aureum* [1], *Athyrium hipponicum* [2], *Briza maxima* [3], *Dacrydium intermedium* [4], *Gomphrena affinis, G. haageana* [5], *Kalanchoe blossfeldiana* [6], *Lastrea thelypteris* [7], *Lemmaphyllum macrophyllum* [8, 9], *Lychnis chalcedonica* [10], *Matteuccia struthiopteris* [2], *Onoclea sensibilis* [7], *Pfaffia iresinoides* [11, 12], *Schizea dichotoma* [1], *Serratula tinctoria* [13], *Vitex glabrata* [14], *V. megapotamica* [15]
$C_{27}H_{44}O_7$: 480.3087
Mp: 214–216°C [4], 229–230°C [7], 228–230°C [12], 227–228°C (MeOH–$CHCl_3$) [14], 218–220, 228–231°C [15]
$[\alpha]_D^{20}$ + 7.4° (c, MeOH) [7]
IR (KBr) ν_{max} cm^{-1}: 3380, 1641 [4, 7], 3420, 1650 [12], 1645, 1625 [15]
UV λ_{max}^{EtOH} nm (ε): 243 (9100) [4], 243 [7]
EI-MS m/z: 480, 462, 444, 426, 408, 363 $[M\text{-}117]^+$, 345 $[M\text{-}117\text{-}H_2O]^+$, 328 $[M + H\text{-}117\text{-}2H_2O]^+$, 117 $[M\text{-}363]^+$, 99 $[M\text{-}363\text{-}H_2O]^+$, 81 $[M\text{-}363\text{-}2H_2O]^+$ [4], 462 $[M\text{-}H_2O]^+$, 444, 429, 426, 419, 411, 408, 401, 383, 363, 345 [13]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.16 (br dt, J = 3.4, 11.8, Ha-2), 4.22 (br s, He-3), 3.02 (dd, J = 4.3, 13.0, H-5), 6.25 (d, J = 2.2, H-7), 3.58 (br t J = 9.2, H-9), 2.60 (dt, J = 5.0, 13.0, Ha-12), 2.47 (q, J = 10.4, Ha-16), 2.94 (t, J = 9.2, H-17), 1.21 (s, CH_3-18), 1.06 (s, CH_3-19), 1.59 (s, CH_3-21), 4.12 (br d, J = 10.6, H-22), 3.94 (dt, J = 4.0, 9.0, H-24), 1.003 (d, J = 6.6, CH_3-26), 1.006 (d, J = 6.6, CH_3-27) [12]
^{13}C NMR (100 MHz, C_5D_5N) [12]:

Table 1

C-1	37.7	C-10	38.6	C-19	24.4
2	68.1	11	21.0	20	76.8
3	68.0	12	31.9	21	21.6
4	32.4	13	48.0	22	77.4
5	51.3	14	84.1	23	35.7
6	203.8	15	31.6	24	76.7
7	121.6	16	21.4	25	33.8
8	166.3	17	49.9	26	17.0
9	34.3	18	17.9	27	19.5

Pharm./Biol.: *Sarcophaga* test: high moulting hormone active; high protein anabolic active [7].

References

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11. N. Nishimoto, Y. Shiobara, S.S. Inoue, M. Fujino, T. Takemoto, C.L. Yeoh, F. De Oliveira, G. Akisue, M.K. Akisue, G. Hashimoto, Phytochemistry **27**, 1665 (1988)

12. N. Nishimoto, Y. Shiobara, M. Fujino, S.S. Inoue, T. Takemoto, F. De Oliveira, G. Akisue, M.K. Akisue, G. Hashimoto, O. Tanaka, R. Kasai, H. Matsuura, Phytochemistry **26**, 2505 (1987)
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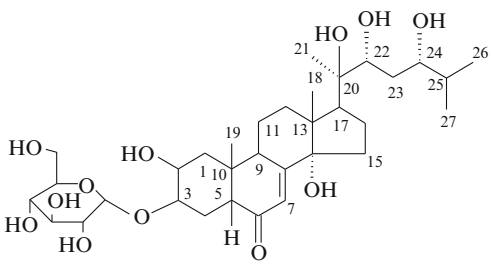
14. A. Suksamrarn, B. Yin, S. Charoensuk, Tetrahedron **55**, 255 (1999)
15. H. Rimpler, Tetrah. Lett. **24**, 329 (1969)

Pterosterone-3-Glucoside

CAS Registry Number: 960198-74-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Sida rhombifolia* [1]

$C_{33}H_{54}O_{12}$: 642.3615

Mp: amorphous [1]

$[\alpha]_D^{20}$ + 29.1° (c 3.4; MeOH) [1]

IR (NaCl) ν_{max} cm^{-1}: 3379, 1648, 1374, 1169, 1074, 1025 [1]

UV λ_{max}^{MeOH} nm (ε): 250 (4832) [1]

HR-ESI-MS m/z: for $C_{33}H_{54}NaO_{12}$ $[M + Na]^+$ calcd. 665.3513, found 665.3658 [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 1.72–1.78 (Ha-1), 2.01–2.06 (He-1), 4.12–4.14 (Ha-2), 4.30 (br s, He-3), 1.66–1.69 (Ha-4), 2.19–2.23 (He-4), 2.91–2.94 (H-5), 6.22 (s, H-7), 3.54 (br s, Ha-9), 1.78–1.80 (Ha-11), 1.89 (t, J = 12.0, He-11), 1.92–1.98 (Ha-12), 2.56–2.58 (He-12), 2.01–2.09 (Ha-15), 2.53–2.56 (Hb-15), 2.45 (br s, Ha-16), 2.48 (br s, Hb-16), 2.89–2.91 (H-17), 1.18 (s, CH_3-18), 0.86 (s, CH_3-19), 1.58 (s, CH_3-21), 4.12–4.14 (H-22), 1.98–2.01 (Ha-23), 2.06–2.09 (Hb-23), 3.95 (q, J = 4.0, H-24), 1.69–1.78 (H-25), 1.02 (d, J = 6.4, CH_3-26), 1.02 (d, J = 6.4, CH_3-27), Other: β-D-Glcp′: 4.91 (d, J = 7.6, H-1), 4.03 (t, J = 8.0, H-2), 3.91 (br s, H-3), 4.22 (m, H-4), 4.21 (m, H-5), 4.33 (m, Ha-6), 4.52 (d, J = 11.6, Hb-6) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.9	C-12	31.7	C-23	35.8
2	67.4	13	48.0	24	76.7
3	77.3	14	84.1	25	33.9
4	30.4	15	31.9	26	16.9
5	51.3	16	21.5	27	19.6
6	203.3	17	49.9	Glc′-1	103.9
7	121.6	18	17.9	2	74.7
8	166.5	19	24.0	3	78.5
9	34.2	20	76.7	4	71.5
10	38.6	21	21.7	5	78.4
11	21.0	22	77.6	6	62.4

References

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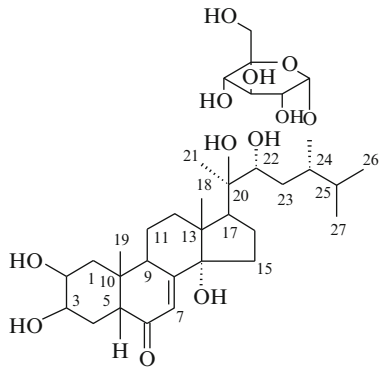
Pterosterone-24-Glucoside

CAS Registry Number: 116424-81-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Pfaffia iresinoides* [1]

$C_{33}H_{54}O_{12}$: 642.3615

Mp: 276–277°C [1]

$[\alpha]_D^{15}$ + 40.9° (c 1.5, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}:3400, 1650 [1]
UV λ_{max}^{EtOH} nm (log ε): 243 (4.04) [1]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 2.98 (dd, J = 13.4, 4.0, H-5), 6.22 (d, J = 2.2, H-7), 3.55 (br t, J = 9.0, H-9), 2.51 (dt, J = 13.2, 5.0, H-12), 2.42 (q, J = 10.2, H-16), 2.89 (t, J = 9.0, H-17), 1.17 (s, CH_3-18), 1.04 (s, CH_3-19), 1.56 (s, CH_3-21), 1.05 (d, J = 6.6, CH_3-26), 1.14 (d, J = 6.6, CH_3-27), Other: β-D-Glcp′: 4.96 (d, J = 7.6, H-1) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.0	C-12	32.1	C-23	36.1
2	68.3	13	48.1	24	84.7
3	68.2	14	84.2	25	32.1
4	32.6	15	31.8	26	17.3
5	51.5	16	21.6	27	19.5
6	203.6	17	49.9	Glc′-1	105.9
7	121.7	18	18.0	2	75.5
8	166.3	19	24.6	3	78.7
9	34.5	20	76.8	4	72.1
10	38.8	21	21.6	5	78.2
11	21.2	22	75.4	6	63.3

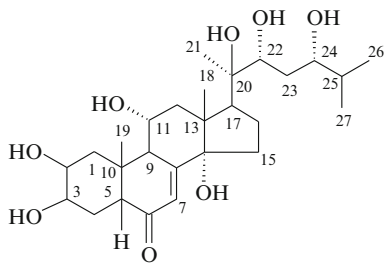
Pharm./Biol.: *Lucilia cuprina* test: weak activities (ca 1/100) compared to 20-hydroxyecdysone [1].

References

1. N. Nishimoto, Y. Shiobara, S.S. Inoue, M. Fujino, T. Takemoto, C.L. Yeoh, F. De Oliveira, G. Akisue, M.K. Akisue, G. Hashimoto, Phytochemistry **27**, 1665 (1988)

Punisterone (Rhapontisterone)

CAS Registry Number: 137476-71-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Blandfordia punicea* [1], *Rhaponticum uniflorum* [2]
$C_{27}H_{44}O_8$: 496.3036
Mp: 234–236°C (decomp) [2]
IR (KBr) ν_{max} cm^{-1}: 3400, 1660, 1440, 1380, 1050, 980, 880 [2]
UV λ_{max}^{EtOH} nm (log ε): 241.4 (4.08) [1]
UV λ_{max}^{MeOH} nm (log ε): 242 (3.97) [2]
EI-MS m/z: 478 $[M\text{-}H_2O]^+$ (2), 460 $[M\text{-}2H_2O]^+$ (1), 442 $[M\text{-}3H_2O]^+$ (5), 424 $[M\text{-}4H_2O]^+$ (2), 409 $[M\text{-}4H_2O\text{–}CH_3]^+$ (1), 361 (15), 343 (50), 325 (30), 301 (10), 300 (13), 267 (24), 249 (4), 225 (8), 213 (9), 187 (12), 143 (14), 125 (16), 99 (10), 81 (19), 69 (19), 43 (100) [2]
CI-MS m/z: 496 $[M + H + NH_3\text{–}H_2O]^+$, 479 $[M + H\text{–}H_2O]^+$, 461 $[479\text{-}H_2O]^+$, 443 $[461\text{-}H_2O]^+$, 425 $[443\text{-}H_2O]^+$, 407, 391, 362 $[M + H\text{-}117]^+$ [1]
FAB-MS m/z: 519 $[M + Na]^+$, 497 $[M + H]^+$, 479, 461, 443, 425, 407, 389, 371 [2]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 3.40 (dd, J = 7.0, 14.0, Ha-1), 2.01 (m, He-1), 4.15 (m, Ha-2), 4.25 (m, He-3), 2.02 (m, Ha-4), 1.83 (m, He-4), 3.05 (m, H-5), 6.27 (br s, H-7), 3.82 (m, Ha-9), 4.59 (m, Ha-11), 2.98 (m, Ha-12), 2.70 (m, He-12), 1.90 or 2.22 (m, Ha-15), 1.90 or 2.22 (m, Hb-15), 2.18 or 2.55 (m, Ha-16), 2.18 or 2.55 (m, Hb-16), 3.01 (m, H-17), 1.25 (s, CH_3-18), 1.30 (s, CH_3-19), 1.54 (s, CH_3-21), 4.14 (m, H-22), 1.82 (m, 10.0, 7.0, Ha-23), 1.95 (m, Hb-23), 3.90 (m, Ha-24), 1.73 (m, H-25), 1.003 (d, J = 7.0, CH_3-26), 1.006 (d, J = 7.0, CH_3-27) [2]
^{13}C NMR (125 MHz, C_5D_5N) [2]:

Table 1

C-1	39.5	C-10	39.3	C-19	24.7
2	68.1	11	68.6	20	76.4
3	67.9	12	43.8	21	21.3
4	32.5	13	47.9	22	77.4
5	52.2	14	83.9	23	35.4
6	203.6	15	31.7	24	76.6
7	121.3	16	21.3	25	33.8
8	163.9	17	49.6	26	16.9
9	42.5	18	18.7	27	19.4

References

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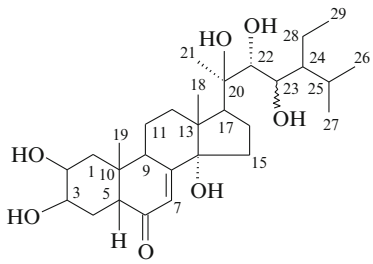
Rapisterone

CAS Registry Number: 113900-73-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum carthamoides* [1]

$C_{29}H_{48}O_7$: 508.3400

Mp: 241–242°C (EtOAc–MeOH) [1]

$[\alpha]_D^{20}$ + 30 ± 2° (c 0.10, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3300–3500, 1655 [1]

UV λ_{max}^{EtOH} nm (log ε): 244 (4.07) [1]

EI-MS m/z: 490 $[M\text{-}H_2O]^+$ (1), 475 (1), 472 (3), 457 (6), 454 (13), 443 (2), 439 (2), 436 (1), 363 (75), 345 (88), 327 (30), 300 (12), 250 (12), 171 (21), 127 (100), 109 (30), 84 (40) [1]

CD (c, 0.10, dioxane): $\Delta\varepsilon$ = +1.52 (340 nm), $\Delta\varepsilon$ = −3.81 (248 nm) [1]

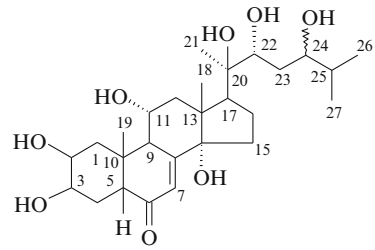
^{1}H NMR (200 MHz, J/Hz, C_5D_5N): 4.12 (m, H-2), 4.12 (m, H-3), 2.90 (H-5), 6.16 (br s, H-7), 3.50 (m, H-9), 1.28 (s, CH_3-18), 0.98 (s, CH_3-19), 1.48 (s, CH_3-21), 3.80 (d, J = 10.0, H-22), 3.50 (m, H-23), 1.13 (d, CH_3-26), 1.13 (d, CH_3-27), 0.92 (d, CH_3-29) [1]

References

1. U.A. Baltaev, N.K. Abubakirov, Chem. Nat. Comp. **23**, 565 (1987)

Rapisterone B

CAS Registry Number: 928621-17-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum carthamoides* [1]

$C_{27}H_{44}O_8$: 496.3036

Mp: amorphous [1]

IR (KBr) ν_{max} cm^{-1}: 3550–3500, 1655 [1]

EI-MS m/z: 462 $[M\text{-}H_2O]^+$ (3), 444 (4), 426 (6), 408 (6), 393 (3), 379 (12), 361 (30), 343 (100), 325 (75), 301 (60), 267 (45), 145 (21), 109 (15), 83 (12), 55 (25) [1]

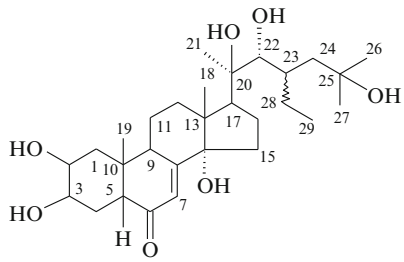
^{1}H NMR (100 MHz, C_5D_5N): 4.45 (m, H-2), 4.12 (m, H-3), 6.11 (s, H-7), 3.61-3.72 (m, H-9), 4.45 (m, H-11), 1.10 (s, CH_3-18), 1.15 (s, CH_3-19), 1.42 (s, CH_3-21), 3.61–3.72 (m, H-24), 0.67 (d, CH_3-26), 0.67 (d, CH_3-27) [1]

References

1. U.A. Baltaev, Chem. Nat. Comp. **27**, 712 (1991)

Rapisterone C

CAS Registry Number: 196399-47-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum carthamoides* [1], *Rh. uniflorum* [2]

$C_{29}H_{48}O_7$: 508.3400

Mp: 249–250°C (EtOAc–CH_3OH) [1], 248–250°C [2]

$[\alpha]_D^{23}$ + 171° (c 0.41, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3340–3500, 1655 [1]

EI-MS m/z: 472 $[M\text{-}2H_2O]^+$ (4), 454 (28), 439 (16), 436 (4), 421 (4), 363 (16), 345 (40), 327 (24), 300 (32), 171 (20), 154 (16), 127 (100), 109 (40), 83 (16), 69 (9) [1]

FAB-MS m/z: 547 $[M + Na]^+$, 531 $[M + Li]^+$ [2]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.16 (m, H-2), 4.22 (m, H-3), 3.00–3.02 (m, H-5), 6.26 (br s, H-7), 3.60 (m, H-9), 3.00–3.02 (m, H-17), 1.22 (s, CH_3-18), 1.08 (s, CH_3-19), 1.56 (s, CH_3-21), 3.87 (d, J = 10.0, H-22), 1.25 (s, CH_3-26), 1.38 (s, CH_3-27), 1.01 (t, CH_3-29) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

C-1	38.01	C-11	21.59	C-21	21.53
2	68.05	12	31.76	22	76.02
3	68.10	13	48.11	23	50.67
4	32.46	14	84.14	24	32.62
5	51.40	15	32.02	25	72.57
6	203.43	16	21.14	26	29.83
7	121.63	17	49.98	27	25.72
8	166.14	18	17.87	28	25.58
9	34.48	19	24.46	29	13.82
10	38.67	20	76.92		

(*continued*)

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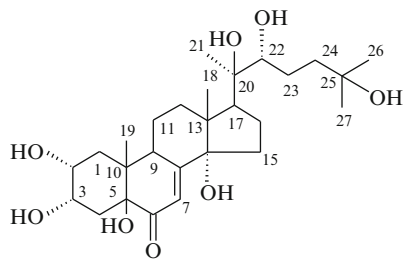
1. U.A. Baltaev, Chem. Nat. Comp. **28**, 198 (1992)
2. J.K. Cheng, Y.H. Zhang, Z.Y. Zhang, D.L. Cheng, G.L. Zhang, Chem. J. Chin. Univ. **23**, 2084 (2002)

Rapisterone D

CAS Registry Number: 148054-07-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum carthamoides* [1]

$C_{27}H_{44}O_8$: 496.3036

Mp: 246–248°C (EtOAc–MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3370–3490, 1690 [1]

EI-MS m/z: 478 $[M\text{-}H_2O]^+$, 463 $[M\text{-}H_2O\text{–}CH_3]^+$, 445 $[M\text{-}2H_2O\text{–}CH_3]^+$, 427 $[M\text{-}3H_2O\text{–}CH_3]^+$, 409 $[M\text{-}4H_2O\text{–}CH_3]^+$, 391 $[M\text{-}5H_2O\text{–}CH_3]^+$, 379 $[M\text{-}117]^+$, 361 $[M\text{-}117\text{-}H_2O]^+$, 325 $[M\text{-}117\text{-}3H_2O]^+$, 301 $[C_{19}H_{25}O_3]$, 99 $[C_6H_{11}O]$, 81 $[C_6H_9]$ [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.14 (k, J = 3.5, H-2), 4.25 (dt, J = 4.0, 12.0, H-3), 6.24 (br s, H-7), 3.61 (m, H-9), 2.95 (t, H-17), 1.12 (s, CH_3-18), 1.18

(s, CH_3-19), 1.56 (s, CH_3-21), 3.83 (dd, H-22), 1.35 (s, CH_3-26), 1.35 (s, CH_3-27) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	36.0	C-10	44.7	C-19	17.8
2	69.8	11	21.3	20	76.8
3	67.9	12	31.6	21	21.6
4	34.8	13	48.1	22	77.5
5	79.8	14	84.0	23	27.4
6	200.9	15	32.0	24	42.6
7	119.8	16	22.0	25	69.6
8	166.8	17	50.0	26	29.9
9	38.2	18	17.1	27	30.1

Pharm./Biol.: *Galleria mellonela* bioassay: EC_{50} = 7.8 µg/g, *Sarcophaga bullata* bioassay: EC_{50} = 7.8 µg/g [2], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.0 \times 10^{-9}$M [3, 4].

References

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2. K. Slama, N.K. Abubakirov, M.B. Gorovits, U.A. Baltaev, Z. Saatov, Insect Biochem. Mol. Biol. **23**, 181 (1993)
3. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
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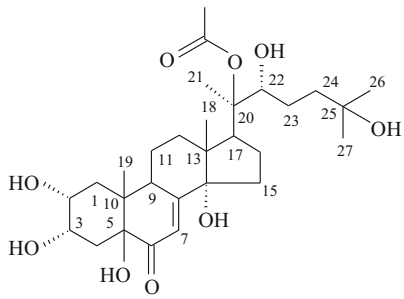
Rapisterone D-20-Acetate

CAS Registry Number: 256510-76-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Leuzea carthamoides* [1]

$C_{29}H_{46}O_9$: 538.3141

Mp: 225–227°C [1]

$[\alpha]_D^{20}$ + 36.5 ± 2° (c 0.7, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3300–3400, 1715, 1662, 1285 [1]

EI-MS m/z: 520 $[M\text{-}H_2O]^+$ (2), 505 (2), 502 (3), 487 (4), 478 (3), 469 (3), 460 (3), 451 (5), 421 (78), 406 (65), 403 (100), 316 (15), 301 (6), 285 (6), 99 (45), 81 (30) [1]

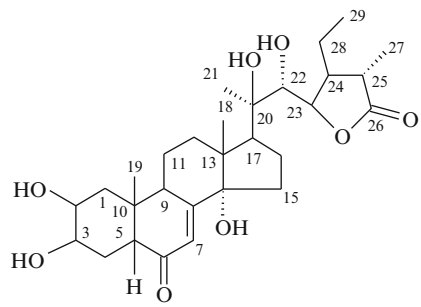
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.14 (q, J = 3.5, H-2), 4.25 (dt, J = 12.0, 4.0, H-3), 6.23 (br s, H-7), 3.62 (m, H-9), 2.95 (t, H-17), 1.12 (s, CH_3-18), 1.18 (s, CH_3-19), 1.56 (s, CH_3-21), 3.84 (dd, H-22), 1.35 (s, CH_3-26), 1.35 (s, CH_3-27), 1.92 (s, CH_3COO-20) [1]

References

1. E.B. Borovikova, G.S. Shangaraeva, U.A. Baltaev, Chem. Nat. Comp. **35**, 184 (1999)

Reptanslactone A

CAS Registry Number: 1145890-74-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *reptans* [1]

$C_{29}H_{44}O_8$: 520.3036

$[\alpha]_D^{25}$ + 17° (c 0.1, MeOH) [1]

UV λ_{max}^{MeOH} nm (log ε): 239.5 (3.931) [1]

ESI-MS m/z: 543 $[M + Na]^+$ (41), 521 $[M + H]^+$ (11), 505 $[M\text{-}CH_3]^+$ (11.5), 503 $[M + H\text{–}H_2O]^+$ (100), 484 $[M\text{-}2H_2O]^+$ (9), 452 $[M + H\text{-}3H_2O\text{–}CH_3]^+$ (15), 437 (24), 413 (23), 391 (37.5), 365 (17) [1]

HR-ESI-MS m/z: for $C_{29}H_{44}O_8$ $[M]^+$ calcd. 520.3024, found 520.3029 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.42 (Ha-1), 1.79 (He-1), 3.85 (Ha-2), 3.95 (He-3), 1.70 (Ha-4), 1.75 (He-4), 2.38 (H-5), 5.80 (H-7), 3.16 (H-9), 1.69 (Ha-11), 1.80 (He-11), 2.19 (Ha-12), 1.87 (He-12), 1.60 (Ha-15), 1.97 (Hb-15), 1.78 (Ha-16), 2.00 (Hb-16), 2.75 (H-17), 0.89 (s, CH_3-18), 0.96 (s, CH_3-19), 1.315 (s, CH_3-21), 3.59 (d, J = 9.8, H-22), 4.40 (dd, J = 2.5, 10.0, H-23), 2.11 (H-24), 2.485 (dq, J = 7.5, 3.0, H-25), 1.29 (d, J = 7.6, CH_3-27), 1.27 (Ha-28), 1.90 (Hb-28), 0.98 (t, J = 7.3, CH_3-29) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

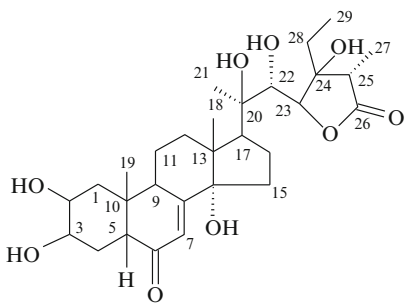
C-1	37.5	C-11	21.65	C-21	21.68
2	68.8	12	32.5	22	72.8
3	68.7	13	48.9	23	81.4
4	33.05	14	85.3	24	48.9
5	52.0	15	31.8	25	41.4
6	206.7	16	21.9	26	182.3
7	122.0	17	50.7	27	15.45
8	168.6	18	18.6	28	21.4
9	35.3	19	24.5	29	12.0
10	39.4	20	77.5		

References

1. A. Vanyolo, A. Simon, G. Toth, L. Polgar, Z. Kele, A. Ilku, P. Matyus, M. Bathori, J. Nat. Prod. **72**, 929 (2009)

Reptanslactone B

CAS Registry Number: 1145890-77-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *reptans* [1]

$C_{29}H_{44}O_9$: 536.2985

$[\alpha]_D^{25}$ + 3° (c 0.1, MeOH) [1]

UV λ_{max}^{MeOH} nm (log ε): 242 (3.5952) [1]

HR-ESI-MS m/z: for $C_{29}H_{44}O_9$ $[M]^+$ calcd. 536.2973, found 536.2961; for $C_{29}H_{44}O_9Na$ $[M + Na]^+$ calcd. 559.2870, found 559.2861 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.42 (Ha-1), 1.79 (He-1), 3.86 (Ha-2), 3.95 (He-3), 1.70 (Ha-4), 1.75 (He-4), 2.37 (H-5), 5.79 (H-7), 3.17 (H-9), 1.68 (Ha-11), 1.80 (He-11), 2.20 (Ha-12), 1.88 (He-12), 1.58 (Ha-15), 1.96 (Hb-15), 1.71 (Ha-16), 2.00 (Hb-16), 2.73 (H-17), 0.89 (s, CH_3-18), 0.96 (s, CH_3-19), 1.33 (s, CH_3-21), 3.54 (d, J = 9.7, H-22), 4.14 (d, J = 9.7, H-23), 2.605 (q, J = 7.3, H-25), 1.18 (d, J = 7.3, CH_3-27), 1.73 (Ha-28), 1.93 (Hb-28), 1.04 (t, J = 7.3, CH_3-29) [1]

^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.97 (Ha-1), 2.18 (He-1), 4.31 (Ha-2), 4.31 (He-3), 1.94 (Ha-4), 2.14 (He-4), 3.08 (H-5), 6.31 (H-7), 3.68 (H-9), 1.73 (Ha-11), 1.85 (He-11), 2.73 (Ha-12), 2.00 (He-12), 6.38 (OH-14), 1.95 (Ha-15), 2.20 (Hb-15), 2.17 (Ha-16), 2.49 (Hb-16), 3.54 (H-17), 1.25 (s, CH_3-18), 1.11 (s, CH_3-19), 1.72 (s, CH_3-21), 4.12 (d, J = 9.5, H-22), 6.88 (s, OH-22), 4.81 (d, J = 9.5, H-23), 6.49 (s, OH-24), 2.90 (q, J = 7.2, H-25), 1.48 (CH_3-27), 2.01 (Ha-28), 2.34 (dq, J = 14.4, 7.3, Hb-28), 1.35 (q, J = 7.3, CH_3-29) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

C-1	37.5	C-11	21.7	C-21	21.5
2	68.8	12	32.5	22	72.9
3	68.7	13	48.9	23	87.2
4	33.0	14	85.2	24	81.2
5	52.0	15	31.8	25	44.3
6	206.8	16	22.0	26	180.2
7	122.0	17	50.7	27	9.4
8	168.6	18	18.7	28	28.2
9	35.3	19	24.5	29	8.4
10	39.4	20	77.4		

^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 2

C-1	38.4	C-11	21.5	C-21	22.2
2	68.5	12	32.3	22	72.5

(*continued*)

Table 2 (continued)

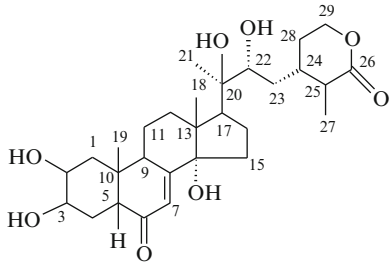
3	68.5	13	48.6	23	87.5
4	33.0	14	84.4	24	80.6
5	51.9	15	32.0	25	43.9
6	204.0	16	22.1	26	178.6
7	121.6	17	50.4	27	9.9
8	167.2	18	18.8	28	28.3
9	34.9	19	24.9	29	9.1
10	39.0	20	76.8		

References

1. A. Vanyolo, A. Simon, G. Toth, L. Polgar, Z. Kele, A. Ilku, P. Matyus, M. Bathori, J. Nat. Prod. **72**, 929 (2009)

Reptansterone

CAS Registry Number: 179308-56-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* [1]

$C_{29}H_{44}O_8$: 520.3036

IR (KBr) ν_{max} cm^{-1}: 3416, 1718, 1654 [1]

TSP-MS m/z: 521 $[M + H]^+$ (38), 503 $[M + H–H_2O]^+$ (100)

TSP-MS m/z: 565 $[M + HCOO]^+$ (100), 547 $[M + HCOO–H_2O]^+$ (55) [1]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 2.13 (Ha-1), 1.93 (He-1), 4.19 (Ha-2), 4.25 (He-3), 2.05 (Ha-4), 1.81 (He-4), 3.03 (m, H-5), 6.27 (d, J = 2.1, H-7), 3.60 (m, H-9), 1.89 (Ha-11), 1.74 (He-11), 2.61 (Ha-12), 2.04 (He-12), 2.40 (m, Ha-16), 1.98 (Hb-16), 2.86 (t, J = 9.1, H-17), 1.22 (s, CH_3-18), 1.06 (s, CH_3-19), 1.56 (s, CH_3-21), 3.89 (m, H-22), 1.88 (Ha-23), 1.57 (Hb-23), 1.94 (H-24), 2.56 (H-25), 1.39 (d, J = 6.9, CH_3-27), 2.04 (Ha-28), 1.82 (Hb-28), 4.26 (Ha-29), 4.14 (Hb-29) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	37.9	C-11	21.0	C-21	21.1
2	68.1	12	32.0	22	75.7
3	68.0	13	48.1	23	36.9
4	32.4	14	84.0	24	37.8
5	51.4	15	31.6	25	41.2
6	203.5	16	21.3	26	174.8
7	121.6	17	49.8	27	16.5
8	166.0	18	17.8	28	29.6
9	34.4	19	24.4	29	67.2
10	38.6	20	76.8		

References

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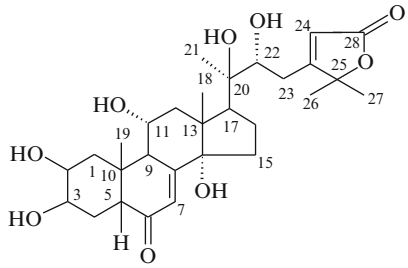
Rhapontisterone

CAS Registry Number: 137476-71-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Rhaponticum uniflorum* [1]

$C_{29}H_{42}O_9$: 534.2828

UV λ_{max}^{MeOH} nm: 244 [1]

EI-MS m/z: 534 $[M]^+$ [1]

^{1}H NMR (C_5D_5N): 4.56 (m, Ha-2), 4.22 (m, He-3), 3.04 (m, H-5), 6.32 (br s, H-7), 3.90 (m, H-9), 4.59 (m, He-11), 3.04 (m, H-17), 1.27 (s, CH_3-18), 1.32

(s, CH_3-19), 1.63 (s, CH_3-21), 1.28 (s, CH_3-26), 1.36 (s, CH_3-27), 6.27 (br s, H-28) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

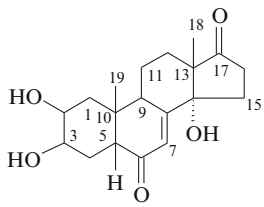
C-1	39.6	C-11	68.4	C-21	21.7
2	68.8	12	44.1	22	76.5
3	68.2	13	48.3	23	30.5
4	32.9	14	84.2	24	176.9
5	52.5	15	32.0	25	87.5
6	203.9	16	21.6	26	24.9
7	122.45	17	50.0	27	24.9
8	164.0	18	18.9	28	115.4
9	42.8	19	24.7	29	172.4
10	39.9	20	75.3		

References

1. X.Q. Li, J.H. Wang, S.X. Wang, X. Li, J. Asian Nat. Prod. Res. **2**, 225 (2000)

Rubrosterone

CAS Registry Number: 19466-41-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Achyranthes fauriei, A. obtusifolia* [1], *A. rubrofusca* [2], *Cucubalis baccifer* [3], *Leuzea carthamoides* [4], *Lychnis flos-culculi* [5], *Palisota schweinfurthii* [6], *Serratula tinctoria* [7], *Silene otites* [8]

$C_{19}H_{26}O_5$: 334.1780

Mp: 240–245°C [1], 230°C (dec.) [2], 238–240°C [9], 235–237°C (MeOH–EtOAc) [10], 240–244°C (dec.) [11]

$[\alpha]_D$ + 119° (c 0.86, MeOH) [2], $[\alpha]_D$ + 125° (MeOH) [11]

IR (KBr) ν_{max} cm^{-1}: 3410, 1741, 1646 [2], 3537, 3036, 1747, 1649 [4], 1740, 1645 [9]

UV λ_{max}^{EtOH} nm: 240 (log ε 4.07) [2], 239 (ε 10600) [9]

FAB-MS m/z: 357 $[M + Na]^+$ (3), 335 $[M + H]^+$ (35), 317 (6), 299 (4), 229 (5), 198 (9), 181 (18), 167 (14), 149 (18), 131 (26), 115 (56), 91 (91), 69 (60), 55 (100) [4]

HR-MS m/z: for $C_{19}H_{27}O_5$ $[M + H]^+$ calcd. 335.1859, found 335.1916 [4]

CD (c, 0.043, dioxane): $[\theta]_{400}0$, $[\theta]_{355} + 3.95 \times 10^3$, $[\theta]_{342} + 4.83 \times 10^3$, $[\theta]_{327} + 3.80 \times 10^3$, $[\theta]_{296}^{sh} + 15.7 \times 10^3$, $[\theta]_{287} + 16.4 \times 10^3$, $[\theta]_{262}0$, $[\theta]_{246} - 41.1 \times 10^3$, $[\theta]_{230}0$, $[\theta]_{220} + 25.4 \times 10^3$, $[\theta]_{210} + 21.0 \times 10^3$ [2]

CD (c, 0.0714, dioxane): $[\theta]_{400}0$, $[\theta]_{331} + 6.22 \times 10^3$, $[\theta]_{287} + 19.8 \times 10^3$, $[\theta]_{266}$ 0, $[\theta]_{240} - 34.0 \times 10^3$, $[\theta]_{232}0$, $[\theta]_{220} + 27.0 \times 10^3$, $[\theta]_{210} + 20.1 \times 10^3$ [2]

^{1}H NMR (500 MHz, CD_3OD): 1.80 (dd, Ha-1), 1.45 (dd, He-1), 3.83 (ddd, Ha-2), 3.96 (bq, He-3), 1.74 (Ha-4), 1.71 (He-4), 2.43 (dd, H-5), 5.91 (d, H-7), 3.18 (ddd, H-9), 1.91 (Ha-11), 1.66 (He-11), 2.13 (Ha-12), 1.58 (He-12), 2.03 (Ha-15), 2.30 (Hb-15), 2.37 (Ha-16), 2.51 (Hb-16), 0.88 (s, CH_3-18), 0.99 (s, CH_3-19) [4]

^{1}H NMR (250 MHz, J/Hz, CD_3OD): 1.45 (dd, J = 12.0, 13.0, Ha-1), 1.80 (dd, He-1), 3.83 (ddd, J = 3.0, 4.0, 12.0, Ha-2), 3.96 (q, J = 3.0, He-3), 1.73 (Ha-4), 1.78 (He-4), 2.45 (H-5), 5.91 (d, J = 2.5, H-7), 3.18 (ddd, J = 2.5, 7.0, 11.0, H-9), 1.90 (Ha-11), 1.70 (He-11), 2.10 (Ha-12), 1.60 (He-12), 2.30 (Ha-15), 2.05 (Hb-15), 2.50 (Ha-16), 2.30 (Hb-16), 0.88 (s, CH_3-18), 0.99 (s, CH_3-19) [4]

^{13}C NMR (125.7 MHz, CD_3OD) [4]:

Table 1

C-1	37.35	C-8	164.69	C-15	29.12
2	68.65	9	35.80	16	34.00
3	68.44	10	39.34	17	220.22
4	32.88	11	20.69	18	17.60
5	51.99	12	24.97	19	24.58
6	205.92	13	54.09		
7	122.44	14	80.47		

Pharm./Biol.: *Sarcophaga peregrine*: very weak activity [2], high anabolic activity [12], stimulating effect on protein synthesis in mouse liver [13], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} > 1.0 \times 10^{-4}$M [14].

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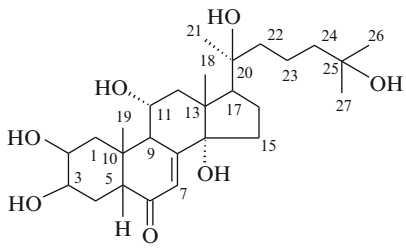
Scabrasterone

CAS Registry Number: 474524-75-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Vitex scabra* [1]

$C_{27}H_{44}O_7$: 480.3087

IR (KBr) ν_{max} cm^{-1}: 3422, 2925, 1654, 1384 [1]

ES-MS m/z: 503 $[M + Na]^+$ (100) [1]

HR-FAB-MS m/z: 479.3011 $[M-H]^-$ (calc. for $C_{27}H_{43}O_7$ 479.3008) [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 3.41 (dd, J = 12.8, 4.2, Hae-1), 4.56 (m, Ha-2), 4.21 (m, He-3), 3.00 (dd, J = 13.1, 3.6, H-5), 6.26 (d, J = 2.1, H-7), 3.84 (dd, J = 8.5, 2.1, H-9), 4.56 (m, H-11), 2.99 (m, Ha-12), 2.65 (dd, J = 11.9, 5.8, He-12), 2.93 (t, J = 9.0, H-17), 1.18 (s, CH_3-18), 1.29 (s, CH_3-19), 1.53 (s, CH_3-21), 1.33 (s, CH_3-26), 1.33 (s, CH_3-27) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	39.6	C-10	39.4	C-19	24.7
2	68.3	11	68.8	20	74.2
3	68.0	12	43.8	21	26.7
4	32.8	13	47.5	22	45.4
5	52.7	14	84.4	23	21.8
6	204.1	15	31.5	24	45.6
7	122.0	16	19.5	25	69.6
8	164.5	17	53.2	26	29.6
9	42.6	18	18.7	27	29.8

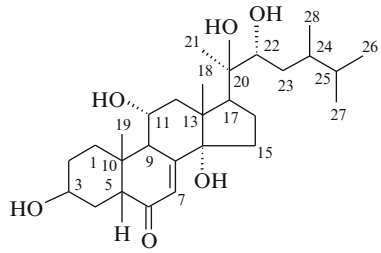
Pharm./Biol.: *Musca* bioassay: $EC_{50} = 1.0 \times 10^{-3}$M very low activity [1].

References

1. A. Suksamrarn, S. Kumpun, B. Yingyongnarongkul, J. Nat. Prod. **65**, 1690 (2002)

Schizaeasterone A

CAS Registry Number: 203871-23-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Schizea dichotoma* [1]

$C_{28}H_{46}O_6$: 478.3294
$[\alpha]_D$ + 45° (c 0.2, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3420, 2955, 1700, 1656, 1466, 1373, 1295, 1260, 1214, 1180, 1138, 1099, 1068, 1034 [1]
UV λ_{max}^{MeOH} nm (log ε): 238 (4.06) [1]
HR-FAB-MS m/z: for $C_{28}H_{45}O_6$ $[M-H]^-$ calcd. 477.322, found 477.323 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.17 (br s, H-3), 6.25 (d, J = 2.1, H-7), 3.92 (H-9), 4.62 (br dd, J = 9.8, 14.6, Ha-11), 1.33 (s, CH_3-18), 1.35 (s, CH_3-19), 1.61 (s, CH_3-21), 3.92 (H-22), 0.77 (d, J = 6.7, CH_3-26), 0.81 (d, J = 7.0, CH_3-27), 0.85 (d, J = 6.7, CH_3-29) [1]
^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

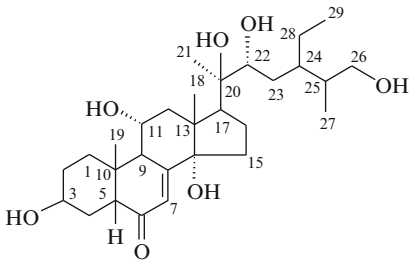
C-1	31.1	C-11	68.9	C-21	21.5
2	32.0	12	44.3	22	74.1
3	64.1	13	48.2	23	36.9
4	34.1	14	84.3	24	35.6
5	53.4	15	29.6	25	33.7
6	204.1	16	21.4	26	20.2
7	122.3	17	49.9	27	18.7
8	164.6	18	19.0	28	15.2
9	41.6	19	25.1		
10	38.2	20	76.9		

References

1. H. Fuchino, H. Nakamura, T. Hakamatsuka, N. Tanaka, R.C. Cambie, J.E. Braggins, Nat. Medicines. **51**, 491 (1997)

Schizaeasterone B

CAS Registry Number: 203871-24-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Schizea dichotoma* [1]
$C_{29}H_{48}O_7$: 508.3400
$[\alpha]_D$ + 5° (c 0.2, MeOH) [1]
IR (KBr) ν_{max} cm^{-1}: 3400, 2955, 1656, 1457, 1373, 1320, 1297, 1123, 1097, 1067, 1033 [1]
UV λ_{max}^{MeOH} nm (log ε): 244 (4.08) [1]
HR-FAB-MS m/z: for $C_{29}H_{47}O_7$ $[M-H]^-$ calcd. 507.332, found 507.332 [1]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 4.19 (br s, H-3), 6.34 (d, J = 2.4, H-7), 3.95 (H-9), 4.60 (br dd, J = 10.4, 15.6, Ha-11), 1.32 (s, CH_3-18), 1.35 (s, CH_3-19), 1.60 (s, CH_3-21), 3.95 (H-22), 1.13 (d, J = 6.7, CH_3-27), 0.93 (t, J = 7.5, CH_3-29) [1]
^{13}C NMR (125 MHz, C_5D_5N) [1]:

Table 1

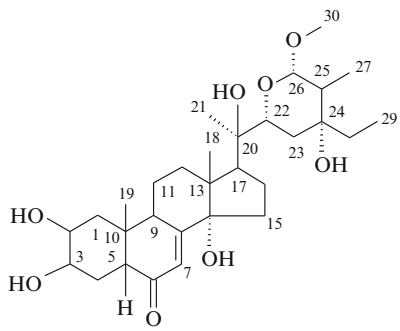
C-1	31.1	C-11	68.9	C-21	21.4
2	31.9	12	44.3	22	75.3
3	64.1	13	48.2	23	34.2
4	34.1	14	84.3	24	39.1
5	53.4	15	29.6	25	39.2
6	204.1	16	21.6	26	65.5
7	122.3	17	49.9	27	14.9
8	164.7	18	19.0	28	23.2
9	41.6	19	25.1	29	12.1
10	38.2	20	76.9		

References

1. H. Fuchino, H. Nakamura, T. Hakamatsuka, N. Tanaka, R.C. Cambie, J.E. Braggins, Nat. Med. **51**, 491 (1997)

Sendreisterone

CAS Registry Number: 1145890-81-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* var. *reptans* [1]

$C_{30}H_{48}O_8$: 536.3349

Mp: 253–255°C [1]

$[\alpha]_D^{28}$ + 22° (c 0.1, MeOH) [1]

UV λ_{max}^{MeOH} nm (log ε): 240 (3.62) [1]

ESI-MS m/z: 560 $[M + Na + H]^+$ (27), 559 $[M + Na]^+$ (100), 537 $[M + H]^+$ (25.5), 521 $[M\text{-}CH_3]^+$ (14), 519 $[M + H\text{–}H_2O]^+$ (26), 505 (19.5), 482 $[M\text{-}3H_2O]^+$ (18), 445 (20.7), 437 (16.5), 413 (27.9), 391 (7.5), 365 (37.9), 356 (14.8) [1]

HR-ESI-MS m/z: for $C_{30}H_{49}O_8$ $[M + H]^+$ calcd. 537.3414, found 537.3424 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.43 (Ha-1), 1.80 (He-1), 3.84 (Ha-2), 3.95 (He-3), 1.70 (Ha-4), 1.75 (He-4), 2.39 (H-5), 5.81 (H-7), 3.16 (H-9), 1.70 (Ha-11), 1.81 (He-11), 2.17 (Ha-12), 1.85 (He-12), 1.63 (Ha-15), 2.00 (Hb-15), 1.81 (Ha-16), 2.01 (Hb-16), 2.50 (H-17), 0.87 (s, CH_3-18), 0.97 (s, CH_3-19), 1.27 (s, CH_3-21), 3.26 (dd, J = 12.0, 1.2, H-22), 1.20 (t, J = 12.4, Ha-23), 2.02 (Hb-23), 1.53 (H-25), 4.13 (d, J = 8.9, H-26), 0.92 (d, J = 7.0, CH_3-27), 1.52 (Ha-28), 1.57 (Hb-28), 0.93 (t, J = 7.4, CH_3-29), 3.50 (s, OCH_3-30) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

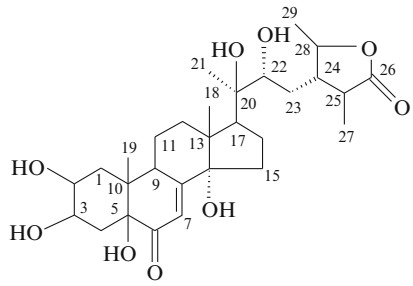
C-1	37.5	C-11	21.65	C-21	21.84
2	68.9	12	32.6	22	77.5
3	68.7	13	48.6	23	36.8
4	33.0	14	85.4	24	74.2
5	52.0	15	31.9	25	49.2
6	206.6	16	22.1	26	106.4
7	122.3	17	50.7	27	8.8
8	168.1	18	18.3	28	25.3
9	35.2	19	24.5	29	7.5
10	39.4	20	77.4	30	57.2

References

1. A. Vanyolo, A. Simon, G. Toth, L. Polgar, Z. Kele, A. Ilku, P. Matyus, M. Bathori, J. Nat. Prod. **72**, 929 (2009)

Sengosterone

CAS Registry Number: 22799-11-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* [1], *Cyathula capitata* [2, 3]

$C_{29}H_{44}O_9$: 536.2985

Mp: 159–161°C [2]

$[\alpha]_D$ + 39.6° (c 0.69, pyridine) [2]

IR (KBr) ν_{max} cm^{-1}: 3425, 1748, 1670 [2, 3]

UV λ_{max}^{EtOH} nm (log ε): 241 (4.01) [2, 3]

EI-MS m/z: 518 $[M\text{-}H_2O]^+$ (4), 500 (10), 482 (4), 464 (2), 446 (1), 379 $[M\text{-}157]^+$ (2), 361 $[M\text{-}157\text{-}H_2O]^+$ (14), 343 $[M\text{-}157\text{-}2H_2O]^+$ (24), 325 $[M\text{-}157\text{-}3H_2O]^+$ (17), 316 (9), 201 (M - 335) (5), 183 (8), 157 $[M\text{-}379]^+$ (18), 113 (13), 43 (100) [3]

CD (c, 0.2039, dioxane): $[\theta]_{380}$ 0, $[\theta]_{328}$ +7.49 × 10^3, $[\theta]_{283}$ 0, $[\theta]_{245}$ −18.07 × 10^3, $[\theta]_{220\text{–}214}$ 0, $[\theta]_{206}$ − 30.66 × 10^3 [3]

ORD (c, 0.2039, dioxane): $[\varphi]_{400}$ + 1960, $[\varphi]_{356}$ + 5620, $[\varphi]_{238}$ + 18420, $[\varphi]_{304}$ − 5050, $[\varphi]_{283}$ − 3720, $[\varphi]_{267}$ − 6320, $[\varphi]_{212}$ − 18850 [3]

^{1}H NMR (J/Hz, C_5D_5N): 5.27 (s, H-2), 4.10 (s, H-3), 6.20 (d, J = 2.0, H-7), 3.58 (ddd, H-9), 1.21 (s, CH_3-18), 1.13 (s, CH_3-19), 1.56 (s, CH_3-21), 4.99 (dd, H-22), 1.36 (d, J = 7.0, CH_3-27), 4.11 (dq, J = 6.0, 7.0, CH-CH_3-28), 1.34 (d, J = 6.0, CH_3-29) [3]

^{1}H NMR (300 MHz, C_5D_5N): 2.08 (Ha-1), 2.22 (He-1), 4.25 (Ha-2), 4.16 (He-3), 1.95 (Ha-4), 2.06 (He-4), 6.31 (H-7), 3.65 (H-9), 1.80 (Ha-11), 1.93 (He-11), 2.05 (Ha-12), 2.64 (He-12), 2.21 (Ha-15), 1.97 (Hb-15), 2.05 (Ha-16), 2.47 (Hb-16), 2.85 (H-17), 1.24 (s, CH_3-18), 1.17 (s, CH_3-19), 1.57 (s, CH_3-21), 3.94 (H-22), 1.70 (Ha-23), 1.72 (Hb-23), 2.22

(H-24), 2.36 (H-25), 1.36 (s, CH_3-27), 4.02 (H-28), 1.31 (s, CH_3-29) [1]

^{13}C NMR (75 MHz, C_5D_5N) [1]:

Table 1

C-1	34.8	C-11	22.0	C-21	20.9
2	67.8	12	32.2	22	73.9
3	69.8	13	48.2	23	34.4
4	35.9	14	83.9	24	48.6
5	79.8	15	31.9	25	42.4
6	200.9	16	21.2	26	179.2
7	120.1	17	49.8	27	15.8
8	166.4	18	17.8	28	79.8
9	38.2	19	17.1	29	19.3
10	44.8	20	76.7		

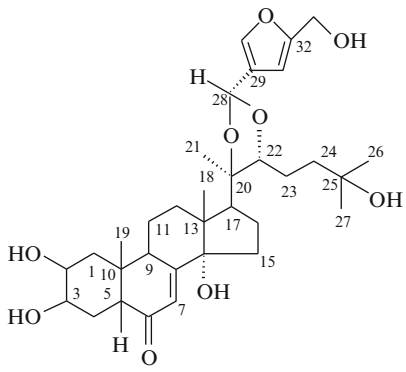
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 9.0 \times 10^{-8}$M [4, 5].

References

1. H. Hikino, K. Nomoto, T. Takemoto, Tetrah. Lett. **18**, 1417 (1969)
2. H. Hikino, K. Nomoto, T. Takemoto, Tetrahedron **26**, 887 (1970)
3. M.P. Calgano, F. Camps, J. Coll, E. Male, F. Sanchez-Baeza, Tetrahedron **52**, 10137 (1996)
4. L. Dinan, R.E. Hormann, T. Fujimoto, J. Comput. Aid. Mol. Des. **13**, 185 (1999)
5. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

Serfurosterone A

CAS Registry Number: 1010731-90-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula wolffii* [1]

$C_{33}H_{48}O_9$: 588.3298

$[\alpha]_D^{25.5}$ + 56° (c 0.0025; DMSO) [1]

UV λ_{max}^{DMSO} nm (log ε): 258.7 (3.925) [1]

EI-MS m/z: 519 $[M + K–C_6H_4O_2]^+$, 463 $[M + H–H_2O\text{-}C_6H_4O_2]^+$, 445 $[M + H–2H_2O–C_6H_4O_2]^+$ [1]

HR-ESI-MS m/z: for $C_{33}H_{49}O_9$ $[M + H]^+$ calcd. 589.3363, found 589.3393 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.79 (dt, J = 4.2, 13.2, Ha-1), 1.42 (dd, J = 12.0, 13.2, He-1), 3.84 (dt, J = 3.4, 12.0, Ha-2), 3.95 (s, br, He-3), 1.75 (Ha-4), 1.71 (He-4), 2.39 (dd, J = 4.2, 12.6, H-5), 5.82 (d, J = 2.6, H-7), 3.15 (ddd, J = 2.6, 8.9, 10.8, Ha-9), 1.62 (Ha-11), 1.62 (He-11), 2.11 (td, J = 4.2, 12.6, Ha-12), 1.85 (He-12), 2.41 (t, J = 9.1, H-17), 0.86 (s, CH_3-18), 0.96 (s, CH_3-19), 1.30 (s, CH_3-21), 3.79 (dd, J = 2.3, 9.4, H-22), 1.53 (td, J = 4.2, 13.2, Ha-24), 1.53 (td, J = 4.2, 13.2, Hb-24), 1.20 (s, CH_3-26), 1.21 (s, CH_3-27), 5.79 (s, H-28), 6.42 (d, J = 3.0, H-30), 6.28 (d, J = 3.0, H-31), 4.51 (s, 2H-33) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

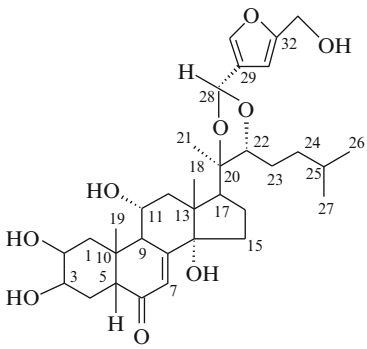
C-1	37.3	C-12	32.2	C-23	
2	68.5	13	48.0	24	41.7
3	68.3	14	85.4	25	71.4
4	32.7	15		26	28.7
5	52.1	16		27	29.2
6		17	51.1	28	98.2
7	122.0	18	17.5	29	
8		19	24.1	30	
9	35.0	20	85.6	31	
10	39.1	21	23.6	32	
11	31.7	22	85.7	33	57.2

References

1. E.L. Busa, A. Simon, G. Toth, M. Bathori, Tetrah. Lett. **49**, 1738 (2008)

Serfurosterone B

CAS Registry Number: 1010830-99-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula wolffii* [1]

$C_{33}H_{48}O_9$: 588.3298

$[\alpha]_D^{25.5}$ + 80° (c 0.0025; DMSO) [1]

UV λ_{max}^{DMSO} nm (log ε): 255.7 (3.874) [1]

EI-MS m/z: 519 $[M + K–C_6H_4O_2]^+$, 463 $[M + H–H_2O–C_6H_4O_2]^+$, 445 $[M + H–2H_2O–C_6H_4O_2]^+$ [1]

HR-ESI-MS m/z: for $C_{33}H_{49}O_9$ $[M + H]^+$ calcd. 589.3363, found 589.3389 [1]

^{1}H NMR (500 MHz, J/Hz, DMSO-d_6): 2.46 (dd, J = 4.1, 12.5, Ha-1), 1.15 (t, J = 11.9, He-1), 3.77 (Ha-2), 3.76 (He-3), 1.62 (Ha-4), 1.46 (He-4), 2.14 (dd, J = 3.8, 13.1, H-5), 5.63 (d, J = 2.6, H-7), 2.98 (dd, J = 2.6, 8.9, 10.8, Ha-9), 3.87 (ddd, J = 5.7, 9.1, 10.9, He-11), 2.08 (dd, J = 10.9, 12.1, Ha-12), 1.93 (dd, J = 5.7, 12.1, He-12), 1.535 (Ha-15), 1.85 (Hb-15), 1.84 (Ha-16), 1.84 (Hb-16), 2.30 (t, J = 8.6, H-17), 0.69 (s, CH_3-18), 0.90 (s, CH_3-19), 1.20 (s, CH_3-21), 3.69 (dd, J = 2.6, 9.4, H-22), 1.44 (Ha-23), 1.51 (Hb-23), 1.25 (Ha-24), 1.40 (Hb-24), 1.58 (dt, J = 6.6, 13.3, H-25), 0.88 (d, J = 7.0, CH_3-26), 0.89 (d, J = 6.6, CH_3-27), 5.74 (s, H-28), 6.45 (d, J = 3.2, H-30), 6.25 (d, J = 3.2, H-31), 4.37 (s, 2H-33) [1]

^{13}C NMR (125 MHz, DMSO-d_6) [1]:

Table 1

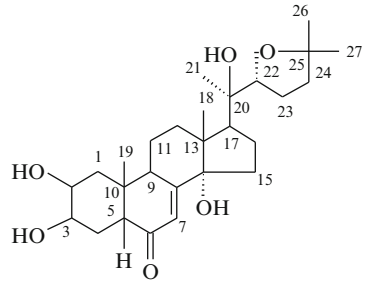
C-1	38.2	C-12	42.0	C-23	26.0
2	66.9	13	46.6	24	35.8
3	66.5	14	82.7	25	27.5
4	32.0	15	30.2	26	22.33
5	51.1	16	21.3	27	22.44
6		17	49.2	28	96.5
7	121.0	18	17.5	29	150.3
8	162.6	19	24.08	30	109.9
9	41.2	20	83.9	31	107.5
10	40.5	21	21.2	32	156.1
11	67.2	22	83.4	33	55.7

References

1. E.L. Busa, A. Simon, G. Toth, M. Bathori, Tetrah. Lett. **49**, 1738 (2008)

Shidasterone (Stachysterone D)

CAS Registry Number: 26361-67-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Achyranthes bidentata* [1], *Blechnum niponicum* [2, 3], *Cyanotis arachnoidea* [4], *Klaseopsis chinensis* [5], *Lychnis chalcedonica* [6], *Stachyurus praecox* [7, 8], *Vitex canescens* [9]

$C_{27}H_{42}O_6$: 462.2981

Mp: 257–258°C [2, 7], 245–250°C (dec.) [3], 255–257°C (EtOAc–MeOH) [6]

$[\alpha]_D^{25}$ + 65.0° (c 0.18, $CHCl_3$) [10]

IR (KBr) ν_{max} cm^{-1}: 3430, 1643 [2], 3400, 1650 [3]

IR ($CHCl_3$) ν_{max} cm^{-1}: 3600, 3400, 1664 [10]

UV λ_{max}^{EtOH} nm: 244 (ε 9.110) [2]

UV λ_{max}^{MeOH} nm: 243 (ε 10.950) [8], 242 [11]

EI-MS m/z: 462 $[M]^+$, 363 $[M-99]^+$, 345 $[M-99-H_2O]^+$, 99 $[M-363]^+$, 81 $[M-363-H_2O]^+$ [1], 462 $[M]^+$, 405 (1) 363 (19), 345 (50), 327 (15), 99 [C_{22}-C_{27}; 60]$^+$, 81 (54), 43 (100) [3], 462 $[M]^+$, 444, 426, 406, 363, 345, 327, 309, 301, 279, 161, 125, 99, 81, 55 [6]

FAB-MS m/z: 485 $[M + Na]^+$ (13.7), 463 $[M + H]^+$ (55.5), 445 $[M + H–H_2O]^+$ (24.2), 123 (100) [10]

HR-MS m/z: for $C_{27}H_{42}O_6$ $[M + H]^+$ calcd. 463.3059, found 463.3028 [10]

ORD (c, 0.118, dioxane): $[\varphi]_{358}^{peak}$ + 3670, $[\varphi]_{307}^{trough}$ − 4060 [2]

CD (c, 0.118, dioxane): $[\theta]_{337}$ +3.2 × 10^3 [2]

^{1}H NMR (100 MHz, C_5D_5N): 4.10 (m, Ha-2), 4.19 (ddd, He-3), 2.95 (dd, H-5), 6.29 (d, H-7), 3.53 (ddd, Ha-9), 1.06 (s, CH_3-18), 1.06 (s, CH_3-19), 1.39 (s, CH_3-21), 4.06 (dd, H-22), 1.22 (s, CH_3-26), 1.22 (s, CH_3-27) [2]

^{1}H NMR (300 MHz, J/Hz, CD_3OD): 1.42 (dd, J = 12.0, 13.0, H-1), 3.84 (ddd, J = 3.0, 3.0, 12.0, Ha-2), 3.94 (m, He-3), 2.36 (m, H-5), 5.81 (d, J = 2.5, H-7), 3.15 (ddd, J = 2.5, 7.5, 12.0, Ha-9), 2.15 (ddd, J = 4.0, 13.0, 13.0, H-12), 2.36 (m, H-17), 0.84 (s, CH_3-18), 0.96 (s, CH_3-19), 1.21 (s, CH_3-21), 3.94 (m, H-22), 1.24 (s, CH_3-26), 1.25 (s, CH_3-27) [10]

^{13}C NMR (25 MHz, C_5D_5N) [2]: **^{13}C NMR** (75.5 MHz, CD_3OD) [10]:

Table 1

C-1	37.7	C-15	31.5	C-1	37.3	C-15	31.6
2	67.9	16	21.5	2	68.6	16	21.6 or 21.4
3	67.9	17	51.2	3	68.4	17	51.7
4	32.2	18	17.8	4	32.7	18	18.0
5	51.2	19	24.3	5	51.7	19	24.3
6	205.5	20	80.3	6	206.4	20	76.9
7	121.5	21	21.0	7	122.0	21	20.6
8	166.0	22	84.8	8	167.9	22	85.4
9	34.2	23	27.6	9	35.0	23	28.4
10	38.5	24	38.8	10	39.2	24	39.5
11	21.0	25	75.4	11	21.6 or 21.4	25	81.7
12	31.5	26	28.2	12	32.2	26	28.3
13	47.5	27	28.7	13	48.6	27	28.9
14	84.0			14	85.2		

Pharm./Biol.: *Sarcophaga* biotest: high hormone activity [2, 3, 8]; *Chilo* test: inactive [7]; Strong stimulating effect on protein synthesis in mouse [7], *Drosophila melanogaster* cell bioassay: 200-fold less active than 20-hydroxyecdysone, the effective dose for a 50% response being 1.6 × 10^{-6} mol dm^{-3} as opposed to 7.5 × 10^{-6} mol dm^{-3} for 20-hydroxyecdysone [10], *Drosophila melanogaster* B_{II} bioassay: EC_{50} = 1.5, 4.0 × 10^{-6} M [11, 12].

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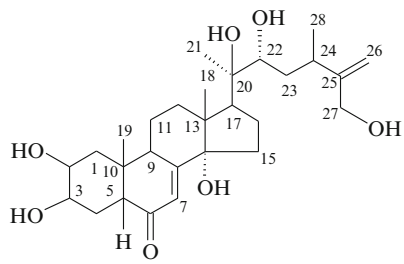
Sidasterone A

CAS Registry Number: 168706-13-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Sida cordifolia* [1, 2], *S. rhombifolia, S. spinosa* [2]
$C_{28}H_{44}O_7$: 492.3087
Mp: 238–240°C [2]
$[\alpha]_D^{20}$ + 67.8° (c, dioxane) [2]
IR (KBr) ν_{max} cm^{-1}: 3500, 3410, 1662, 1632, 890 [2]
UV λ_{max}^{EtOH} nm (log ε): 243 (4.08) [1, 2]
UV $\lambda_{max}^{(MeOH-HCl)}$ nm: 243, 293 [1]
EI-MS m/z: 363, 345, 301 [1], 474 $[M-H_2O]^+$ [2]
Pharm./Biol.: *Musca domestica* bioassay: active [1].

References

1. S. Ghosal, *4th Indo-Soviet Symposium on the Chemistry and Pharmacology of Natural Products*, Lucknow, 1976, p. 142
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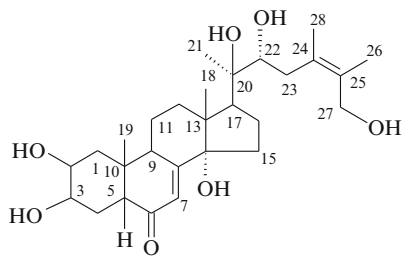
Sidasterone B

CAS Registry Number: 169063-72-3



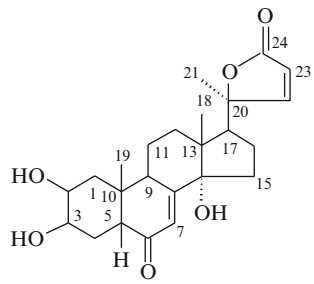
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Sida cordifolia* [1, 2], *S. rhombifolia, S. spinosa* [2]
$C_{28}H_{44}O_7$: 492.3087
Mp: 235–237°C [2]
$[\alpha]_D^{20}$ + 53.8° (c, $CHCl_3$) [2]
IR (KBr) ν_{max} cm^{-1}: 3520, 3412, 1670, 1662, 792 [2]
UV λ_{max}^{EtOH} nm (log ε): 243 (4.11) [2]
UV $\lambda_{max}^{(MeOH–HCl)}$ nm: 243, 293 [1]
EI-MS m/z: 363, 345, 301 [1], 474 $[M-H_2O]^+$ [2]
Pharm./Biol.: *Musca domestica* bioassay: active [1].

References

1. S. Ghosal, *4th Indo-Soviet Symposium on the Chemistry and Pharmacology of Natural Products*, Lucknow, 1976, p. 142
2. A. Prakash, S. Ghosal, J. Sci. Ind. Res. **38**, 632 (1979)

Sidisterone

CAS Registry Number: 176391-32-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Briza maxima* [1], *Silene dioica, Silene otites* [2]
$C_{24}H_{32}O_6$: 416.2198
IR (KBr) ν_{max} cm^{-1}:1749, 1643 [2]
UV λ_{max}^{EtOH} nm (ε): 240 (13300), 209 (14500) [2]
CI-MS m/z: 434 $[M + H + NH_3]^+$, 417 $[M + H]^+$, 399 $[M + H–2H_2O]^+$ [2]
HR-MS m/z: for $C_{24}H_{32}O_6$ $[M]^+$ calcd. 416.21978, found 416.21988 [2]
^{1}H NMR (500 MHz, J/Hz, C_5D_5N): 1.43 (t, J = 12.0, Ha-1), 1.78 (He-1), 3.82 (ddd, J = 12.0, 3.5, 3.0, Ha-2), 3.94 (q b, He-3), 1.65 (Ha-4), 1.75 (He-4), 2.38 (dd, J = 11.3, 5.4, H-5), 5.78 (d, J = 2.5, H-7), 3.14 (m, Ha-9), 1.65 (Ha-11), 1.80 (He-11), 2.19 (dt, J = 13.0, 5.0, Ha-12), 1.85 (He-12), 1.95 (Ha-15), 1.65 (Hb-15), 1.80 (Ha-16), 1.45 (Hb-16), 2.77 (t, J = 9.2, H-17), 0.76 (s, CH_3-18), 0.95 (s, CH_3-19), 1.52 (s, CH_3-21), 7.76 (d, J = 5.4, H-22), 6.01 (d, J = 5.4, H-23) [2]
^{13}C NMR (125 MHz, C_5D_5N) [2]:

Table 1

C-1	37.38	C-9	35.07	C-17	52.20
2	68.70	10	39.20	18	18.16
3	68.49	11	21.46	19	24.37
4	32.85	12	31.92	20	92.80
5	51.80	13	48.20	21	25.17
6	206.20	14	85.00	22	163.92
7	122.32	15	31.56	23	120.05
8	167.10	16	22.56	24	175.50

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} > 1.0 \times 10^{-4}$M [3].

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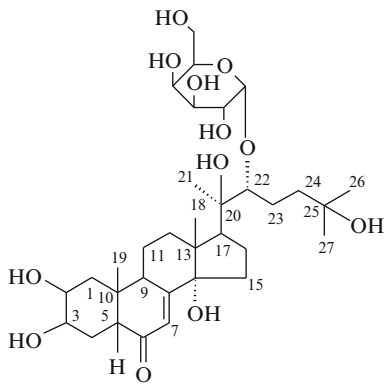
Sileneoside A

CAS Registry Number: 81655-86-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1], *S. viridiflora* [2]

$C_{33}H_{54}O_{12}$: 642.3615

Mp: 254–256°C (MeOH-H_2O) [1]

$[\alpha]_D^{22}$ + 93.1 ± 2° (c 1.03, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3370–3440, 1645 [1]

UV λ_{max}^{EtOH} nm (log ε): 246 (4.15) [1]

EI-MS m/z: 624 $[M\text{-}H_2O]^+$ (0.3), 606 (0.8), 588 (0.5), 570 (0.2), 507 (2.5), 489 (1.1), 473 (2.0), 463 (2.2), 455 (3.8), 445 (5), 444 (4), 427 (34), 426 (35), 409 (12), 408 (11), 393 (3.8), 363 (3.7), 358 (5), 352 (17), 345 (100), 344 (94), 327 (67), 309 (22), 300 (34), 163 (20), 145 (22), 143 (33), 99 (66), 81 (44), 69 (42) [1]

CD (c, 0.10, MeOH): Δε = +2.01 (330 nm), Δε = −5.03 (249 nm) [1]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.00–4.20 (br m, H-2), 4.00–4.20 (br m, H-3), 6.11 (br s, H-7), 3.42 (br m, H-9), 1.09 (s, CH_3-18), 0.90 (s, CH_3-19), 1.49 (s, CH_3-21), 3.59 (br m, H-22), 1.24 (s, CH_3-26), 1.30 (s, CH_3-27), Other: α-D-Galp′: 5.50 (d, J = 3.4, H-1) [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.38 (t, J = 13.0, Ha-1), 1.88 (He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (Ha-4), 1.75 (He-4), 2.36 (t-like, H-5), 5.97 (d, J = 2.3, H-7), 3.11 (m, H-9), 1.73 (Ha-11), 1.87 (He-11), 1.98 (Ha-12), 1.75 (He-12), 2.05 (Ha-15), 1.66 (Hb-15), 1.92 (Ha-16), 1.78 (Hb-16), 2.28 (t, J = 9.0, H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.326 (s, CH_3-21), 3.44 (d, J = 8.7, H-22), 1.49 (Ha-23), 1.70 (Hb-23), 1.85 (Ha-24), 1.54 (td, J = 2.7, 12.3, Hb-24), 1.219 (s, CH_3-26), 1.232 (s, CH_3-27), Other: α-D-Galp′: 5.11 (d, J = 3.8, H-1), 3.89 (dd, J = 3.6, 10.5, H-2), 3.93 (dd, J = 2.8, 10.5, H-3), 4.03 (m, H-4), 4.10 (t, J = 6.5, H-5), 3.77 (dd, J = 6.0, 11.5, Ha-6), 3.72 (dd, J = 7.1, 11.5, Hb-6) [3]

^{13}C NMR (125 MHz, D_2O) [3]:

Table 1

C-1	37.8	C-12	33.4	C-23	28.3
2	69.9	13	50.3	24	43.0
3	69.7	14	87.7	25	74.3
4	33.7	15	32.6	26	30.2
5	53.1	16	22.4	27	30.9
6	211.0	17	51.7	Gal′-1	104.4
7	123.0	18	19.5	2	72.0
8		19	25.5	3	72.0
9	36.3	20	82.1	4	71.8
10	40.6	21	23.2	5	73.8
11	22.4	22	92.0	6	63.3

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.1 \times 10^{-5}$M [3], *Drosophila melanogaster in vitro* bioassay: inactive [4].

References

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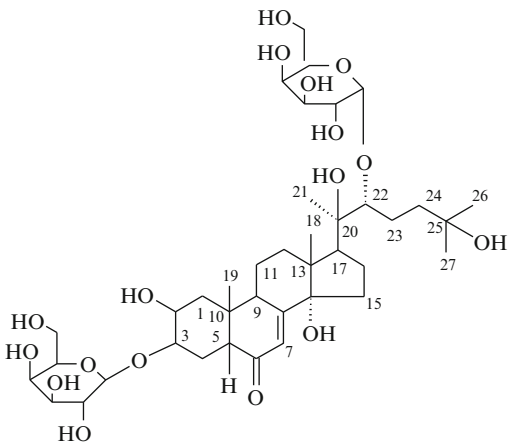
Sileneoside B

CAS Registry Number: 84699-93-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1]

$C_{39}H_{64}O_{17}$: 804.4144

Mp: 236–238°C (MeOH–EtOAc) [1]

$[\alpha]_D^{22}$ + 110.7±2° (c 0.51, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3370–3420, 1660 [1]

UV λ_{max}^{EtOH} nm (log ε): 246 (4.11) [1]

EI-MS m/z: 642 $[M\text{-}162]^+$ (0.5), 624 (1), 606 (3), 588 (17), 570 (3), 490 (3), 462 (10), 444 (12), 429‘(17), 426 (41), 411 (19), 409 (20), 363 (11), 345 (45), 327 (46), 309 (27), 300 (27), 163 (10), 161 (10), 145 (11), 143 (10), 99 (100), 81 (36), 69 (35) [1]

CD (c, 0.10, MeOH): Δε = +2.8 (330 nm), Δε = −6.3 (250 nm) [1]

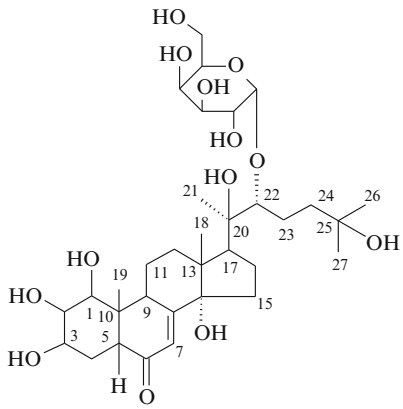
^{1}H NMR (J/Hz, C_5D_5N): 3.96 (m, H-2), 3.96 (m, H-3), 6.03 (br s, H-7), 3.34 (m, H-9), 1.09 (s, CH_3-18), 0.86 (s, CH_3-19), 1.51 (s, CH_3-21), 3.61 (d, J = 7.5, H-22), 1.26 (s, CH_3-26), 1.31 (s, CH_3-27), Other: β-D-Galp′: 5.40 (d, J = 3.9, H-1), β-D-Galp″: 5.45 (d, J = 3.9, H-1) [1]

References

1. Z. Saatov, M.B. Gorovits, N.D. Abdullaev, B.Z. Usmanov, N.K. Abubakirov, Chem. Nat. Comp. **18**, 578 (1982)

Sileneoside C

CAS Registry Number: 83207-65-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1]

$C_{33}H_{54}O_{13}$: 658.3564

Mp: 232–234°C (EtOAc–MeOH) [1]

$[\alpha]_D^{22}$ + 48.0 ± 2° (c 1.02, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3370–3440, 1658 [1]

UV λ_{max}^{EtOH} nm (log ε): 245 (4.01) [1]

EI-MS m/z: 460 $[M\text{-sugar-}H_2O]^+$ (0.6), 442 (4), 427 (4), 424 (2), 368 (2), 361 (4), 360 (4), 343 (8), 325 (4), 316 (4), 309 (2), 301 (2), 163 (3), 145 (4), 143 (6), 125 (5), 99 (100), 81 (98) [1]

CD (c, 0.12, MeOH): Δε = +1.36 (338 nm), Δε = −3.81 (245 nm) [1]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.13 (br m, H-1), 4.13 (m, H-2), 4.13 (m, H-3), 6.06 (br s, H-7), 3.41 (H-9), 1.11 (s, CH_3-18), 1.26 (s, CH_3-19), 1.48 (s,

CH_3-21), 3.58 (m, H-22), 1.24 (s, CH_3-26), 1.29 (s, CH_3-27), Other: α-D-Galp′: 5.46 (d, J = 3.3, H-1) [1]

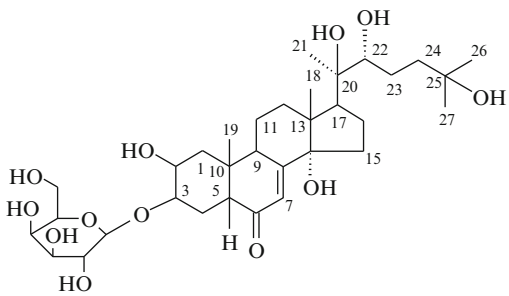
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.0 \times 10^{-4}$M [2].

References

1. Z. Saatov, M.B. Gorovits, N.D. Abdullaev, B.Z. Usmanov, N.K. Abubakirov, Chem. Nat. Comp. **18**, 193 (1982)
2. A. Maria, J.P. Girault, Z. Saatov, J. Harmatha, L. Dinan, R. Lafont, J. Chrom. Sci. **43**, 149 (2005)

Sileneoside D

CAS Registry Number: 93552-68-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1], *S. tatarica* [2], *S. viridiflora* [3]

$C_{33}H_{54}O_{12}$: 642.3615

Mp: 240–242°C (MeOH-acetone) [1]

$[\alpha]_D^{20}$ + 91.2±2° (c 1.01, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3380–3430, 1648 [1]

UV λ_{max}^{EtOH} nm (log ε): 247 (4.15) [1]

EI-MS m/z: 624 $[M\text{-}H_2O]^+$ (0.5), 606 (0.8), 588 (5), 570 (1), 514 (0.8), 507 (0.7), 490 (0.9), 473 (0.6), 462 (1), 444 (1), 426 (11), 411 (2), 408 (3), 393 (1), 375 (1), 363 (5), 345 (55), 327 (13), 309 (10), 300 (11), 284 (11), 145 (10), 143 (12), 135 (11), 99 (100), 81 (55), 69 (53) [1]

CD (c, 0.10, MeOH): Δε = +2.2 (327 nm), Δε = −5.5 (250 nm) [1]

^{1}H NMR (J/Hz, C_5D_5N): 3.96 (m, H-2), 3.96 (m, H-3), 6.10 (br s, H-7), 3.37 (m, H-9), 1.09 (s, CH_3-18), 0.86 (s, CH_3-19), 1.48 (s, CH_3-21), 3.75 (m, H-22), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27), Other: β-D-Galp′: 5.48 (d, J = 3.9, H-1) [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.04 (H-2), 4.07 (H-3), 3.46 (H-9), 1.19 (s, CH_3-18), 0.97 (s, CH_3-19), 1.57 (s, CH_3-21), 3.86 (H-22), 1.35 (s, CH_3-26), 1.35 (s, CH_3-27), Other: β-D-Galp′: 5.75 (d, J = 4.0, H-1) [2]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.51 (t, J = 12.5, Ha-1), 1.94 (He-1), 4.03 (m, Ha-2), 4.05 (m, He-3), 1.74 (Ha-4), 1.95 (He-4), 2.37 (dd, J = 1.8, 13.7, H-5), 5.97 (d, J = 2.0, H-7), 3.10 (m, H-9), 1.73 (Ha-11), 1.86 (He-11), 1.97 (Ha-12), 1.75 (He-12), 2.05 (Ha-15), 1.65 (Hb-15), 1.87 (Ha-16), 1.80 (Hb-16), 2.32 (t, J = 9.0, H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.24 (s, CH_3-21), 3.43 (d, J = 10.0, H-22), 1.32 (m, Ha-23), 1.65 (Hb-23), 1.78 (Ha-24), 1.49 (Hb-24), 1.22 (s, CH_3-26), 1.23 (s, CH_3-27), Other: β-D-Galp′: 5.14 (d, J = 3.8, H-1), 3.83 (dd, J = 3.9, 10.4, H-2), 3.95 (dd, J = 3.3, 10.4, H-3), 4.04 (m, H-4), 4.15 (m, H-5), 3.76 (dd, J = 7.6, 11.8, Ha-6), 3.79 (dd, J = 5.4, 12.0, Hb-6) [4]

^{13}C NMR (125 MHz, D_2O) [4]:

Table 1

C-1	39.1	C-12	33.1	C-23	28.4
2	70.3	13	50.1	24	43.1
3	79.9	14	87.7	25	74.6
4	33.5	15	32.8	26	30.0
5	54.1	16	22.4	27	30.6
6	211.0	17	51.7	Gal′-1	103.7
7	123.7	18	19.5	2	71.7
8	171.1	19	25.5	3	72.1
9	36.5	20	80.6	4	72.0
10	40.5	21	22.0	5	74.3
11	22.4	22	79.9	6	63.8

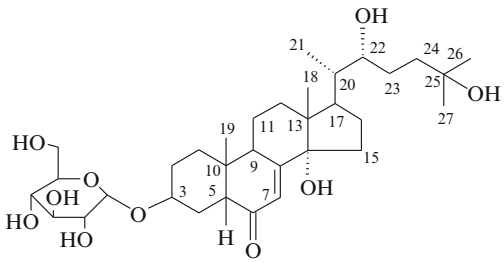
Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 3.0 \times 10^{-5}$M [4].

References

1. Z. Saatov, N.D. Abdullaev, M.B. Gorovits, N.K. Abubakirov, Chem. Nat. Comp. **20**, 700 (1984)
2. U.A. Baltaev, Phytochemistry **47**, 1233 (1998)
3. N.Z. Mamadalieva, L.N. Zibareva, Z. Saatov, R. Lafont, Chem. Nat. Comp. **39**, 199 (2003)
4. A. Maria, J.P. Girault, Z. Saatov, J. Harmatha, L. Dinan, R. Lafont, J. Chrom. Sci. **43**, 149 (2005)

Silenoside E (Blechnoside A)

CAS Registry Number: 104406-79-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Blechnum minus* [1], *Silene brahuica* [2]

$C_{33}H_{54}O_{10}$: 610.3716

Mp: 195–196°C (Me_2CO) [2]

$[\alpha]_D^{20}$ + 44.4 ± 2° (c 0.80, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}: 3400, 1648 [1], 3380–3430, 1655 [2]

UV λ_{max}^{EtOH} nm (log ε): 243 (4.02) [1], 245 (4.00) [2]

EI-MS m/z: 446 $[M-164]^+$ (0.2), 430 (1), 412 (5), 403 (1.5), 398 (2), 395 (2), 379 (2), 361 (4), 343 (3), 332 (4), 314 (4), 311 (4), 299 (7), 285 (8), 284 (15), 264 (7), 251 (8), 234 (6), 233 (6), 185 (7), 149 (100), 135 (11), 129 (1), 99 (15), 81 (27), 69 (30) [2]

CD (c, 0.12, EtOH): Δε = −1.28 (253 nm), Δε = +1.35 (330 nm) [2]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 3.86 (br m, J = 10.0, He-3), 2.89 (H-5), 6.19 (br d, J = 2.0, H-7), 3.48 (m, Ha-9), 0.72 (s, CH_3-18), 0.88 (s, CH_3-19), 1.29 (d, J = 6.5, CH_3-21), 4.10 (Hb-22), 1.40 (s, CH_3-26), 1.40 (s, CH_3-27), Other: β-D-Glcp′: 4.90 (d, J = 7.5, H-1) [2]

^{13}C NMR (C_5D_5N) [2]:

Table 1

C-1	29.5	C-12	31.7	C-23	25.6
2	27.5	13	48.1	24	42.5
3	78.6	14	84.0	25	69.7
4	29.6	15	31.7	26	30.2
5	51.5	16	26.7	27	30.0
6	203.9	17	48.3	Glc′-1	103.3
7	121.3	18	15.8	2	75.2
8	165.9	19	24.0	3	78.6
9	34.5	20	43.0	4	71.8
10	36.7	21	13.6	5	78.2
11	21.5	22	74.0	6	62.9

(*continued*)

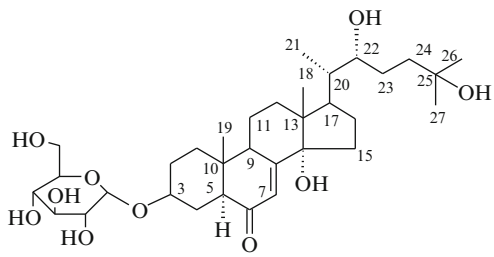
Pharm./Biol.: *Calliphora* bioassay: high active [1], *Drosophila melanogaster* B_{II} bioassay: inactive [3].

References

1. A. Suksamrarn, J.S. Wilkie, D.H.S. Horn, Phytochemistry **25**, 1301 (1986)
2. Z. Saatov, M.B. Gorovits, N.D. Abdullaev, B.Z. Usmanov, N.K. Abubakirov, Chem. Nat. Comp. **22**, 297 (1986)
3. A. Maria, J.P. Girault, Z. Saatov, J. Harmatha, L. Dinan, R. Lafont, J. Chrom. Sci. **43**, 149 (2005)

5α-Silenoside E

CAS Registry Number: 176166-62-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1]

$C_{33}H_{54}O_{10}$: 610.3716

EI-MS m/z: 592 $[M-H_2O]^+$ (3), 574 (7), 556 (1.4), 476 (2), 448 (6), 446 (7), 430 (10), 412 (60), 395 (16), 394 (16), 379 (8), 343 (8), 314 (11), 311 (12), 285 (50), 284 (100), 269 (15), 163 (9), 145 (12), 143 (8), 99 (80), 81 (80), 69 (50) [1]

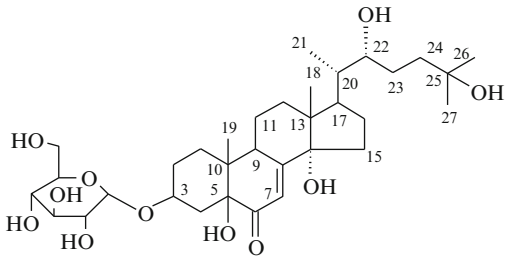
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 6.10 (br s, H-7), 3.44 (br m, Ha-9), 0.71 (s, CH_3-18), 0.81 (s, CH_3-19), 1.28 (d, J = 6.5, CH_3-21), 1.40 (s, CH_3-26), 1.40 (s, CH_3-27), Other: β-D-Glcp′: 4.98 (d, J = 7.5, H-1) [1]

References

1. M.H. Djukharova, Z. Saatov, N.D. Abdullaev, Chem. Nat. Comp. **31**, 207 (1995)

Sileneoside F

CAS Registry Number: 170663-52-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1]

$C_{33}H_{54}O_{11}$: 626.3666

Mp: amorphous [1]

IR (KBr) ν_{max} cm^{-1}: 3300–3500, 1680 [1]

UV λ_{max}^{EtOH} nm (log ε): 243 (4.09) [1]

EI-MS m/z: 608 $[M\text{-}H_2O]^+$ (0.4), 590 (3), 572 (3), 492 (2), 447 (23), 446 (23), 429 (98), 428 (100), 426 (24), 418 (26), 411 (50), 410 (98), 395 (16), 392 (17), 377 (42), 348 (56), 330 (26), 99 (57), 81 (55) [1]

^{1}H NMR (J/Hz, C_5D_5N): 4.10 (m, H-3), 6.24 (br s, H-7), 3.53 (m, H-9), 0.74 (s, CH_3-18), 1.14 (s, CH_3-19), 1.30 (d, J = 6.5, CH_3-21), 1.40 (s, CH_3-26), 1.40 (s, CH_3-27), Other: β-D-Glcp′: 4.90 (d, J = 7.5, H-1), 3.70-4.50 (H-2-H-6) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

C-1	25.5	C-12	31.4	C-23	25.5
2	27.1	13	47.0	24	42.3
3	71.5	14	83.7	25	69.6
4	32.4	15	31.7	26	30.0
5	78.4	16	26.5	27	29.9
6	202.2	17	48.1	Glc′-1	101.3
7	120.2	18	15.7	2	75.2
8	166.4	19	17.1	3	78.3
9	36.7	20	42.8	4	71.7
10	42.8	21	13.5	5	78.3
11	21.7	22	73.9	6	62.6

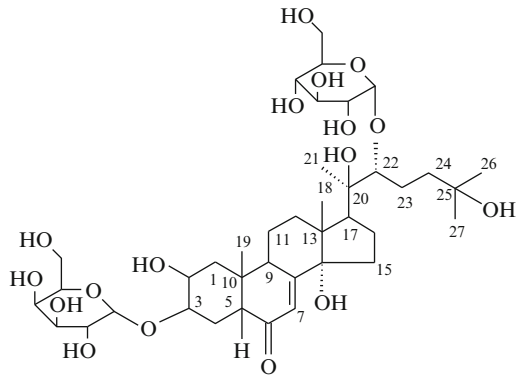
(*continued*)

References

1. M.H. Djukharova, Z. Saatov, N.D. Abdullaev, N.K. Abubakirov, Chem. Nat. Comp. **34**, 680 (1994)

Sileneoside G

CAS Registry Number: 241478-02-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1]

$C_{39}H_{64}O_{17}$: 804.4143

Mp: 225–227°C (MeOH-acetone)

$[\alpha]_D^{20}$ + 121 ± 2° (c 0.10, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3372, 1653 [1]

UV λ_{max}^{EtOH} nm (log ε): 245 (4.01) [1]

EI-MS m/z: 588 $[M\text{-}162\text{-}3H_2O)^+$ (2.5), 570 (2), 426 (38), 363 (35), 345 (40), 327 (41), 311 (35), 309

(38), 300 (35), 145 (50), 143 (52), 99 (100), 81 (97), 69 (98) [1]

^{1}H NMR (J/Hz, C_5D_5N): 4.10 (m, H-2), 4.10 (m, H-3), 2.79 (dd, J = 13.4, 3.6, H-5), 6.02 (s, H-7), 3.50 (t, J = 7.9, H-9), 2.96 (t, J = 8.5, H-17), 1.24 (s, CH_3-18), 0.97 (s, CH_3-19), 1.67 (s, CH_3-21), 3.78 (d, J = 9.1, H-22), 1.40 (s, CH_3-26), 1.47 (s, CH_3-27), Other: α-D- Glcp ′: 5.69 (d, J = 4.03, H-1), α-D-Galp ′: 5.62 (d, J = 3.9, H-1) [1]

^{13}C NMR (C_5D_5N) [1]:

Table 1

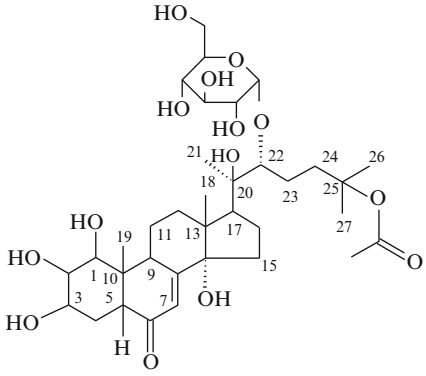
C-1	39.36	C-11	21.01	C-21	22.28	Gal′-4	71.15
2	68.05	12	31.97	22	90.96	5	72.44
3	79.72	13	48.05	23	27.11	6	62.59
4	31.61	14	84.15	24	41.75	Glc′-1	104.04
5	51.41	15	31.72	25	69.72	2	73.44
6	203.01	16	21.42	26	29.73	3	79.10
7	121.46	17	49.85	27	29.73	4	71.19
8	166.54	18	18.05	Gal′-1	103.68	5	78.30
9	34.22	19	24.24	2	70.93	6	62.74
10	38.50	20	77.81	3	71.75		

References

1. Z.T. Sadikov, Z. Saatov, Chem. Nat. Comp. **34**, 602 (1998)

Sileneoside H

CAS Registry Number: 289622-72-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene brahuica* [1]

$C_{35}H_{56}O_{14}$: 700.3670

Mp: 210–212°C [1]

IR (KBr) ν_{max} cm^{-1}:3398, 1707, 1655, 1282 [1]

UV λ_{max}^{EtOH} nm (log ε): 242 (4.00) [1]

CI-MS m/z: 700 $[M]^+$, 682 $[M\text{-}H_2O]^+$, 664 $[M\text{-}2H_2O]^+$, 640 $[M\text{-}CH_3COOH]^+$, 623, 605, 587, 569, 479, 461, 443, 180 [hexose] [1]

HRCI-MS m/z: for $C_{35}H_{58}O_{13}N$ $[M\text{-}H_2O + NH_4]^+$ calcd. 700.3907, found 700.3893 [1]

^{1}H NMR (500 MHz, J/Hz, D_2O): 3.93 (br s, He-1), 4.05 (br t, J = 3.1, Ha-2), 4.15 (br s, He-3), 1.79 (Ha-4), 1.82 (He-4), 2.62 (br dd, J = 11.0, 6.0, H-5), 5.99 (br s, H-7), 3.05 (m, H-9), 1.75 (Ha-11), 1.80 (He-11), 1.95 (Ha-12), 1.75 (He-12), 1.67 (Ha-15), 2.06 (Hb-15), 1.90 (Ha-16), 1.75 (Hb-16), 2.29 (t, J = 8.7, H-17), 0.87 (s, CH_3-18), 1.09 (s, CH_3-19), 1.30 (s, CH_3-21), 3.42 (d, J = 9.5, H-22), 1.47 (Ha-23), 1.59 (Hb-23), 1.95 (Ha-24), 2.06 (Hb-24), 1.42 (s, CH_3-26), 1.47 (s, CH_3-27), Other: 2.04 (s, CH_3COO-25), α-D-Galp′: 5.10 (d, J = 3.4, H-1), 3.91 (dd, J = 10.3, 3.4, H-2), 3.94 (H-3), 4.04 (dd, J = 3.0, 1.2, H-4), 4.11 (dt, J = 6.5, 1.2, H-5), 3.74 (dd, J = 11.7, 5.8, H-6), 3.76 (dd, J = 11.7, 6.7, H-6′) [1]

^{13}C NMR (125 MHz, D_2O) [1]:

Table 1

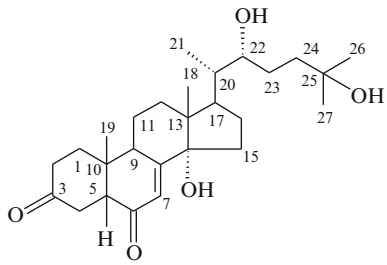
C-1	75.6	C-13	48.4	C-25	85.9
2	68.2	14	86.0	26	26.5
3	70.0	15	31.5	27	26.7
4	32.7	16	21.2	CH_3COO	23.1
5	46.5	17	50.1	CH_3COO	174.9
6		18	18.2	Gal′-1	102.9
7	122.1	19	20.0	2	70.9
8		20	80.6	3	70.1
9	35.4	21	21.8	4	70.3
10	43.2	22	90.6	5	72.2
11	21.3	23	26.4	6	61.8
12	31.9	24	38.5		

References

1. Z.T. Sadikov, Z. Saatov, J.P. Girault, R. Lafont, J. Nat. Prod. **63**, 987 (2000)

Silenosterone

CAS Registry Number: 74396-16-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene praemixta* [1]

$C_{27}H_{42}O_5$: 446.3032

Mp: 115–117°C (MeOH) [1], 114–115°C ($CHCl_3$–C_6H_6)[2]

$[\alpha]_D^{28}$ + 86.9 ± 2° (c 0.92, MeOH) [1], $[\alpha]_D^{25}$ + 86.5 ± 2° (c 0.35, MeOH) [2]

IR (KBr) ν_{max} cm^{-1}:3420, 1710, 1660 [1], 3425, 1710, 1660 [2]

UV λ_{max}^{EtOH} nm (log ε): 246 (4.05) [1]

EI-MS m/z: 446 $[M]^+$ (0.3), 428 (5), 413 (4), 410 (8), 400 (3), 395 (10), 377 (3), 359 (3), 341 (8), 330 (7), 312 (10), 297 (10), 283 (14), 282 (16), 261 (10), 233 (33), 232 (25), 231 (17), 99 (100), 81 (92) [1], 446 $[M]^+$ (9), 428 (98), 413 (40), 410 (50), 395 (98), 377 (8), 359 (40), 341 (50), 330 (95), 312 (96), 297 (50), 283 (30), 232 (35), 99 (100), 81 (98) [2]

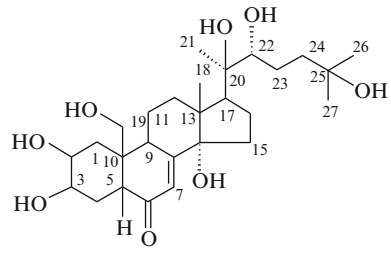
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 6.00 (br s, H-7), 3.45 (m, H-9), 0.60 (s, CH_3-18), 0.94 (s, CH_3-19), 1.15 (d, CH_3-21), 3.90 (m, H-22), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27) [1], 5.96 (br s, H-7), 3.45 (m, H-9), 0.62 (s, CH_3-18), 0.94 (s, CH_3-19), 1.16 (d, J = 6.0, CH_3-21), 3.90 (m, H-22), 1.27 (s, CH_3-26), 1.27 (s, CH_3-27) [2]

References

1. Z. Saatov, B.Z. Usmanov, N.K. Abubakirov, Chem. Nat. Comp. **15**, 700 (1979)
2. N.Z. Mamadalieva, N.Sh. Ramazanov, Z. Saatov, Chem. Nat. Comp. **35**, 653 (1999)

Sogdisterone

CAS Registry Number: 58347-83-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Serratula sogdiana* [1]

$C_{27}H_{44}O_8$: 496.3036

$[\alpha]_D^{20}$ + 43.9° (c 0.41, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3300–3550, 1665 [1]

UV λ_{max}^{EtOH} nm (log ε): 242 (3.98) [1]

EI-MS m/z: 478 $[M\text{-}H_2O]^+$, 460 $[M\text{-}2H_2O]^+$, 442 $[M\text{-}3H_2O]^+$, 424 $[M\text{-}4H_2O]^+$, 409 $[M\text{-}4H_2O\text{-}CH_3]^+$, 406 $[M\text{-}5H_2O]^+$, 379, 361, 343, 325, 99, 81, 69 [1]

CD (c, dioxane): $[\theta]_{358}$ +3.52 × 10^3, $[\theta]_{315}$ −0.622 × 10^3, a = +41°, $[\theta]_{260}$ −3.8 × 10^3, $[\theta]_{233}$ +14.3 × 10^3, a = −181° [1]

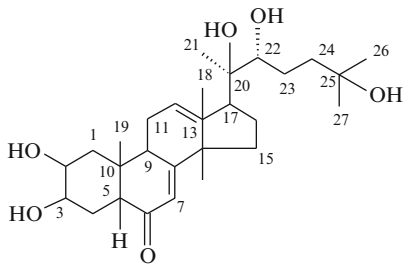
^{1}H NMR (100 MHz, C_5D_5N): 4.07–4.04 (m, H-2), 4.07–4.04 (m, H-3), 6.15 (H-7), 3.50 (m, H-9), 1.06 (s, CH_3-18), 4.07–4.04 (m, H-19), 1.46 (s, CH_3-21), 3.75 (m, H-22), 1.25 (s, CH_3-26), 1.25 (s, CH_3-27) [1]

References

1. I.L. Novoselskaya, M.B. Gorovits, N.K. Abubakirov, Chem. Nat. Comp. **11**, 445 (1975)

Stachysterone A

CAS Registry Number: 30655-78-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Stachyurus praecox* [1]

$C_{27}H_{42}O_6$: 462.2981

Mp: amorphous [1]

IR (KBr) ν_{max} cm^{-1}: 3400, 1640, 1590 [1]

UV λ_{max}^{MeOH} nm (ε): 248 (10700) [1]

EI-MS m/z: 462 $[M]^+$; 426 $[M - 2H_2O]^+$, 345 $[M- C_{22}\text{-}C_{27}]^+$ (9), 327 (4), 143 $[C_{20}\text{-}C_{27}]^+$ (96), 125 (34), 99 $[C_{22}\text{-}C_{27}]^+$ (20), 81 (28), 43 (100) [1]

HR-MS m/z: for $C_{27}H_{38}O_4$ calcd. 426.2769, found 426.2699 [1]

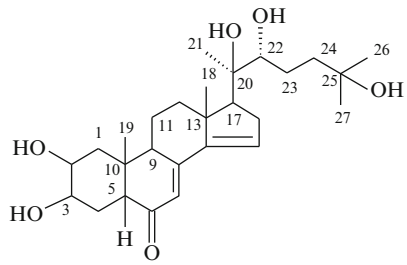
^{1}H NMR (J/Hz, C_5D_5N): 4.09 (m, Ha-2), 4.31 (m, He-3), 6.14 (d, J = 2.5, H-7), 5.98 (m, H-12), 0.92 (s, CH_3-19), 1.51 (s, CH_3-21), 3.85 (m, H-22), 1.41 (s, CH_3-26), 1.41 (s, CH_3-27), 1.20 (s, CH_3-14) [1].

References

1. S. Imai, E. Murata, S. Fugioka, T. Matsuoka, M. Koreeda, K. Nakanishi, J. Am. Chem. Soc. **92**, 7510 (1970)

Stachysterone B

CAS Registry Number: 30655-79-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Asparagus filicinus* [1], *Serratula wolffii* [2], *Stachyurus praecox* [3]

$C_{27}H_{42}O_6$: 462.2981

Mp: amorphous [3]

IR (KBr) ν_{max} cm^{-1}: 3400, 1640, 1590 [3]

UV λ_{max}^{MeOH} nm (ε): 298 (12800) [3]

EI-MS m/z: 462 $[M]^+$ 444 $[M - H_2O]^+$, 345 $[M- C_{22}\text{-}C_{27}]^+$ (5), 327 (7), 99 $[C_{22}\text{-}C_{27}]^+$ (86), 81 (45), 43 (100) [3]

HR-MS m/z: for $C_{28}H_{40}O_5$ calcd. 444.2815, found 444.2861 [3]

^{1}H NMR (500 MHz, CD_3OD): 1.81 (Ha-1), 1.465 (He-1), 3.80 (Ha-2), 3.94 (He-3), 1.65 (Ha-4), 1.72 (He-4), 2.385 (H-5), 6.08 (H-7), 2.72 (H-9), 1.86 (Ha-11), 1.77 (He-11), 1.64 (Ha-12), 2.31 (He-12), 6.08 (H-15), 2.25 (Ha-16), 2.625 (Hb-16), 2.20 (H-17), 1.14 (s, CH_3-18), 0.97 (s, CH_3-19), 1.25 (s, CH_3-21), 3.335 (H-22), 1.32 (Ha-23), 1.61 (Hb-23), 1.425 (Ha-24), 1.81 (Hb-24), 1.185 (s, CH_3-26), 1.21 (s, CH_3-27) [2]

^{1}H NMR (J/Hz, C_5D_5N): 3.82 (m, Ha-2), 4.40 (m, He-3), 2.96 (dd, J = 13.5, 5.0, H-5), 6.31 (d, J = 2.5, H-7), 5.94 (dd, J = 3.0, 3.0, H-15), 1.33 (s, CH_3-18), 1.00 (s, CH_3-19), 1.49 (s, CH_3-21), 3.76 (m, H-22), 1.42 (s, CH_3-26), 1.42 (s, CH_3-27) [3]

^{13}C NMR (125 MHz, CD_3OD) [3]:

Table 1

C-1	37.2	C-10	40.06	C-19	24.15
2	68.71	11	21.8	20	77.3
3	68.67	12	41.2	21	20.5
4	33.0	13	49.1	22	78.7
5	51.6	14	150.8	23	27.4
6	205.9	15	130.4	24	42.4
7	121.2	16	32.1	25	71.4
8	158.9	17	50.1	26	29.0
9	39.96	18	20.2	27	30.0

References

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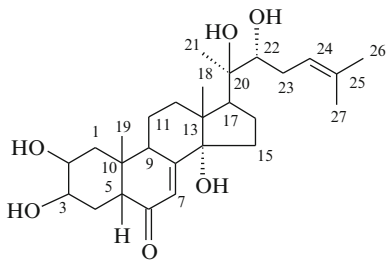
Stachysterone C

CAS Registry Number: 26362-25-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Klaseopsis chinensis* [1], *Stachyurus praecox* [2, 3]

$C_{27}H_{42}O_6$: 462.2981

Mp: white amorphous powder [1], 235–240°C [2], 225–227°C (MeOH–$CHCl_3$) [3]

$[\alpha]_D^{25}$ + 40° (c 0.005; MeOH) [1], $[\alpha]_D^{20}$ + 43° (c; dioxane) [2]

IR (KBr) ν_{max} cm^{-1}: 3400, 1640 [2], 3414, 2926, 1647, 1445, 1382, 1116, 1056, 875 [3]

UV λ_{max}^{MeOH} nm: 241.5 [1]

UV λ_{max}^{EtOH} nm (ε): 242 (10500) [2]

EI-MS m/z: 462 $[M]^+$; 444 $[M–H_2O]^+$, 363 (25), 345 (74), 327 (25), 99 $[C_{22}$-$C_{27}]^+$ (9), 81 (23), 69 $[C_{23}$-$C_{27}]$ (49), 43 (100) [2]

ESI-MS m/z: 461 $[M\text{-}H]^-$; 521 $[M + CH_3COO]^-$, 559 $[M + HSO_4]^-$ [1]

FAB-MS m/z: 463 $[M + H]^+$ (54), 445 (29), 427 (6) [3]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 4.175 (br d, J = 10.4, Ha-2), 4.238 (br s, He-3), 3.015 (dd, J = 3.6, 12.2, H-5), 6.252 (1H, d, J = 2.1, H-7), 3.594 (m, H-9), 2.607 (1H, dt, J = 4.8, 13.2, Ha-12), 2.950 (br t, J = 9.0, H-17), 1.217 (s, CH_3-18), 1.075 (s, CH_3-19), 1.598 (s, CH_3-21), 3.890 (br d, J = 9.6, H-22), 5.549 (br t, J = 6.8, H-24), 1.598 (s, CH_3-26), 1.660 (s, CH_3-27), 4.751 (1H, br s, OH), 5.938 (1H, s, OH), 6.029 (2H, br s, OH), 6.130 (1H, s, OH), 6.284 (1H, s, OH) [1]

^{1}H NMR (J/Hz, C_5D_5N): 1.05 (CH_3-18), 1.17 (CH_3-19), 1.55 (CH_3-21), 5.51 (dd, J = 7.0, 7.0, H-24), 1.60 (CH_3-26), 1.66 (CH_3-27) [2]

^{1}H NMR (J/Hz, C_5D_5N): 4.17 (m, Ha-2), 4.24 (br s, He-3), 3.02 (dd, J = 13.2, 3.5, H-5), 6.25 (d, J = 2.1, H-7), 3.60 (m, Ha-9), 2.95 (t, J = 9.3, H-17), 1.21 (s, CH_3-18), 1.07 (s, CH_3-19), 1.59 (s, CH_3-21), 3.89 (dd, J = 9.7, 1.5, H-22), 5.55 (br t, J = 7.0, H-24), 1.59 (s, CH_3-26), 1.63 (s, CH_3-27) [3]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	38.26	C-10	38.94	C-19	24.70
2	68.38	11	21.86	20	76.96
3	68.33	12	32.29	21	21.73

(*continued*)

Table 1 (continued)

4	32.73	13	48.35	22	77.30
5	51.66	14	84.42	23	32.03
6	203.73	15	32.03	24	124.15
7	121.95	16	21.38	25	132.20
8	166.37	17	50.35	26	18.22
9	34.72	18	18.15	27	26.15

Pharm./Biol.: *Chilo* test: active [2], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.4 \times 10^{-8}$M [4, 5].

References

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3. B. Yindyongnarongkul, A. Suksamrarn, Tetrahedron **54**, 2795 (1998)
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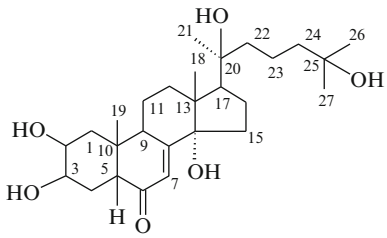
5. M. Ravi, A.J. Hopfinger, R.E. Hormann, L. Dinan, J. Chem. Inf. Comput. Sci. **41**, 1587 (2001)

Taxisterone

CAS Registry Number: 19536-24-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Coronaria flos-cuculi* [1], *Cucubalis baccifer* [2], *Leuzea carthamoides* [3], *Lychnis flos-cuculi* [4], *Penstemon venustus* [5], *Serratula coronata* [6], *Silene italica* ssp. *nemoralis* [7], *S. nutans* [8], *S. viridiflora* [9], *Taxis cuspidata* [10, 11]

$C_{27}H_{44}O_6$: 464.3138

Mp: 141–141.5°C [6], 241–242°C (EtOAc–MeOH) [8], 120–125°C [10], 131–133°C (EtOAc–MeOH) [12]

$[\alpha]_D^{17}$ + 42.7° (c 0.88, MeOH) [6], $[\alpha]_D^{20}$ + 80.9 ± 2° (c 0.42, MeOH) [8]

IR (KBr) ν_{max} cm^{-1}:3392, 3318, 1639 [3], 3400–3430, 1647 [8], 3400, 1650 [10]

UV λ_{max}^{EtOH} nm (log ε): 244 (4.03) [8], 242 (4.17) [12]

EI-MS m/z: 464 $[M]^+$ (0.3), 446 (1.4), 431 (0.8), 428 (35), 418 (1), 413 (16), 410 (28), 400 (2.5), 395 (12), 385 (0.7), 377 (0.8), 367 (7.0), 363 (11), 361 (1.0), 354 (11), 345 (43), 343 (5), 327 (54), 325 (20), 320 (20), 309 (10), 302, 301 (19), 300 (35), 299 (27), 250 (30), 249 (15), 145 (20), 127 (97), 109 (100), 81 (20), 69 (54) [6], 464 $[M]^+$ (0.05), 446 (0.1), 428 (6), 410 (12), 363 (7), 345 (13), 320 (12), 302 (10), 145 (33), 127 (97), 109 (100) [12]

FAB-MS m/z: 487 $[M + Na]^+$ (2), 465 $[M + H]^+$ (6), 447 (11), 429 (12), 411 (10), 397 (3), 371 (3), 355 (5), 303 (10), 301 (12), 263 (6), 249 (10), 239 (8), 227 (9), 213 (11), 181 (18), 165 (19), 145 (21), 128 (27), 109 (48), 91 (65), 69 (100) [3]

HR-MS m/z: for $C_{27}H_{45}O_6$ $[M + H]^+$ calcd. 465.3216, found 465.3202 [3]

CD (c, MeOH): $\Delta\varepsilon = +1.26$ (338 nm), $\Delta\varepsilon = -3.87$ (246 nm) [8]

^{1}H NMR (500 MHz, CD_3OD): 1.79 (dd, Ha-1), 1.42 (dd, He-1), 3.84 (ddd, Ha-2), 3.95 (q, He-3), 1.75 (Ha-4), 1.70 (He-4), 2.38 (dd, H-5), 5.81(d, H-7), 3.15 (ddd, H-9), 1.78 (Ha-11), 1.68 (He-11), 2.12 (dt, Ha-12), 1.84 (He-12), 1.95 (Ha-15), 1.61 (Hb-15), 1.71 (Ha-16), 1.92 (Hb-16), 2.34 (dd, H-17), 0.86 (s, CH_3-18), 0.96 (s, CH_3-19), 1.28 (s, CH_3-21), 1.38-1.52 (H-22), 1.38-1.52 (Ha-23), 1.38-1.52 (Hb-23), 1.38-1.52 (Ha-24), 1.38-1.52 (Hb-24), 1.19 (s, CH_3-26), 1.19 (s, CH_3-27) [3]

^{1}H NMR (100 MHz, C_5D_5N): 4.04 (m, H-2), 4.04 (m, H-3), 6.02 (br s, H-7), 3.41 (m, H-9), 0.99 (s, CH_3-18), 0.92 (s, CH_3-19), 1.41 (s, CH_3-21), 1.22 (s, CH_3-26), 1.22 (s, CH_3-27) [8]

^{13}C NMR (125.7 MHz, CD_3OD) [3]: **^{13}C NMR** (125.7 MHz, CD_3OD) [6]:

Table 1

C-1	37.37	C-15	31.58	C-1	37.37 (t)	C-15	31.57 (t)
2	68.72	16	21.96	2	68.69 (d)	16	21.49 (t)
3	68.53	17	53.36	3	68.51 (d)	17	51.77 (d)
4	32.86	18	18.12	4	32.84 (d)	18	18.17 (q)
5	51.80	19	24.39	5	53.30 (d)	19	24.41 (q)
6	206.51	20	75.99	6	206.67 (s)	20	76.03 (s)
7	122.10	21	26.46	7	122.07 (d)	21	26.46 (q)
8	168.14	22	45.89	8	168.26 (s)	22	45.85 (t)
9	35.05	23	20.10	9	35.04 (d)	23	20.12 (t)
10	39.26	24	45.50	10	39.28 (s)	24	45.44 (t)
11	21.51	25	71.48	11	21.97 (t)	25	71.55 (s)
12	32.38	26	29.33	12	32.36 (t)	26	29.12 (q)
13	48.07	27	29.10	13		27	29.34 (q)
14	85.54			14	85.57 (s)		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 9.5 \times 10^{-8}$M [6], *Bombyx mori* growth: exhibited a potential moulting effect although slightly less than that of 20-hydroxyecdysone [10], *Calliphora* bioassay: 1/100 to 1/50 of 20-hydroxyecdysone [12].

References

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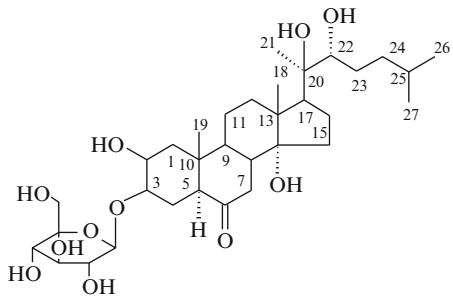
Tenuifolioside A

CAS Registry Number: 126239-75-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Lilium tenuifolium* [1]

$C_{33}H_{56}O_{10}$: 612.3873

Mp: amorphous [1]

$[\alpha]_D^{28}$ −9.8° (c 0.54, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3420, 2950, 2870, 1695, 1465, 1455, 1380, 1250, 1165, 1075, 1030, 955, 905, 890 [1]

UV λ_{max}^{EtOH} nm (ε): 230 sh (714), 279 (240), 316 sh (159) [1]

SI-MS m/z: 433 $[aglycone\text{-}OH]^+$, 415 $[aglycone\text{-}OH–H_2O]^+$, 397 $[aglycone\text{-}OH–2H_2O]^+$ [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 3.94 (m, He-3), 2.88 (dd, J = 12.7, 12.7, Ha-7), 2.45 (dd, J = 12.7, 4.3, He-7), 2.29 (ddd, J = 12.7, 12.7, 4.2, H-8), 2.13 (ddd, J = 12.7, 12.7, 4.2, Ha-9), 2.84 (t, J = 9.5, H-17), 1.34 (s, CH_3-18), 0.73 (s, CH_3-19), 1.56 (s, CH_3-21), 3.79 (br d, J = 10.3, H-22), 0.84 (d, J = 6.5, CH_3-26), 0.83 (d, J = 6.5, CH_3-27), Other: β-D-Glcp′: 5.04 (d, J = 7.7, H-1), 4.04 (dd, J = 8.7, 7.7, H-2), 4.28 (dd, J = 8.7, 8.7, H-3), 4.22 (dd, J = 8.7, 8.7, H-4), 4.00 (ddd, J = 8.7, 5.6, 2.2, H-5), 4.61 (dd, J = 11.7, 2.2, Ha-6), 4.39 (dd, J = 11.7, 5.6, Hb-6) [1]

^{1}H NMR (400 MHz, J/Hz, CD_3OD): 3.70 (m, He-3), 2.28 (dd, J = 12.2, 2.2, H-5), 2.48 (dd, J = 12.7, 12.7, Ha-7), 2.09 (dd, J = 12.7, 4.5, He-7), 2.17 (ddd, J = 12.7, 12.7, 4.5, H-8), 2.31 (t, J = 9.3, H-17), 1.02 (s, CH_3-18), 0.76 (s, CH_3-19), 1.15

(s, CH_3-21), 3.37–3.21 (H-22), 0.91 (d, J = 6.5, CH_3-26), 0.90 (d, J = 6.5, CH_3-27), Other: β-D-Glcp′: 4.39 (d, J = 7.8, H-1), 3.14 (dd, J = 9.0, 7.8, H-2), 3.37–3.21 (H-3), 3.37–3.21 (H-4), 3.37–3.21 (H-5), 3.85 (dd, J = 12.3, 1.7, Ha-6), 3.64 (dd, J = 12.3, 5.4, Hb-6) [1]

^{13}C NMR (100.6 MHz, C_5D_5N) [1]:

Table 1

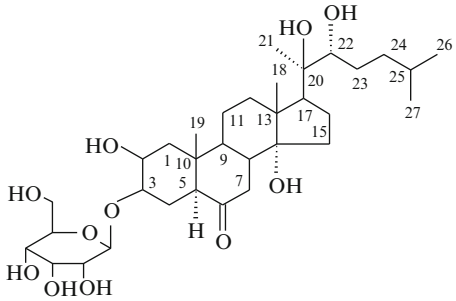
C-1	37.0	C-12	33.0	C-23	30.3
2	27.1	13	48.8	24	37.2
3	76.9	14	83.8	25	28.2
4	29.6	15	32.4	26	22.5
5	56.4	16	21.6	27	23.2
6	211.4	17	50.2	Glc′-1	102.0
7	42.8	18	17.8	2	75.4
8	40.9	19	12.8	3	78.6
9	46.7	20	76.8	4	71.9
10	40.7	21	21.3	5	78.6
11	21.2	22	76.7	6	63.0

References

1. Y. Mimaki, Y. Sashida, H. Shimomura, Phytochemistry **28**, 3454 (1989)

Tenuifolioside B

CAS Registry Number: 126239-76-7



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Lilium tenuifolium* [1]

$C_{33}H_{56}O_{10}$: 612.3873

Mp: amorphous [1]

$[\alpha]_D^{26}$ − 19.0° (c 0.20, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3430, 2945, 2870, 1695, 1460, 1380, 1360, 1245, 1075, 1020, 955, 900, 880 [1]

UV λ_{max}^{EtOH} nm (ε): 230 sh (589), 281 (249), 320 sh (147) [1]

SI-MS m/z: 635 $[M + Na]^+$ [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 3.89 (m, He-3), 2.87 (dd, J = 12.6, 12.6, Ha-7), 2.44 (dd, J = 12.6, 4.5, He-7), 2.28 (ddd, J = 12.6, 12.6, 4.2, H-8), 2.12 (ddd, J = 12.6, 12.6, 4.2, Ha-9), 2.85 (t, J = 9.1, H-17), 1.34 (s, CH_3-18), 0.72 (s, CH_3-19), 1.57 (s, CH_3-21), 3.79 (br d, J = 10.2, H-22), 0.84 (d, J = 6.4, CH_3-26), 0.83 (d, J = 6.5, CH_3-27), Other: β-D-Glcp′: 5.49 (d, J = 7.8, H-1), 3.98 (dd, J = 7.8, 2.8, H-2), 4.76 (dd, J = 2.8, 2.8, H-3), 4.22 (dd, J = 9.6, 2.8, H-4), 4.51 (ddd, J = 9.6, 5.3, 2.1, H-5), 4.57 (dd, J = 11.6, 2.1, Ha-6), 4.39 (dd, J = 11.6, 5.3, Hb-6) [1]

^{1}H NMR (400 MHz, J/Hz, CD_3OD): 3.73–3.58 (He-3), 2.28 (dd, J = 12.4, 2.4, H-5), 2.49 (dd, J = 12.6, 12.6, Ha-7), 2.08 (dd, J = 12.6, 4.4, He-7), 2.17 (ddd, J = 12.6, 12.6, 4.4, H-8), 2.31 (t, J = 9.4, H-17), 1.02 (s, CH_3-18), 0.76 (s, CH_3-19), 1.15 (s, CH_3-21), 3.31 (H-22), 0.91 (d, J = 6.5, CH_3-26), 0.90 (d, J = 6.5, CH_3-27), Other: β-D-Allp′: 4.76 (d, J = 8.0, H-1), 3.26 (dd, J = 8.0, 3.0, H-2), 4.04 (dd, J = 3.0, 3.0, H-3), 3.46 (dd, J = 9.5, 3.0, H-4), 3.75–3.58 (H-5), 3.82 (br d, J = 9.6, Ha-6), 3.75–3.58 (Hb-6) [1]

^{13}C NMR (100.6 MHz, C_5D_5N) [1]:

Table 1

C-1	37.0	C-12	33.0	C-23	30.3
2	27.2	13	48.8	24	37.2
3	76.9	14	83.9	25	28.2
4	29.6	15	32.4	26	22.5
5	56.4	16	21.7	27	23.2
6	211.4	17	50.2	All′-1	99.6
7	42.8	18	17.8	2	73.0
8	40.9	19	12.8	3	72.4
9	46.7	20	76.8	4	69.3
10	40.7	21	21.3	5	76.0
11	21.2	22	76.7	6	63.2

References

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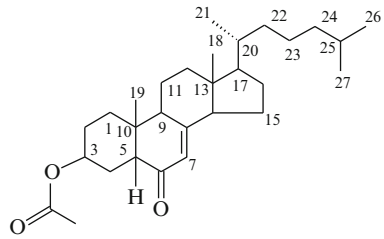
2,14,22,25-Tetradeoxyecdysone

CAS Registry Number: 39219-58-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Peniocereus greggi* [1]
$C_{29}H_{46}O_3$: 442.3447
Mp: 176–177°C [1], 172–175°C (MeOH) [2]
IR (KBr) ν_{max} cm^{-1}: 1725, 1710 [2]

References

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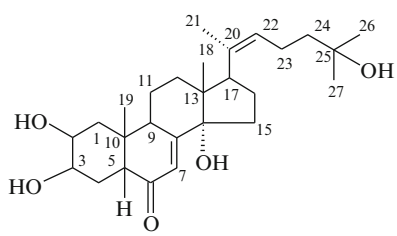
2β,3β,14α,25-Tetrahydroxy-5β-Cholesta-7,20(22)-dien-6-one

CAS Registry Number: 894408-16-3



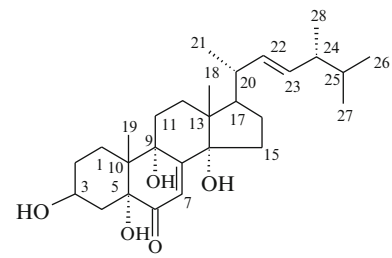
Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Serratula wolffii* [1]
$C_{27}H_{42}O_5$: 446.3032

References

1. E. Liktor-Busa, A. Simon, M. Bathori, *55th International Congress & Annual Meeting of the Society for Medicinal Plant Research*, vol. 364, Graz, 2007, p. 936

3β,5α,9α,14α-Tetrahydroxyergosta-7,22-dien-6-one

CAS Registry Number: 211486-14-5



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Hypsizigus marmoreus, Lentinus edodes, Pholiota nameko, Pleurotus ostreatus* [1]
$C_{28}H_{44}O_5$: 460.3188
Mp: amorphous [1]
$[\alpha]_D^{19}$ − 22.7° (c 0.04, $CHCl_3$) [1]
IR (KBr) ν_{max} cm^{-1}: 3354, 1687 [1]
UV λ_{max}^{EtOH} nm (log ε): 225 (3.9) [1]
EI-MS m/z: 338 $[M\text{-}4H_2O]^+$, 263 [M-4H_2O-side-chain]$^+$ [1]
HR-MS m/z: for $C_{28}H_{42}O_4$ $[M\text{-}H_2O]^+$, calcd. 442.3083, found 442.3095 [1]
^{1}H NMR (600 MHz, J/Hz, C_5D_5N): 2.70 (ddd, J = 14.0, 14.0, 3.8, Ha-1), 4.61 (m, He-3), 6.36 (d, J = 4.8, OH-3), 2.82 (dd, J = 12.0, 5.3, Ha-4), 8.45 (s,

OH-5), 6.25 (s, H-7), 6.81 (s, OH-9), 0.73 (s, CH_3-18), 1.13 (s, CH_3-19), 2.13 (m, H-20), 1.09 (d, J = 6.6, CH_3-21), 5.26 (dd, J = 15.4, 8.1, H-22), 5.31 (dd, J = 15.4, 7.3, H-23), 0.85 (d, J = 7.0, CH_3-26), 0.86 (d, J = 6.6, CH_3-27), 0.94 (d, J = 7.0, CH_3-28) [1]

^{13}C NMR (150 MHz, C_5D_5N) [1]:

Table 1

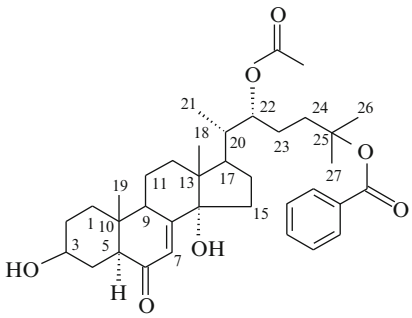
C-1	25.7	C-11	31.0	C-21	21.5
2	31.3	12	28.5	22	135.2
3	66.6	13	47.3	23	132.4
4	37.8	14	86.2	24	43.1
5	79.6	15	27.4	25	33.3
6	199.3	16	28.0	26	19.9
7	122.1	17	50.5	27	20.2
8	158.9	18	16.6	28	17.8
9	77.2	19	20.2		
10	42.8	20	40.4		

References

1. Y. Yaoita, K. Amemiya, H. Ohnuma, K. Furumura, A. Masaki, T. Matsuki, M. Kikichi, Chem. Pharm. Bull. **46**, 944 (1998)

Tomentesterone A

CAS Registry Number: 178405-18-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene tomentella* [1]

$C_{36}H_{50}O_7$: 594.3556

Mp: 139 – 140°C (MeOH–H_2O) [1]

IR (KBr) ν_{max} cm^{-1}: 3420, 1730, 1720, 1645, 1610, 1590, 1290, 1250, 1225, 715 [1]

EI-MS m/z: 576 $[M\text{-}H_2O]^+$ (0.8), 566 (0.5), 474 (46), 472 (10), 452 (46), 444 (46), 439 (9), 412 (46), 397 (46), 379 (11), 332 (30), 331 (35), 284 (100), 234 (13), 231 (12), 122 (50), 105 (45), 99 (46), 81 (47) [1]

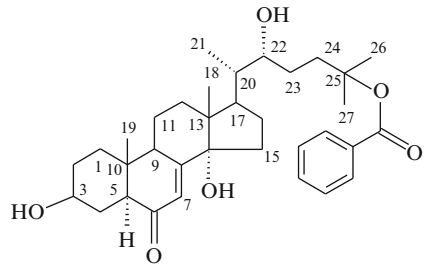
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.10 (m, H-3), 6.19 (d, J = 3.0, H-7), 0.74 (s, CH_3-18), 0.89 (s, CH_3-19), 1.13 (d, J = 6.5, CH_3-21), 5.34 (m, H-22), 1.60 (s, CH_3-26), 1.60 (s, CH_3-27), Other: 2.14 (s, CH_3COO-22), Ar: 7.48 (3H), 8.18 (2H) [1].

References

1. N.Sh. Ramazanov, E.S. Maksimov, Z. Saatov, N.D. Abdullaev, Chem. Nat. Comp. **31**, 600 (1995)

Tomentesterone B

CAS Registry Number: 181939-54-8



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene tomentella* [1]

$C_{34}H_{48}O_6$: 552.3451

Mp: 145 – 147°C (MeOH–H_2O) [1]

IR (KBr) ν_{max} cm^{-1}: 3429, 1712, 1662, 1584, 1292, 713 [1]

EI-MS m/z: 430 $[M\text{-}122]^+$ (24), 415 (24), 412 (44), 397 (24), 379 (24), 332 (44), 284 (84), 234 (82), 122 $[C_7H_6O_2]^+$ (100), 105 $[C_7H_5O]^+$ (66), 99 (32), 77 $[C_6H_5]^+$ (42) [1]

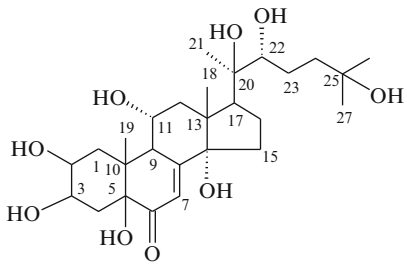
^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.09 (m, H-3), 6.16 (d, J = 3.0, H-7), 0.71 (s, CH_3-18), 0.89 (s, CH_3-19), 1.30 (d, J = 6.0, CH_3-21), 4.09 (m, H-22), 1.65 (s, CH_3-26), 1.65 (s, CH_3-27), Other: Ar: 7.49 (3H), 8.22 (2H) [1].

References

1. N.Sh. Ramazanov, E.S. Maksimov, Z. Saatov, N.D. Abdullaev, Chem. Nat. Comp. **32**, 47 (1996)

5β,11α,20-Trihydroxyecdysone

CAS Registry Number: 1040923-81-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Dioscorea dumetorum* [1]

$C_{27}H_{44}O_9$: 512.2985

Mp: amorphous [1]

$[\alpha]_D^{20}$ − 55.6° (c 0.048, CH_3OH) [1]

IR ($CHCl_3$) ν_{max} cm^{-1}: 3373, 3055, 2371, 1683, 1227 [1]

HR-ESI-MS m/z: for $C_{27}H_{44}O_9Na$ $[M + Na]^+$ calcd. 535.6226, found 535.6231 [1]

FAB-MS m/z: 511 $[M-H]^-$ [1]

^{1}H NMR (600 MHz, J/Hz, C_5D_5N): 3.14 (Ha-1), 2.17 (He-1), 4.60 (m, Ha-2), 4.60 (m, He-3), 2.18 (Ha-4), 1.70 (He-4), 6.12 (s, H-7), 3.78 (m, H-9), 4.43 (m, H-11), 2.76 (t, J = 11.5, Ha-12), 2.51 (m, He-12), 1.90 (Ha-15), 1.98 (Hb-15), 1.98 (Ha-16), 2.23 (Hb-16), 2.84 (t, J = 9.0, H-17), 1.00 (s, CH_3-18), 2.10 (s, CH_3-19), 1.43 (s, CH_3-21), 3.74 (m, H-22), 1.92 (Ha-23), 2.13 (Hb-23), 1.70 (Ha-24), 2.18 (Hb-24), 1.26 (s, CH_3-26), 1.30 (s, CH_3-27) [1]

^{13}C NMR (150 MHz, C_5D_5N) [1]:

Table 1

C-1	34.7	C-10	45.0	C-19	23.8
2	67.5	11	69.0	20	76.7
3	69.0	12	43.0	21	20.6
4	41.5	13	47.5	22	77.1
5	79.6	14	83.7	23	35.5
6	201.0	15	30.8	24	41.5
7	120.2	16	20.7	25	69.8
8	164.1	17	49.2	26	29.1
9	45.3	18	18.3	27	29.1

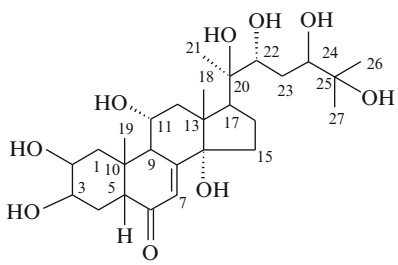
Pharm./Biol.: *Candida* tests: Not active (MIC > 200 μg/ml) [1].

References

1. M. Santour, F. Canon, T. Miyamoto, A. Dongmo, M.A. Lacaille-Dubois, Biochem. Sys. Ecol. **36**, 559 (2008)

11α,20,24-Trihydroxyecdysone

CAS Registry Number: 280116-12-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Vitex canescens* [1]

$C_{27}H_{44}O_9$: 512.2985

IR (KBr) ν_{max} cm^{-1}: 3408, 2967, 1654, 1384, 1052 [1]

HR-FAB-MS m/z: for $C_{27}H_{44}O_9$ $[M-H]^-$ calcd. 511.2907, found 511.2912 [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 3.43 (dd, J = 3.8, 12.5, H-1), 4.57 (m, Ha-2), 4.20 (br s, He-3), 3.00 (dd, J = 3.2, 12.7, H-5), 6.25 (d, J = 2.0, H-7), 3.84 (br d, J = 7.0, H-9), 4.60 (m, H-11), 3.04 (H-12), 3.16 (t, J = 9.1, H-17), 1.26 (s, CH_3-18), 1.29 (s, CH_3-19), 1.61 (s, CH_3-21), 4.50 (br d, J = 8.6, H-22), 4.35 (br d, J = 8.8, H-24), 1.45 (s, CH_3-26), 1.45 (s, CH_3-27) [1]

^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

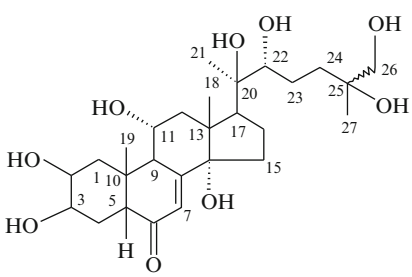
C-1	39.64	C-10	39.31	C-19	24.65
2	68.19	11	68.63	20	76.62
3	67.94	12	43.96	21	21.47
4	32.61	13	48.00	22	73.53
5	52.25	14	84.06	23	35.00
6	203.73	15	31.64	24	75.73
7	122.00	16	21.18	25	72.40
8	164.11	17	49.73	26	25.85
9	42.54	18	18.72	27	25.92

References

1. A. Suksamrarn, N. Promrangsan, A. Jintasirikul, Phytochemistry **53**, 921 (2000)

11α,20,26-Trihydroxyecdysone

CAS Registry Number: 280116-13-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Vitex canescens* [1]

$C_{27}H_{44}O_9$: 512.2985

IR (KBr) ν_{max} cm^{-1}: Epimer 1: 3448, 2952, 1660, 1385, 1053; Epimer 2: 3448, 2927, 1660, 1385, 1053 [1]

HR-FAB-MS m/z: for $C_{27}H_{44}O_9$ $[M-H]^-$ calcd. 511.2907, found 511.2906 (Epimer 1), 511.2908 (Epimer 2) [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N) (Epimer 1): 3.43 (dd, J = 3.5, 12.4, H-1), 4.58 (m, Ha-2), 4.20 (br s, He-3), 3.00 (H-5), 6.28 (d, J = 2.0, H-7), 3.85–3.89 (H-9), 4.58 (m, H-11), 3.02 (H-12), 3.09 (t, J = 9.1, H-17), 1.24 (s, CH_3-18), 1.30 (s, CH_3-19), 1.56 (s, CH_3-21), 3.85–3.89 (H-22), 3.85–3.89 (H-26), 1.45 (s, CH_3-27) [1]

^{1}H NMR (400 MHz, J/Hz, C_5D_5N) (Epimer 2): 3.44 (dd, J = 3.5, 12.5, H-1), 4.58 (m, Ha-2), 4.21 (br s, He-3), 3.00 (H-5), 6.28 (br s, H-7), 3.85–3.89 (H-9), 4.58 (m, H-11), 3.02 (H-12), 3.09 (t, J = 8.9, H-17), 1.24 (s, CH_3-18), 1.30 (s, CH_3-19), 1.55 (s, CH_3-21), 3.85–3.89 (H-22), 3.85–3.89 (H-26), 1.44 (s, CH_3-27) [1]

^{13}C NMR (100 MHz, C_5D_5N) (Epimer 1): **^{13}C NMR** (100 MHz, C_5D_5N) (Epimer 2):

Table 1

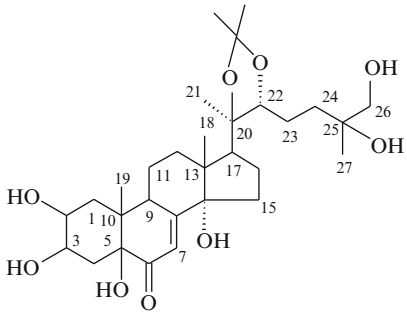
C-1	39.65	C-15	31.65	C-1	39.64	C-15	31.65
2	68.20	16	21.40	2	68.20	16	21.41
3	67.94	17	49.78	3	67.94	17	49.78
4	32.64	18	18.68	4	32.66	18	18.68
5	52.26	19	24.65	5	52.26	19	24.65
6	203.74	20	76.62	6	203.76	20	76.61
7	122.02	21	21.29	7	122.01	21	21.32
8	164.07	22	77.39	8	164.09	22	77.43
9	42.53	23	26.57	9	42.53	23	26.51
10	39.30	24	37.35	10	39.30	24	37.31
11	68.62	25	72.41	11	68.62	25	72.37
12	43.93	26	70.63	12	43.93	26	70.44
13	47.96	27	24.32	13	47.96	27	24.52
14	84.01			14	84.01		

References

1. A. Suksamrarn, N. Promrangsan, A. Jintasirikul, Phytochemistry **53**, 921 (2000)

5,20,26-Trihydroxyecdysone-20,22-Acetonide

CAS Registry Number: 1039035-97-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *S. viridiflora* [1]

$C_{30}H_{48}O_9$: 552.3298

$[\alpha]_D^{25}$ + 89° (c 0.05, MeOH) [1]

UV λ_{max}^{MeOH} nm: 242 (log ε 3.76) [1]

ESI-MS m/z: 575 $[M + Na]^+$ (46), 553 $[M + H]^+$ (100), 537 $[M\text{-}CH_3]^+$ (5), 535 $[M + H–H_2O]^+$ (2), 520 $[M + H–H_2O–CH_3]^+$ (2), 495 [M + H-acetone]$^+$ (59), 481 (1), 477 (3), 437 (3), 359 (3), 328 (14) [1]

HR-ESI-MS m/z: for $C_{30}H_{49}O_9$ $[M + H]^+$ calcd. 553.3363, found 553.3366 [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.73 (m, Ha-1), 1.73 (m, He-1), 3.95 (ddd, J = 10.0, 7.4, 3.6, He-2), 3.99 (q, J = 3.0, He-3), 2.075 (dd, J = 14.7, 3.0, Ha-4), 1.77 (dd, J = 14.9, 3.0, He-4), 5.86 (d, J = 2.8, H-7), 3.19 (ddd, J = 11.3, 7.0, 2.7, H-9), 1.74 (m, Ha-11), 1.81 (m, Hb-11), 2.12 (td, J = 13.1, 5.0, Ha-12), 1.86 (m, He-12), 1.61 (m, Ha-15), 1.96 (dd, J = 12.4, 6.5, Hb-15), 1.87 (m, Ha-16), 2.03 (m, Hb-16), 2.31 (dd, J = 9.4, 8.1, H-17), 0.83 (s, CH_3-18), 0.915 (s, CH_3-19), 1.18 (s, CH_3-21), 3.695 (t, J = 6.0, H-22), 1.53 (m, Ha-23), 1.55 (m, Hb-23), 1.52 (m, Ha-24), 1.71 (m, Hb-24), 3.355 (d, J = 11.0, Ha-26), 3.375 (d, J = 11.0, Hb-26), 1.15 (s, CH_3-27), Other: 1.32 and 1.39 (s, 20,22-iPr) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

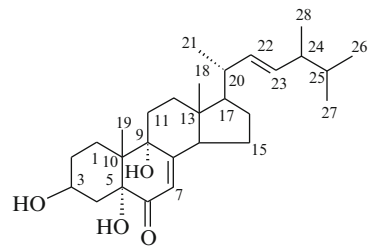
C-1	34.3	C-11	22.65	C-21	22.7
2	68.6	12	32.6	22	83.6
3	70.4	13	48.7	23	24.0
4	36.3	14	85.3	24	37.2
5	80.4	15	31.8	25	73.6
6	202.5	16	22.5	26	70.7
7	120.7	17	50.5	27	23.9
8	167.4	18	17.8	20,22-iPr	27.3
9	39.2	19	17.1		29.5
10	45.5	20	86.0		108.2

References

1. N. Toth, A. Simon, G. Toth, Z. Kele, A. Hunyadi, M. Bathori, J. Nat. Prod. **71**, 1461 (2008)

3β,5α,9α-Trihydroxyergosta-7,22-Diene-6-one

CAS Registry Number: 88191-14-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Agaricus blazei* [1], *Hericum erinacens* [2], *Polyporus versicolor* [3]

$C_{28}H_{44}O_4$: 444.3239

Mp: 226–230°C ($CHCl_3$-hexane) [1], 225–228 C [3]

$[\alpha]_D^{20}$ −60° (c 0.14, $CHCl_3$) [1], $[\alpha]_D^{28}$ −64° (c, 0.056, $CHCl_3$) [3]

IR (KBr) ν_{max} cm^{-1}: 3400, 1670, 1620 [1], 3440, 1678, 1071, 998, 968, 758 [2]

IR ($CDCl_3$) ν_{max} cm^{-1}: 3590, 3400, 1670, 1620 [3]

UV λ_{max}^{EtOH} nm (ε): 236 (7200) [2], 237 (10000) [3]

EI-MS m/z: 426 $[M\text{-}H_2O]^+$, 390 $[M\text{-}3H_2O]^+$ [1], 444 $[M]^+$ (0.4), 426 $[M\text{-}H_2O]^+$ (34.1), 408 $[M\text{-}2H_2O]^+$ (9.6), 390 $[M\text{-}3H_2O]^+$ (4.0), 369 (65.6), 300 (31.1), 81 (66.0), 69 (100), 55 (99.7) [2], 426 $[M\text{-}H_2O]^+$, 408 $[M\text{-}2H_2O]^+$, 390 $[M\text{-}3H_2O]^+$, 300 $[M\text{-}H_2O\text{-}C_9H_{18}]^+$, 282 $[M\text{-}2H_2O\text{-}C_9H_{18}]^+$ [3]

FAB-MS m/z: 467 $[M + Na]^+$ [2]

HR-MS m/z: for $C_{28}H_{44}O_4$ $[M + H]^+$ calcd. 444.3240, found 444.3209 [2]

FD-MS m/z: 444 $[M]^+$ (100) [1]

^{1}H NMR (400 MHz, J/Hz, $CDCl_3$): 4.06 (m, H-3), 5.65 (d, J = 2.25, H-7), 0.62 (s, CH_3-18), 1.01 (s, CH_3-19), 1.03 (d, J = 6.54, CH_3-21), 5.16 (dd, J = 7.89, 15.10, H-22), 5.24 (dd, J = 7.32, 15.10, H-23), 0.82 (d, J = 6.67, CH_3-26), 0.84 (d, J = 6.54, CH_3-27), 0.92 (d, J = 6.76, CH_3-28) [1]

^{1}H NMR (J/Hz, $CDCl_3$): 4.06 (m, H-3), 5.65 (d, J = 1.9, H-7), 0.61 (s, CH_3-18), 1.01 (s, CH_3-19), 1.02 (d, J = 6.5, CH_3-21), 0.82 (d, J = 6.8, CH_3-26), 0.83 (d, J = 6.8, CH_3-27), 0.91 (d, J = 6.8, CH_3-28) [3]

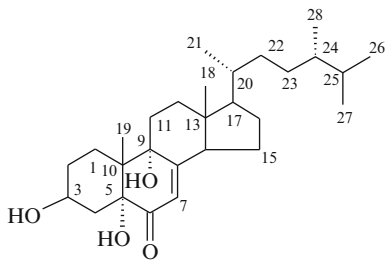
Pharm./Biol.: *HeLa* cells bioassay: showed growth inhibition of *HeLa* cells in concentration 8 μg/ml [1], *Hepatoma* cell biotest: cytotoxic activity [2].

References

1. H. Kawagishi, R. Katsumi, T. Sazawa, T. Mizuno, T. Hagiwara, T. Nakamura, Phytochemistry **27**, 2777 (1988)
2. Y. Takashi, M. Uda, T. Ohashi, K. Nakano, K. Murakami, T. Tomimatsu, Phytochemistry **30**, 4117 (1991)
3. J. Valisolalao, B. Luu, G. Ourisson, Tetrahedron **39**, 2779 (1983)

3β,5α,9α-Trihydroxy-(24S)-Ergost-7-en-6-one

CAS Registry Number: 211486-13-4



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Hypsizigus marmoreus, Lentinus edodes, Pholiota nameko, Pleurotus ostreatus* [1]

$C_{28}H_{46}O_4$: 446.3396

Mp: amorphous [1]

$[\alpha]_D^{28}$ −21.5° (c 0.09, $CHCl_3$) [1]

IR ($CHCl_3$) ν_{max} cm^{-1}: 3600, 3427, 1675, 1625 [1]

UV λ_{max}^{MeOH} nm (log ε): 236 (3.8) [1]

EI-MS m/z: 428 $[M\text{-}H_2O]^+$, 301 $[M\text{-}H_2O\text{-side-chain}]^+$, 265 $[M\text{-}3H_2O\text{-side-chain}]^+$ [1]

HR-MS m/z: for $C_{28}H_{44}O_3$ $[M\text{-}H_2O]^+$ calcd. 428.3290, found 428.3288 [1]

^{1}H NMR (270 MHz, J/Hz, $CDCl_3$): 4.06 (m, H-3), 5.67 (d, J = 2.0, H-7), 2.74 (m, H-14), 0.61 (s, CH_3-18), 1.02 (s, CH_3-19), 0.94 (d, J = 5.8, CH_3-21), 0.78 (d, J = 6.8, CH_3-26 or CH_3-28), 0.79 (d, J = 6.4, CH_3-26 or CH_3-28), 0.86 (d, J = 6.8, CH_3-27), 4.02 (br s, OH) [1]

^{1}H NMR (600 MHz, J/Hz, C_5D_5N): 2.84 (m, Ha-1), 4.65 (m, He-3), 2.84 (m, Ha-4), 2.35 (dd, J = 11.4, 13.9, He-4), 5.93 (d, J = 1.8, H-7), 2.97 (m, H-14), 0.61 (s, CH_3-18), 1.15 (s, CH_3-19), 0.94 (d, J = 5.9, CH_3-21), 0.81 (d, J = 6.6, CH_3-26), 0.87 (d, J = 6.6, CH_3-27), 0.80 (d, J = 6.2, CH_3-28), 6.33 (d, J = 4.8, OH-3), 8.62 (s, OH-5), 6.30 (s, OH-9) [1]

^{13}C NMR (150 MHz, C_5D_5N) [1]:

Table 1

C-1	26.5	C-11	29.0	C-21	19.2
2	31.5	12	35.5	22	33.8
3	66.8	13	45.5	23	31.0
4	38.2	14	51.9	24	39.3
5	79.8	15	22.8	25	31.7
6	199.2	16	28.0	26	17.7
7	120.3	17	56.3	27	20.7
8	164.2	18	12.2	28	15.6
9	75.0	19	20.4		
10	42.2	20	36.7		

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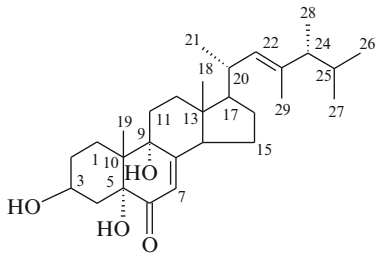
3β,5α,9α-Trihydroxy-(22E,24R)-23-Methyl-Ergosta-7,22-dien-6-one

CAS Registry Number: 211486-12-3



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Lentinus edodes* [1]

$C_{29}H_{46}O_4$: 458.3396

Mp: amorphous

$[\alpha]_D^{18}$ −40.0° (c 0.05, $CHCl_3$) [1]

IR ($CHCl_3$) ν_{max} cm^{-1}: 3588, 3413, 1676, 1626 [1]

UV λ_{max}^{MeOH} nm (log ε): 297 (4.0) [1]

EI-MS m/z: 404 $[M\text{-}3H_2O]^+$, 265 [M-3H_2O-side-chain]$^+$ [1]

HR-MS m/z: for $C_{29}H_{46}O_4$ $[M]^+$ calcd. 458.3396, found 458.3384 [1]

^{1}H NMR (270 MHz, J/Hz, $CDCl_3$): 4.02 (m, H-3), 5.67 (d, J = 2.1, H-7), 2.74 (m, H-14), 0.64 (s, CH_3-18), 1.03 (s, CH_3-19), 0.96 (d, J = 6.6, CH_3-21), 4.91 (d, J = 9.9, H-22), 0.85 (d, J = 6.4, CH_3-26), 0.79 (d, J = 6.4, CH_3-27), 0.94 (d, J = 6.8, CH_3-28), 1.514 (d, J = 1.3, CH_3-29), 3.03 (br s, OH), 4.02 (br s, OH) [1]

^{1}H NMR (600 MHz, J/Hz, C_5D_5N): 2.83 (m, Ha-1), 4.65 (m, He-3), 2.83 (m, Ha-4), 2.35 (dd, J = 11.4, 14.3, He-4), 5.95 (d, J = 1.8, H-7), 3.00 (m, H-14), 0.68 (s, CH_3-18), 1.15 (s, CH_3-19), 1.00 (d, J = 6.6, CH_3-21), 0.85 (d, J = 6.2, CH_3-26), 0.82 (d, J = 6.6, CH_3-27) 0.96 (d, J = 7.3, CH_3-28), 1.51 (s, CH_3-29), 6.34 (d, J = 4.8, OH-3), 8.63 (s, OH-5), 6.32 (br s, OH-9) [1]

^{13}C NMR (150 MHz, C_5D_5N) [1]:

Table 1

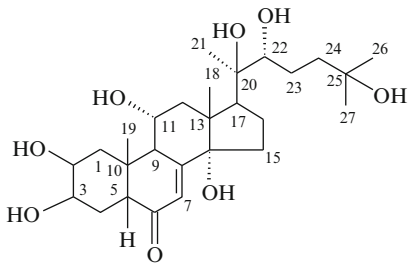
C-1	26.4	C-11	29.0	C-21	20.3
2	31.5	12	35.5	22	131.6
3	66.8	13	45.4	23	135.6
4	38.2	14	52.0	24	50.4
5	79.8	15	22.7	25	31.0
6	199.2	16	27.8	26	21.0
7	120.3	17	57.0	27	22.0
8	164.2	18	12.5	28	17.2
9	75.1	19	20.4	29	13.3
10	42.3	20	35.0		

References

1. Y. Yaoita, K. Amemiya, H. Ohnuma, K. Furumura, A. Masaki, T. Matsuki, M. Kikuchi, Chem. Pharm. Bull. **46**, 944 (1998)

Turkesterone

CAS Registry Number: 41451-87-0



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga turkestanica* [1], *Blandfordia punicea* [2], *Cyanotis arachnoidea* [3], *Leuzea carthamoides* [4], *Rhaponticum uniflorum* [5], *Sida spinosa* [6], *Silene linicola* [7], *Tapinella panuoides* [8], *Vitex canescens* [9], *V. fisherii* [10], *V. glabrata* [11], *V. polygama* [12], *V. scabra* [13]

$C_{27}H_{44}O_8$: 496.3036

Mp: amorphous [1, 6], 173–175°C [6]

$[\alpha]_D^{20}$ + 52.0° (c 1.46, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}:3300–3500, 1660 [1], 3414, 1658, 1446, 1381, 1053, 957, 880 [5], 3433, 1657, 1052 [8]

UV λ_{max}^{EtOH} nm (log ε): 244 (3.95) [1]

UV λ_{max}^{MeOH} nm (log ε): 241 (3.96) [5]

EI-MS m/z: 460, 442, 424, 409, 379, 361, 343, 325, 300, 143, 125, 99, 81, 69 [1], 442 $[M\text{-}3H_2O]^+$ (3), 361 (12), 343 (23), 325 (20), 301 (4), 300 (7), 267 (16), 249 (4), 231 (2), 216 (20), 213 (7), 143 (12), 125 (11), 99 (27), 81 (29), 69 (24), 43 (100) [5], 463 $[M + H\text{–}2H_2O]^+$ (6), 443 (6), 442 (6), 423 (18), 379 (18), 368 (16), 361 (6), 354 (10), 343 (5), 71 (100) [6]

FAB-MS m/z: 520 $[M + H + Na]^+$, 495 $[M\text{-}H]^-$ [5], 519 $[M + Na]^+$ (100), 497 $[M + H]^+$ (66), 479 $[M + H\text{-}H_2O]^+$ (84), 461 $[M + H\text{–}2H_2O]^+$ (89), 443 $[M + H\text{–}3H_2O]^+$ (78), 425 $[M + H\text{–}4H_2O]^+$ (36) [8]

HR-MS m/z: for $C_{27}H_{45}O_8$ $[M + H]^+$ calcd. 497.3114, found 497.3101 [8]

^{1}H NMR (100 MHz, C_5D_5N): 4.45 (m, H-2), 4.06 (m, H-3), 6.12 (s, H-7), 3.75 (m, H-9), 4.45 (m, H-11), 1.12 (s, CH_3-18), 1.18 (s, CH_3-19), 1.45 (s, CH_3-21), 3.75 (m, H-22), 1.24 (s, CH_3-26), 1.24 (s, CH_3-27) [1]

^{1}H NMR (300 MHz, J/Hz, DMSO): 1.19 (t, J = 7.0, Ha-1), 2.42 (dd, J = 4.0, 12.5, He-1), 3.85 (Ha-2), 3.75 (He-3), 1.52 (Ha-4), 1.62 (t, J = 4.0, He-4), 2.18 (dd, J = 3.5, 13.0, H-5), 5.63 (d, J = 2.4, H-7), 3.01 (dd, J = 3.1, 10.0, H-9), 4.11 (m, H-11), 2.03 (dd, J = 10.0, 12.0, Ha-12), 1.98 (dd, J = 6.0, 12.0, He-12), 1.78 (Ha-15), 1.49 (Hb-15), 1.85 (Ha-16), 1.68 (Hb-16), 2.25 (dd, J = 3.9, 12.6, H-17), 0.76 (s, CH_3-18), 0.84 (s, CH_3-19), 1.05 (s, CH_3-21), 3.14 (dd, J = 1.8, 10.0, H-22), 1.13 (t, J = 7.0, Ha-23), 1.52 (Hb-23), 1.70 (Ha-24), 1.23 (t, J = 10.0, Hb-24), 1.05 (s, CH_3-26), 1.08 (s, CH_3-27) [6]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.38 (dd, J = 12.3, 13.0, Ha-1), 2.59 (dd, J = 4.3, 13.0, He-1), 4.01 (ddd, J = 3.4, 4.3, 12.0, Ha-2), 3.95 (q, J = 2.9, He-3), 1.78 (Ha-4), 1.68 (dt, J = 3.7, 3.7, 14.2, He-4), 2.33 (dd, J = 3.9, 13.2, H-5), 5.80 (dd, J = 1.0, 2.6, H-7), 3.15 (dd, J = 2.6, 9.0, H-9), 4.10 (ddd, J = 6.2, 9.0, 10.6, H-11), 2.22 (dd, J = 10.6, 12.4, Ha-12), 2.16 (dd, J = 6.2, 12.4, He-12), 1.95 (Ha-15), 1.58 (Hb-15), 2.00 (Ha-16), 1.75 (Hb-16), 2.43 (H-17), 0.877 (s, CH_3-18), 1.057 (s, CH_3-19), 1.193 (s, CH_3-21), 3.32 (dd, J = 1.8, 11.0, H-22), 1.66 (Ha-23), 1.29 (Hb-23), 1.80 (Ha-24), 1.43 (ddd, J = 4.3, 11.6, 13.6, Hb-24), 1.206 (s, CH_3-26), 1.220 (s, CH_3-27) [8]

^{1}H NMR (400 MHz, C_5D_5N): 3.46 (H-1), 4.60 (Ha-2), 4.22 (He-3), 3.10 (H-5), 6.32 (H-7), 3.62 (H-9), 4.60 (H-11), 3.05 (Ha-12), 2.83 (He-12), 1.33 (s, CH_3-18), 1.28 (s, CH_3-19), 1.59 (s, CH_3-21), 3.62 (H-22), 5.54 (H-24), 1.37 (s, CH_3-26), 1.37 (s, CH_3-27) [10]

^{13}C NMR (75 MHz, DMSO) [6]: **^{13}C NMR** (125.7 MHz, CD_3OD) [8]:

Table 1

C-1	36.6	C-15	31.2	C-1	39.09	C-15	31.86
2	66.9	16	20.6	2	68.94	16	21.52
3	67.1	17	49.0	3	68.57	17	50.35
4	31.8	18	17.5	4	33.28	18	18.89
5	50.4	19	24.1	5	52.78	19	24.62
6	203.5	20	76.5	6	206.66	20	77.83
7	120.7	21	21.2	7	122.74	21	21.02
8	165.9	22	76.6	8	165.74	22	78.42
9	40.9	23	26.4	9	42.94	23	27.35
10	38.0	24	41.6	10	39.91	24	42.40
11	69.2	25	69.3	11	69.51	25	71.29
12	41.5	26	29.2	12	43.79	26	29.73
13	47.2	27	30.1	13		27	28.95
14	83.4			14	84.87		

^{13}C NMR (100 MHz, C_5D_5N) [10]:

Table 2

C-1	39.9	C-10	39.5	C-19	24.9
2	68.1	11	68.8	20	76.8
3	68.4	12	44.2	21	21.6
4	32.9	13	48.2	22	77.5
5	52.5	14	84.2	23	27.5
6	203.0	15	32.0	24	42.6
7	122.0	16	21.5	25	69.5
8	164.0	17	50.0	26	30.0
9	42.8	18	19.0	27	30.1

Pharm./Biol.: *Galleria mellonella* bioassay: ED_{50} = 62.5 μg/g, *Sarcophaga bullata* bioassay: ED_{50} = 0.3 μg/g, *Dermestes vulpinus* bioassay: ED_{50} = 4.2 μg/g [14], *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 1.3 \times 10^{-6}$ M, $EC_{50} = 3.0 \times 10^{-7}$ M [15–17], antidiabetic activity [18, 19], anabolic activity [20–22].

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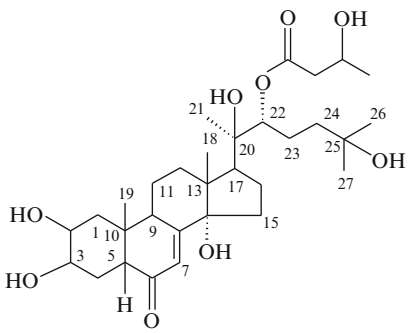
Venustone

CAS Registry Number: 166197-90-6



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Penstemon venustus* [1]

$C_{31}H_{50}O_9$: 566.3454

$[\alpha]_D^{23}$ + 57° (c 2.0, MeOH) [1]

EI-MS m/z: 530 $[M\text{-}2H_2O]^+$ (0.5), 512 (0.9), 494 (1), 468 (2), 444 (2), 426 (11), 387 (6), 363 (32), 345 (100), 327 (40), 285 (18), 269 (16), 215 (16), 173 (19), 99 (51), 81 (28), 69 (40), 45 (56) [1]

FAB-MS m/z: 565 $[M\text{-}H]^-$ (7), 479 (12), 183 (100), 103 (20), 91 (43) [1]

^{1}H NMR (500 MHz, J/Hz, CD_3OD): 1.42 (Ha-1), 1.79 (He-1), 3.83 (Ha-2), 3.94 (He-3), 1.70 (Ha-4), 1.70 (He-4), 2.38 (H-5), 5.80 (d, J = 2.0, H-7), 3.15 (Ha-9), 1.69 (Ha-11), 1.81 (He-11), 2.15 (ddd, J = 13.1, 13.1, 4.9, Ha-12), 1.86 (He-12), 1.95 (Ha-15), 1.61 (Hb-15), 2.03 (Ha-16), 1.75 (Hb-16), 2.38 (H-17), 0.87 (s, CH_3-18), 0.95 (s, CH_3-19), 1.28 (s, CH_3-21), 4.92 (H-22), 1.14 (Ha-23), 1.47 (Hb-23), 1.77 (Ha-24), 1.42 (Hb-24), 1.17 (s, CH_3-26), 1.15 (s, CH_3-27), Other: 2.43 (dd, J = 15.1, 8.3, H-2'a), 2.57 (dd, J = 15.1, 4.8, H-2'b), 4.23 (H-3'), 1.23 (d, J = 6.2, CH_3-4') [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

C-1	37.4	C-12	32.6	C-23	26.1
2	68.7	13	48.7	24	41.5
3	68.5	14	85.2	25	71.0
4	32.8	15	31.8	26	29.5
5	51.8	16	21.5	27	28.9
6	206.4	17	50.8	ac1'	173.5
7	122.2	18	18.1	ac2'	45.2
8	167.8	19	24.4	ac3'	65.6
9	35.1	20	77.6	ac4'	23.2
10	39.3	21	21.9		
11	21.5	22	80.8		

References

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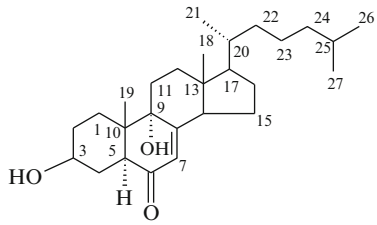
Viperidone

CAS Registry Number: 861-63-2



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Wilcoxia viperina* [1]
$C_{27}H_{44}O_3$: 416.3290
Mp: 208–210°C (MeOH–H_2O) [1]
$[\alpha]_D^2$ −49.1° (c 1.12) [1]
UV λ_{max}^{EtOH} nm (ε): 237 (10780) [1]
IR (KBr) ν_{max} cm^{-1}: 1660 [1]

References

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Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates
Biological sources: *Vitex fisherii* [1]
$C_{27}H_{42}O_7$: 478.2930
IR (KBr) ν_{max} cm^{-1}: 3400, 1655 [1]
UV λ_{max}^{MeOH} nm: 234 [1]
EI-MS m/z: 461 $[M + H–H_2O]^+$ [1]
^{1}H NMR (400 MHz, J/Hz, C_5D_5N): 3.44 (Ha-1), 4.60 (Ha-2), 4.22 (He-3), 3.03 (H-5), 6.29 (H-7), 3.88 (H-9), 4.60 (He-11), 3.03 (Ha-12), 2.71 (He-12), 1.33 (CH_3-18), 1.26 (CH_3-19), 1.59 (CH_3-21), 3.88 (H-22), 5.53 (H-24), 1.59 (CH_3-26), 1.66 (CH_3-27) [1]
^{13}C NMR (100 MHz, C_5D_5N) [1]:

Table 1

C-1	39.9	C-10	39.5	C-19	24.9
2	68.2	11	68.9	20	76.9
3	68.9	12	44.1	21	21.5
4	32.9	13	48.2	22	76.7
5	52.5	14	84.2	23	31.8
6	203.6	15	31.9	24	123.7
7	122.3	16	21.5	25	131.9
8	164.2	17	50.0	26	18.0
9	42.8	18	19.0	27	25.9

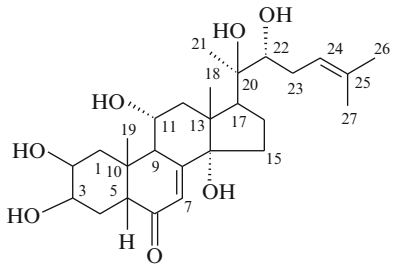
Pharm./Biol.: *Pectinophora gossypiella* test: growth inhibition in larvae [1].

References

1. I. Kubo, Y. Asaka, M.J. Stout, T. Nakatsu, J. Chem. Ecol. **16**, 2581 (1990)

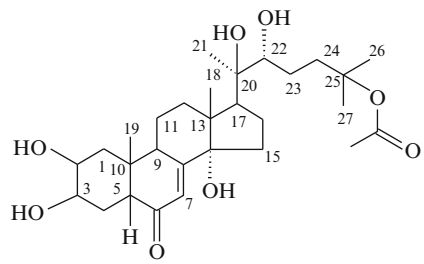
Vitexirone

CAS Registry Number: 130369-79-8



Viticosterone E

CAS Registry Number: 22033-96-1



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Ajuga reptans* [1], *Dianthus hoeltzeri* [2], *Coronaria coreacea* [3], *Lychnis flos-cuculi* [4], *L. chalcedonica* [5], *Serratula centauroides* [6], *S. coronata* [7, 8], *S. procumbens* [6], *S. sogdiana* [9], *S. tinctoria* [10], *Silene brachuica* [11], *S. linicola* [12], *S. praemixta* [13], *S. tomentella* [14], *S. wallichiana* [15], *Vitex agnus-castus* [16], *V. megapotamica* [17]

$C_{29}H_{46}O_8$: 522.3193

Mp: 196–198°C (acetone) [2, 5], 196–198°C (acetone-hexane) [7], 197–198°C (acetone) [9], 195–196°C [12], 194–196°C (acetone) [15], 198–199°C [17]

$[\alpha]_D^{20}$ + 59.7 ± 2° (c 0.87, MeOH) [2], $[\alpha]_D$ + 58.9 ± 2° (c 0.72, MeOH) [5], $[\alpha]_D^{20}$ + 60.1 ± 2° [7], $[\alpha]_D$ + 60° (c 1.31, MeOH) [9], $[\alpha]_D^{22}$ + 59.2 ± 2° (c 0.5, MeOH) [12], $[\alpha]_D^{20}$ + 58.6 ± 2° (c 0.52, MeOH) [15], $[\alpha]_D^{22}$ + 59.8 ± 2° (c, MeOH) [16]

IR (KBr) ν_{max} cm^{-1}: 3400, 1725, 1655, 1275 [2], 3430, 1730, 1670, 1275 [5], 3400, 1660, 1725 [7], 3400, 1725, 1660 [9], 3430–3450, 1730, 1670, 1275 [12], 3430, 1730, 1670, 1275 [16], 1720, 1650, 1615 [17], 3428, 2950, 1725, 1709, 1648, 1444, 1370, 1277, 1207, 1127, 1056, 1022, 950, 876 [18]

UV λ_{max}^{EtOH} nm (log ε): 245 (4.00) [7, 9]

EI-MS m/z: 522 $[M]^+$, 462, 444, 426, 411, 408, 393, 375, 363, 301, 99, 81 [5], 444 $[M\text{-}CH_3COOH\text{–}H_2O]^+$, 426, 411, 408, 393, 375, 363, 345, 327, 310, 301, 300, 99, 81 [9], 504 $[M\text{-}H_2O]^+$, 486, 468, 462 $[M\text{-}CH_3COOH]^+$, 444, 426, 411, 408, 393, 363, 345, 300, 99, 81 [17], 444 $[M\text{-}CH_3COOH\text{-}H_2O]^+$, 426 $[M\text{-}CH_3COOH\text{-}2H_2O]^+$ (0.7), 363 (27), 345 (88), 327 (36), 309 (13), 203 (2), 185 (6), 159 (8), 143 (14), 141 (2), 125 (16), 117 (3), 99 (36), 81 (39) [18]

^{1}H NMR (500 MHz, J/Hz, D_2O): 1.38 (t, J = 13.0, Ha-1), 1.88 (m, He-1), 3.99 (m, Ha-2), 4.07 (m, He-3), 1.75 (t, Ha-4), 1.75 (t, He-4), 2.34 (t, H-5), 5.97 (d, J = 2.0, H-7), 3.11 (m, H-9), 1.76 (m, Ha-11), 1.90 (m, He-11), 1.95 (m, Ha-12), 1.75 (m, He-12), 1.66 (m, Ha-15), 2.05 (m, Hb-15), 1.88 (m, Ha-16), 1.74 (m, Hb-16), 2.32 (t, J = 9.0, H-17), 0.87 (s, CH_3-18), 1.00 (s, CH_3-19), 1.234 (s, CH_3-21), 3.42 (br d, J = 10.0, H-22), 1.59 (m, Ha-23), 1.35 (m, Hb-23), 1.67 (m, Ha-24), 1.43 (s, CH_3-26), 1.49 (s, CH_3-27), 2.03 (s, Ac-25) [8]

^{1}H NMR ($CDCl_3$): 3.90-4.18 (m, H-2), 6.11 (br s, H-7), 1.09 (s, CH_3-18), 0.94 (s, CH_3-19), 1.48 (s, CH_3-21), 1.30 (s, CH_3-26), 1.38 (s, CH_3-27) [9]

^{1}H NMR (300 MHz, J/Hz, C_5D_5N): 4.16 (br d, J = 10.5, Ha-2), 4.23 (br s, He-3), 3.02 (dd, J = 3.5, 13.2, H-5), 6.24 (d, J = 2.2, H-7), 3.58 (m, H-9), 2.98 (t, J = 9.1, H-17), 1.21 (s, CH_3-18), 1.05 (s, CH_3-19), 1.60 (s, CH_3-21), 3.83 (br d, J = 10.0, H-22), 1.39 (s, CH_3-26), 1.46 (s, CH_3-27) [18]

^{13}C NMR (125 MHz, D_2O) [8]:

Table 1

C-1	36.4 (t)	C-11		C-21	20.6 (q)
2	68.5 (d)	12	32.0 (t)	22	78.5 (d)
3	68.2 (d)	13	48.3 (s)	23	
4	32.3 (t)	14	86.0 (s)	24	38.6 (t)
5	51.4 (d)	15		25	85.5 (s)
6		16		26	26.4 (q)
7	122.1 (d)	17	50.4 (d)	27	26.5 (q)
8		18	17.9 (q)	CH_3COO	23.0 (q)
9	34.9 (d)	19	24.2 (q)	CH_3COO	174.8 (s)
10	39.1 (s)	20	79.4 (s)		

Pharm./Biol.: *Drosophila melanogaster* B_{II} bioassay: $EC_{50} = 4.2 \times 10^{-8}$ M [8], $EC_{50} = 1.0 \times 10^{-7}$ M [19–21], Bioassay in rats: anabolic activity [22, 23].

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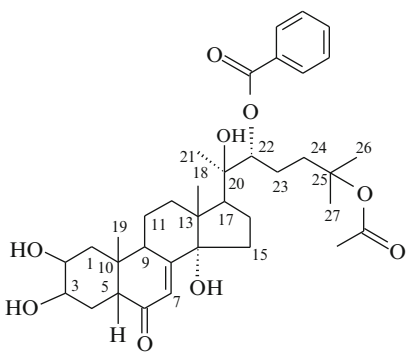
Viticosterone E-22-Benzoate

CAS Registry Number: 118201-53-9



Taxonomy: Physicochemical and Biological Properties of Phytoecdysteroids – Phytoecdysteroids and Their Conjugates

Biological sources: *Silene wallichiana* [1]

$C_{36}H_{50}O_9$: 626.3454

Mp: 147–149°C (CH_3OH-H_2O) [1]

$[\alpha]_D^{20}$ + 63.2 ± 2° (c 0.65, MeOH) [1]

IR (KBr) ν_{max} cm^{-1}: 3220–3300, 1730, 1660, 1610, 1585, 1285, 730 [1]

UV λ_{max}^{EtOH} nm (log ε): 234 (4.11) [1]

EI-MS m/z: 566 $[M\text{-}CH_3COOH]^+$ (0.2), 548 (0.6), 530 (0.7), 514 (0.3), 486 (0.5), 468 (2), 444 (6), 426 (40), 416 (10), 408 (23), 398 (5), 393 (13), 383 (4), 375 (13), 365 (12), 363 (13), 329 (12), 327 (12), 301 (23), 300 (23), 250 (60), 249 (30), 185 (12), 161 (23), 122 (100), 105 (80), 99 (16), 81 (26), 77 (43), 69 (27), 51 (27) [1]

^{1}H NMR (100 MHz, J/Hz, C_5D_5N): 4.00–4.14 (m, H-2), 4.00–4.14 (m, H-3), 6.12 (br s, H-7), 3.50 (m, H-9), 1.10 (s, CH_3-18), 0.98 (s, CH_3-19), 1.68 (s, CH_3-21), 5.54 (m, H-22), 1.30 (s, CH_3-26), 1.33 (s, CH_3-27), Other: 1.84 (s, CH_3COO-25), Ar: 7.34 (3H), 8.18 (2H) [1].

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