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Supporting Information

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Bisnorditerpene, Norditerpene and Lipo-alkaloids from *Aconitum toxicum*

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List of Supporting Information:

Table S1. ¹H NMR data for delavaconine, dolaconine, aconosine, and neolineine

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S1. Physical and spectroscopic data for delavaconitine, delavaconine, dolaconine, aconosine, and neolineine

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Table S1. ¹H NMR data for delavaconine, dolaconine, aconosine, and neolinine [500 MHz, CDCl₃, δ (ppm), (J = Hz)].

position	delavaconine	dolaconine	aconosine	neolinine
1	3.09 dd (10.9, 6.6)	3.13 dd (10.3, 6.6)	3.10 dd (9.4, 7.7)	3.69 s
2a	1.94 m	1.93 m	1.93 m	1.60 m
2b	2.16 m	2.20 m	2.15 m	1.50 m
3a	1.42 m	1.46 brt (13.0)	1.40 brt (13.0)	1.68 m
3b	1.75 m	1.80 m	1.75 m	1.68 m
4	1.69 m	1.66 brs	1.68 m	—
5	1.75 m	1.75 m	1.73 m	2.17 d (6.3)
6a	2.04 dd (13.2, 6.6)	2.10 m	2.14 m	4.23 m (1H)
6b	1.35 m	1.34 dd (14.5, 7.9)	1.32 dd (14.5, 7.8)	
7	2.22 m	2.20 m	2.18 m	2.02 s
9	2.42 m	2.33 t (5.6)	2.29 t (5.4)	2.21 t (6.0)
10	1.86 m	1.83 m	1.70 m	1.89 m
12a	2.20 m	2.07 m	1.83 m	2.05 m
12b	1.93 d (11.5)	1.94 m	1.75 m	1.74 dd (14.6, 5.0)
13	—	2.60 m	2.34 m	2.30 t (5.9, 6.8)
14	4.02 m	4.83 t (4.8)	4.15 t (5.0)	4.23 m
15a	2.51 dd (17.3, 9.0)	2.40 dd (16.1, 9.5)	2.43 dd (17.5, 8.6)	2.39 dd (15.9, 9.2)
15b	2.27 d (17.3)	1.90 m	2.07 d (17.5)	2.05 m
16	3.44 d (7.2)	3.20 dd (9.4, 4.8)	3.40 brd (8.6)	3.39 m
17	3.12 s	2.93 s (1H)	3.10 s	2.71 s (1H)
18a	—	—	—	3.72 d (10.7)
18b	—	—	—	3.52 d (10.7)
19a	2.61 d (11.5)	2.70 brd (10.5)	2.60 brd (11.4)	2.72 d (10.6)
19b	2.47 m	2.52 m	2.49 m	2.33 d (10.6)
20a	2.49 m	2.53 m (2H)	2.49 m (2H)	2.58 dq (12.4, 7.2)
20b	2.40 m			2.51 dq (12.4, 7.2)
21	1.07 t (7.2) (3H)	1.07 t (7.1) (3H)	1.06 t (7.1) (3H)	1.14 t (7.1) (3H)
OCH ₃ -1	3.26 s	3.23 s	3.34 s ^a	—
OCH ₃ -6	—	—	—	3.39 s
OCH ₃ -16	3.43 s	3.27 s	3.27 s ^a	3.35 s
OAc-14	—	2.05 s	—	—
OH-13	4.02 m	—	—	—

^a interchangeable signals

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S1. Physical and spectroscopic data for delavaconitine, delavaconine, dolaconine, aconosine, and neolinine

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Delavaconitine: amorphous solid; $[\alpha]_D^{27}$ -25 (*c* 0.1, CHCl₃); ¹H NMR and ¹³C NMR (CDCl₃), data identical with those published by Niitsu et al.¹³

Delavaconine: amorphous solid; $[\alpha]_D^{27}$ +5 (*c* 0.1, CHCl₃); ¹H NMR, see Table S1, Supporting Information; ¹³C NMR (CDCl₃, 125 MHz), data identical with those published by Niitsu et al.¹³

Dolaconine: amorphous solid; $[\alpha]_D^{27}$ +2 (*c* 0.01, CHCl₃); ¹H NMR: see Table S1, Supporting Information; ¹³C NMR (CDCl₃, 125 MHz), data identical with those published by Niitsu et al.¹³

Aconosine: amorphous solid; $[\alpha]_D^{27}$ -12 (*c* 0.2, CHCl₃); ¹H NMR, see Table S1, Supporting Information; ¹³C NMR (CDCl₃, 125 MHz), data identical with those published by Niitsu et al.¹³

Neolinine: amorphous solid; $[\alpha]_D^{27}$ +17 (*c* 0.1, CHCl₃); ¹H NMR, see Table S1, Supporting Information; ¹³C NMR (CDCl₃, 125 MHz) δ 12.3 (C-21), 29.3 (C-12), 29.7 (C-2), 29.8 (C-3), 39.0 (C-4), 40.2 (C-13), 42.8 (C-15), 44.2 (C-10), 47.1 (C-5), 48.3 (C-9), 48.5 (C-20), 49.7 (C-11), 51.6 (C-7), 56.3 (OMe-16), 56.7 (C-19), 57.9 (OMe-6), 63.9 (C-17), 71.2 (C-18), 72.1 (C-1), 74.0 (C-8), 75.9 (C-14), 81.7 (C-16), 82.5 (C-6).

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