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Saponins from *Chenopodium album*

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The isolation and spectral data of three saponins from the roots of *Chenopodium album* L. are reported. One of them is a *seco*-glycoside analogous to compounds that were previously found in species belonging to Caryophyllales.

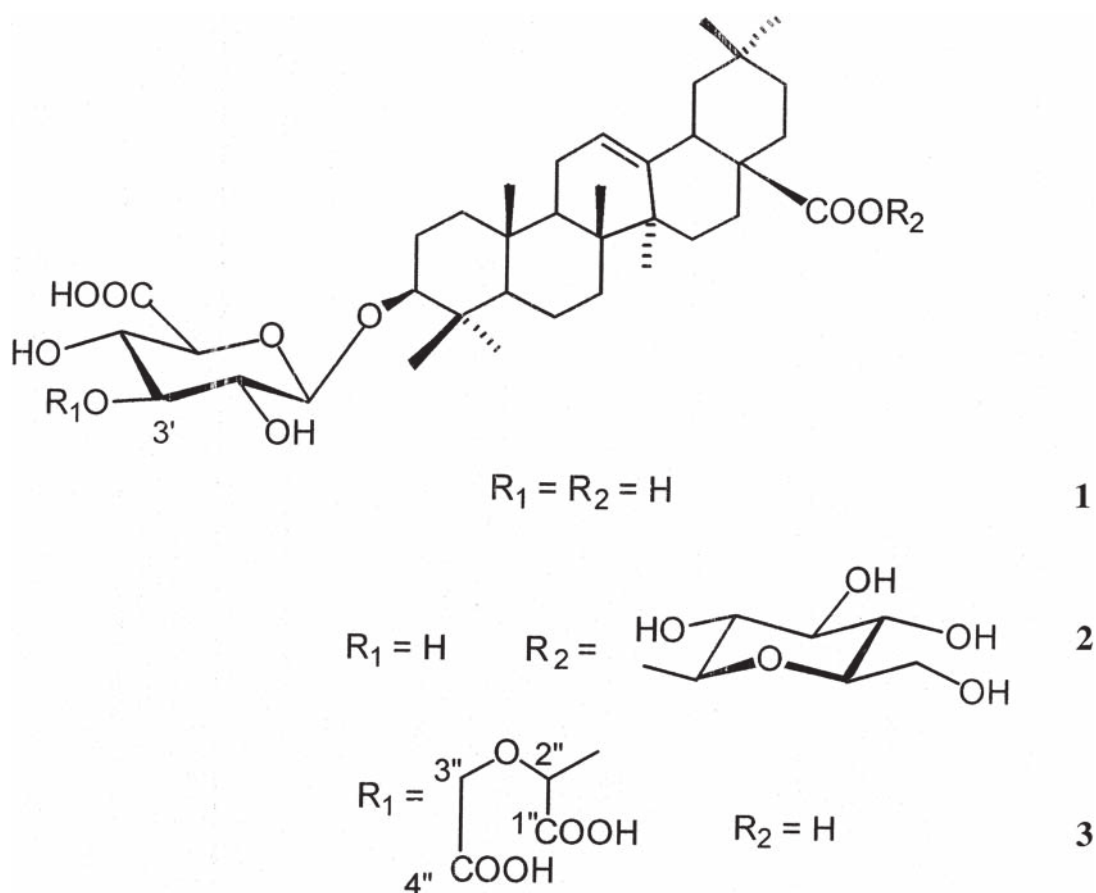
Keywords: *Chenopodium album*; Triterpenoids; Saponins; *Seco*-glycosides

Plant. *Chenopodium album* L. subsp. *album* (Chenopodiaceae) roots were collected in the Champagne region in France in July and August, 1996. It is also known as lamb's quarters and is one of most common agricultural weeds.

Uses and biological activity. Formerly, leaves were consumed as vegetable until replaced by spinach; seeds were ground to a flour and fruits were eaten by poultry 1. The young leaves are used as a salad for human consumption. Plant possesses diuretic, laxative and sedative properties, leaves are used as poultice 2.

Previously isolated classes of constituents. Betalain alkaloids, phenolic acids in fruits, betain and oxalic acid in leaves 3, oleanolic acid and sitosterol in flowers 4, furanocoumarins 5 and saponins from the seeds 6.

New-isolated constituents. 3-*O*- β -D-Glucuronopyranosyl oleanolic acid (1) or calenduloside E 7–9 (0.0013%), 3-*O*- β -D-glucuronopyranosyl-28-*O*- β -D-glucopyranosyl oleanolic acid (2) or chikusetsusaponin IVa 8–10 (0.0025), 3-*O*-3'-*O*-(2''-*O*-glycolyl)-glyoxylyl β -D-glucuronopyranosyl oleanolic acid (3) 9 (0.003).



Calenduloside E (1). $^1\text{H-NMR}$ (500 MHz, CD_3OD): δ 0.79 (1H, *brd*, J 12 Hz, H-5), 0.84 (3H, *s*, H-26), 0.86 (3H, *s*, H-24), 0.90 (3H, *s*, H-29), 0.95 (6H, *s*, H-25 and H-30), 1.07 (3H, *s*, H-23), 1.15 (3H, *s*, H-27), 2.88 (3H, *m*, H-18), 3.22 (1H, *dd*, J 11.7, 4.2 Hz, H-3), 3.27 (1H, *t*, J 7.8 Hz, gluA-2), 3.40 (3H, *t*, J 9 Hz, gluA-3), 3.45 (1H, *t*, J 9 Hz, gluA-4), 3.56 (1H, *d*, J 9, 5 Hz, gluA-5), 4.35 (1H, *d*, J 7.8 Hz, gluA-1), 5.24 (1H, *m*, W_{1-2} 7 Hz, H-12); $^{13}\text{C-NMR}$ (125 MHz, CD_3OD): δ 91 (C-3), 57.1 (C-5), 123 (C-12), 145.5 (C-13) 43.1 (C-18), 28.7 (C-23), 17.2 (C-24), 16.2 (C-25), 18.1 (C-26), 26.7 (C-27), 34 (C-29), 24.4 (C-30), 106.7 (gluA-1), 75.5 (gluA-2), 78 (gluA-3), 73.8 (gluA-4), 75.9 (gluA-5).

Chikusetsusaponin IVa (2). ¹H-NMR (500 MHz, CD₃OD): δ 0.77 (1H, *m*, H-5), 0.81 (3H, *s*, H-26), 0.87 (3H, *s*, H-24), 0.92 (3H, *s*, H-25), 0.93 (3H, *s*, H-29), 0.95 (3H, *s*, H-30), 1.07 (3H, *s*, H-23), 1.17 (3H, *s*, H-27), 2.87 (3H, *dd*, *J* 13.7, 3 Hz, H-18), 3.16 (1H, *t*, *J* 7.8 Hz, gluA-2), 3.21 (1H, *dd*, *J* 11.7, 4.1 Hz, H-3), 3.30 (1H, *m*, glu-2), 3.37 (1H, *m*, glu-5), 3.39 (3H, *t*, *J* 9 Hz, gluA-3), 3.43 (1H, *m*, glu-3), 3.45 (1H, *t*, *J* 9 Hz, gluA-4), 3.50 (1H, *m*, glu-4), 3.56 (1H, *d*, *J* 9, 7 Hz, gluA-5), 3.70 (1H, *dd*, *J* 11, 4.3 Hz, glu-6), 3.84 (1H, *brd*, *J* 11.5 Hz, glu-6), 4.35 (1H, *d*, *J* 7.8 Hz, gluA-1), 5.27 (1H, *m*, *W*_{1 2} 8 Hz, H-12), 5.40 (1H, *d*, *J* 8.1 Hz, glu-1); ¹³C-NMR (125 MHz, CD₃OD): δ 89.2 (C-3), 55.5 (C-5), 122.4 (C-12), 143.3 (C-13), 41.1 (C-18), 27 (C-23), 15.5 (C-24), 14.6 (C-25), 16.3 (C-26), 24.8 (C-27), 176.6 (C-28), 32 (C-29), 22.5 (C-30), 105.3 (gluA-1), 74.1 (gluA-2), 76.6 (gluA-3), 72.3 (gluA-4), 75.1 (gluA-5), 175.6 (gluA-6), 94.2 (glu-1), 72.4 (glu-2), 76.8 (glu-3), 69.6 (glu-4), 77.2 (glu-5), 60.9 (glu-6).

3-O-[3'-O-(2''-O-Glycolyl)-glyoxylyl β-D-glucuronopyranosyl] oleanolic acid (3). ¹H-NMR (500 MHz, CD₃OD): δ 0.79 (1H, *m*, H-5), 0.85 (6H, *s*, H-24 and H-29), 0.89 (3H, *s*, H-26), 0.96 (3H, *s*, H-25), 0.97 (3H, *s*, H-30), 1.07 (3H, *s*, H-23), 1.15 (3H, *s*, H-27), 2.93 (3H, *brdd*, *J* 13.5, 3 Hz, H-18), 3.23 (1H, *dd*, *J* 11.7, 4.5 Hz, H-3), 3.44 (1H, *m*, gluA-2), 3.58 (2H, *m*, gluA-3 and gluA-4), 3.62 (1H, *m*, gluA-5), 4.05 (1H, *d*, *J* 14.8 Hz, H-3''), 4.35 (*d*, *J* 14.8 Hz, H-3''), 4.42 (1H, *d*, *J* 7.8 Hz, gluA-1), 5.04 (1H, *s*, H-2''), 5.22 (1H, *m*, *W*_{1 2} 8 Hz, H-12); ¹³C-NMR (125 MHz, CD₃OD): δ 89.4 (C-3), 55.6 (C-5), 128.4 (C-12), 145.5 (C-13), 42 (C-18), 27.1 (C-23), 15.6 (C-24), 14.5 (C-25), 16.7 (C-26), 25 (C-27), 179.8 (C-28), 32.5 (C-29), 22.9 (C-30), 104.8 (gluA-1), 73.6 (gluA-2), 85.7 (gluA-3), 71.2 (gluA-4), 74 (gluA-5), 178.1 (gluA-6), (C-1'' not determined), 101.4 (C-2''), 67.6 (C-3''), 175.7 (C-4''); ESI-MS (positive mode) *m/z*: 803.3 (M⁺ K⁺), (negative mode) *m/z* 846.8 (M⁻ 2Na⁺ K⁺ 3H⁺), 786.5 (M⁻ Na⁺ H⁺), 613.5, 569.5, 455.5 (aglycone H⁺) 100%, MS-MS (negative mode; *m/z* 763.5) *m/z* 746.3 (M-H₂O), 663.5, 631.5 (M⁻ 133) 100%.

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