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► **To cite this version:**

Catherine Lavaud, Laurence Voutquenne, Philippe Bal, Isabelle Pouny. Saponins from *Chenopodium album*. *Fitoterapia*, 2000, 71 (3), pp.338-340. 10.1016/S0367-326X(99)00166-5 . hal-01996992

**HAL Id: hal-01996992**

**<https://hal.univ-reims.fr/hal-01996992v1>**

Submitted on 6 Dec 2021

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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.

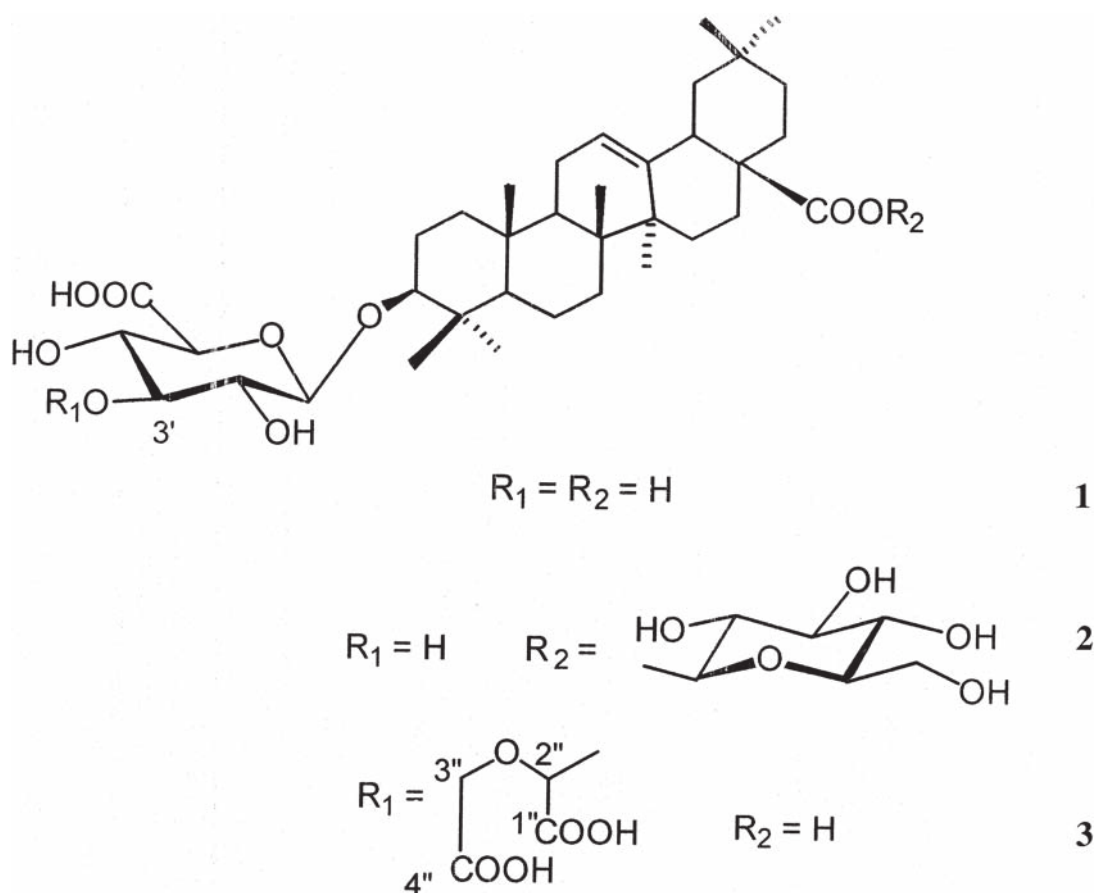
*Keywords:* *Chenopodium album*; Triterpenoids; Saponins; *Seco*-glycosides

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



*Calenduloside E* (1).  $^1\text{H-NMR}$  (500 MHz,  $\text{CD}_3\text{OD}$ ):  $\delta$  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,  $\text{CD}_3\text{OD}$ ):  $\delta$  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)*. <sup>1</sup>H-NMR (500 MHz, CD<sub>3</sub>OD): 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*<sub>1 2</sub> 8 Hz, H-12), 5.40 (1H, *d*, *J* 8.1 Hz, glu-1); <sup>13</sup>C-NMR (125 MHz, CD<sub>3</sub>OD): 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)*. <sup>1</sup>H-NMR (500 MHz, CD<sub>3</sub>OD): 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*<sub>1 2</sub> 8 Hz, H-12); <sup>13</sup>C-NMR (125 MHz, CD<sub>3</sub>OD): 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<sup>+</sup> K<sup>+</sup>), (negative mode) *m/z* 846.8 (M<sup>-</sup> 2Na<sup>+</sup> K<sup>+</sup> 3H<sup>+</sup>), 786.5 (M<sup>-</sup> Na<sup>+</sup> H<sup>+</sup>), 613.5, 569.5, 455.5 (aglycone H<sup>+</sup>) 100%, MS-MS (negative mode; *m/z* 763.5) *m/z* 746.3 (M-H<sub>2</sub>O), 663.5, 631.5 (M<sup>-</sup> 133) 100%.

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