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# TRITERPENES AND FLAVONOIDS FROM *Mosla chinensis*

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*Mosla chinensis* Maxim. cv. Jiangxiangru (Lamiaceae), an annotinous herbaceous plant, is distributed mainly in hilly regions of Jiangxi province in China. It is known for its use in Chinese medicine to treat cold, cough, fever, edema, and pain [1]. Chemical investigation of this plant led to the isolation of eight known compounds, which were identified by spectral data as betulinic acid (**1**), oleanolic acid (**2**), negletein (**3**), luteolin (**4**), quercetin (**5**), chrysoeriol (**6**), apigenin (**7**), and ursolic acid (**8**). Compounds **1–7**, two triterpenes and five flavone derivatives, were isolated from the *Molsa* genus for the first time. Compounds **1–8** were first isolated from this plant.

**Plant Materials.** The whole plants of *M. chinensis* Jiangxiangru were collected at Xinyu City in Jiangxi Province, China, in July 2007. A voucher specimen (20070703) was deposited at the Department of pharmacognosy, School of Pharmacy, Jiangxi University of TCM.

**Extraction and Isolation.** The dried whole plants (3.5 kg) were cut and refluxed three times with 80% EtOH at 65°C for 2 h. The combined extracts evaporated under reduced pressure to yield a residue (980 g). The residue was suspended in $H_2O$ and then partitioned successively with petroleum ether, EtOAc, and *n*-butanol to give three corresponding portions. The EtOAc portion (100 g) was subjected to silica gel column chromatography (200–300 mesh, 1 kg), eluting with gradient petroleum ether–EtOAc (10:1–5:1–1:1–0:1) and EtOAc–MeOH (0:1) to yield five fractions. Fraction I (20 g) was purified by repeated column chromatography on Sephadex LH-20 eluting with $CHCl_3$–MeOH (1:1) and MeOH, and silica gel eluting with petroleum ether–$CHCl_3$–MeOH (10:5:1) to yield compounds **1** (250 mg), **2** (100 mg), **3** (6 mg), **4** (2.4mg), **5** (20 mg), and **6** (50 mg). Fraction II (25 g) was subjected to Sephadex LH-20 eluting with $CHCl_3$–$(CH_3)_2CO$ (10:1–1:1) and column chromatography on Sephadex LH-20 eluting with $CHCl_3$–MeOH (1:1) to afford compound **7** (21.6 mg). Fraction III (30 g) was separated over Sephadex LH-20 eluting with $CHCl_3$–MeOH (1:1) and silica gel eluting with $CHCl_3$–MeOH–$H_2O$ (20:1:0.5) to give compound **8** (30.6 mg).

**General Procedures**. NMR spectra were recorded on Bruker DRX-300 and DRX-600 spectrometers in DMSO-$d_6$ or MeOH-$d_4$ with TMS as an internal standard. ESI-MS spectra were measured with an Agilent MSD-Trap-XCT spectrometer.

**Betulinic Acid (1)**. $C_{30}H_{48}O_3$, colorless needles (MeOH), mp 258–259°C. ESI-MS (–) *m/z* 455 $[M - H]^-$. $^1H$ NMR spectrum (300 MHz, DMSO-$d_6$, δ, ppm, J/Hz): 4.65 (1H, br.s, H-29$\beta$), 4.52 (1H, br.s, H-29$\alpha$), 4.25 (1H, d, J = 6.0, OH-3$\alpha$), 2.91 (1H, m, H-3), 1.76 (3H, s, H-30), 0.88 (3H, s, H-27), 0.82 (6H, s, H-26, 23), 0.72 (3H, s, H-25), 0.60 (3H, s, H-24). $^{13}C$ NMR spectrum (75 MHz, DMSO-$d_6$, δ, ppm): 177.7 (C-28), 150.8 (C-20), 109.7 (C-29), 77.2 (C-3), 55.8 (C-5), 55.3 (C-9), 50.4 (C-18), 49.0 (C-17), 47.1 (C-19), 42.4 (C-14), 41.4 (C-8), 38.9 (C-4), 38.7 (C-1), 38.0 (C-10), 37.2 (C-13), 36.8 (C-7), 34.3 (C-16), 32.2 (C-21), 30.6 (C-22), 29.6 (C-24), 28.5 (C-15), 27.6 (C-2), 25.5 (C-12), 20.9 (C-11), 19.4 (C-30), 18.4 (C-6), 16.4 (C-25), 16.2 (C-26, 23), 14.8(C-27) [2].

**Oleanolic Acid (2)**. $C_{30}H_{48}O_3$, mp 249–250°C. ESI-MS (–) *m/z* 455 $[M - H]^-$. $^{13}C$ NMR spectrum (75 MHz, DMSO-$d_6$, δ, ppm): 179.1 (C-28), 144.3 (C-13), 121.9 (C-12), 77.3 (C-3), 55.2 (C-5), 47.5 (C-9), 46.1 (C-17), 45.9 (C-19), 41.7 (C-14), 41.2 (C-18), 38.8 (C-4), 38.5 (C-8), 37.0 (C-10), 33.7 (C-21), 33.2 (C-29), 32.8 (C-7), 32.5 (C-22), 30.8 (C-20), 28.6 (C-23), 27.6 (C-15), 27.3 (C-2), 26.0 (C-27), 23.8 (C-30), 23.3 (C-16), 23.0 (C-11), 18.4 (C-6), 17.3 (C-26), 16.4 (C-24), 15.5 (C-25) [3].

**Negletein (3)**. $C_{16}H_{12}O_5$, Yellow needles ($CHCl_3$–MeOH), mp 202–204°C; ESI-MS (+) *m/z* 285 $[M + H]^+$. $^1H$ NMR spectrum (400 MHz, DMSO-$d_6$, δ, ppm, J/Hz): 12.52 (1H, br.s, 5-OH), 8.79 (1H, br.s, 6-OH), 8.10 (2H, d, J = 7.2, H-2′, 6′), 7.61 (3H, m, H-3′, 4′, 5′), 6.99 (1H, s, H-3), 6.96 (1H, s, H-8), 3.94 (3H, br.s, $OCH_3$) [4].

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**Luteolin (4)**. $C_{15}H_{10}O_6$, yellow crystal ($CHCl_3$–MeOH), mp > 320°C; ESI-MS (–) *m/z* 285 $[M - H]^-$. $^1H$ NMR spectrum (300 MHz, DMSO-$d_6$, δ, ppm, J/Hz): 12.97 (1H, s, OH-5), 7.42 (1H, dd, J = 8.0, 2.0, H-6′), 7.39 (1H, br.s, H-2′), 6.88 (1H, d, J = 8.0, H-5′), 6.66 (1H, s, H-3), 6.44 (1H, d, J = 2.0, H-8), 6.18 (1H, d, J = 2.0, H-6) [3].

**Quercetin (5)**. $C_{15}H_{10}O_7$, mp 313–314°C; ESI-MS (–) *m/z* 301 $[M - H]^-$ [5].

**Chrysoeriol (6)**. $C_{16}H_{12}O_6$, yellow amorphous powder ($CHCl_3$–MeOH), mp > 320°C; ESI-MS (+) *m/z* 301 $[M + H]^+$, ESI-MS (–) *m/z* 299 $[M - H]^-$. $^1H$ NMR spectrum (300 MHz, DMSO-$d_6$, δ, ppm, J/Hz): 12.93 (1H, s, 5-OH), 6.86 (1H, s, H-3), 6.17 (1H, d, J = 1.7, H-6), 6.49 (1H, d, J = 1.7, H-8), 6.91 (1H, d, J = 8.6, H-5′), 7.53 (1H, d, J = 1.8, H-2′), 7.54 (1H, dd, J = 6.6, 1.8, H-6′) [5].

**Apigenin (7)**. $C_{15}H_{10}O_5$, pale yellow amorphous powder ($CHCl_3$–MeOH), mp > 320°C. ESI-MS (+) *m/z* 271 $[M + H]^+$, ESI-MS (–) *m/z* 269 $[M - H]^-$ [6].

**Ursolic Acid (8)**. $C_{30}H_{48}O_3$, white amorphous powder (MeOH), mp 244–246°C. ESI-MS (–) *m/z* 455 $[M - H]^-$. $^{13}C$ NMR spectrum (75 MHz, DMSO-$d_6$, δ, ppm): 178.7 (C-28), 138.6 (C-13), 125.0 (C-12), 77.3 (C-3), 55.2 (C-5), 52.8 (C-18), 47.4 (C-9), 47.3 (C-17), 42.1 (C-14), 39.5 (C-8), 39.0 (C-19), 38.9 (C-20), 38.8 (C-4), 38.7 (C-1), 37.0 (C-22), 36.7 (C-10), 33.2 (C-7), 30.6 (C-21), 28.7 (C-15), 28.0 (C-23), 27.4 (C-2), 24.3 (C-16), 23.7 (C-11), 23.3 (C-27), 21.5 (C-30), 18.4 (C-6), 17.4 (C-29), 17.3 (C-26), 16.5 (C-24), 15.7 (C-25) [7].

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