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STEROLS FROM THE LEAFY CULMS OF *Desmostachya bipinnata*

Sabina Shrestha, Ha-Na Lyu, Ji-Hae Park, Dae-Young Lee, Jin Gyeong Cho, En-ji Cui, In-Sik Chung, and Nam-In Baek*

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Desmostachya bipinnata (L.) Stapf (Poaceae), also known as sacrificial grass, is a perennial herbaceous plant distributed from north Africa to South Asia [1]. The leafy culms and roots of the plant are used as an aphrodisiac and diuretic in traditional Ayurvedic medicine [2]. *D. bipinnata* has also been reported to have antifungal [3] and antiurolithiatic [4] activities. So far, flavonoids such as kaempferol, quercetin, quercetin-3-glucoside, trycin, trycin-7-glucoside, and 4′-methoxy quercetin-7-*O*-glucoside have been reported from this plant [5, 6]. *D. bipinnata* has pharmacological components such as trycin and trycin-7-glucoside, which are reported to be anti-ulcerogenic [5], and 4′-methoxy quercetin-7-*O*-glucoside, which is reported as an anti-helicobacter [6].

Fresh leafy culms of *D. bipinnata* were collected from Birgunj, Nepal in August 2008. The dried leafy culms of *D. bipinnata* (1.3 kg) were extracted with an 80% aqueous MeOH (20 L × 3) solution at room temperature. The concentrated extracts were successively partitioned with water (3.5 L), EtOAc (3 L × 3), and *n*-BuOH (2 L × 3). The concentrated EtOAc fraction (16 g) was subjected to silica gel (SiO_2) column (8 × 15 cm) chromatography (c.c.) and eluted with *n*-hexane–EtOAc (8:1→6:1→4:1, v/v) and $CHCl_3$–MeOH (10:1→6:1→3:1→1:1, v/v). Each eluant was monitored by thin-layer chromatography (TLC), and 23 fractions (DBLE-1 to DBLE-23) were obtained. Fraction DBLE-9 (621.5 mg) was subjected to ODS c.c. and eluted with MeOH–H_2O (5:1→12:1, v/v) to yield 23 subfractions (DBLE-9-1 to DBLE-9-23). Compound **1** [DBLE-9-21, 9.4 mg, R_f 0.27 on the TLC (RP-18 F_{254}s) in acetone–acetonitrile 1:2] and compound **2** [DBLE-9-22, 40.6 mg, R_f 0.25 on the TLC (RP-18 F_{254}s) in acetone–acetonitrile 1:2] were isolated. Fraction DBLE-21 (5.8 g) was subjected to SiO_2 c.c. and eluted with $CHCl_3$–MeOH (20:1→10:1, v/v) to yield 18 subfractions (DBLE-21-1 to DBLE-21-18). Subfraction DBLE-21-13 (795.9 mg) was subjected to ODS c.c. and eluted with MeOH–H_2O (1:1.5→6:1, v/v) to yield 23 subfractions (DBLE-21-13-1 to DBLE-21-13-23). Compound **3** [DBLE-21-13-22, 75 mg, R_f 0.20 on the TLC (RP-18 F_{254}s) in MeOH–H_2O 25:1] was isolated. Subfraction DBLE-21-8 (852.7 mg) was subjected to ODS c.c. and eluted with acetone–H_2O (1:1.5→1:1, v/v) to yield 18 subfractions (DBLE-21-8-1 to DBLE-21-8-18). Subfraction DBLE-21-8-16 (47.8 mg) underwent flash chromatography over silica gel (Biotage® SNAP cartridge KP-Sil – 10 g) and was eluted with *n*-hexane–EtOAc (4:1, v/v) to yield 14 subfractions (DBLE-21-8-16-1 to DBLE-21-8-16-14), which ultimately yielded compound **4** [DBLE-21-8-16-9, 6.7 mg, R_f 0.68 on the TLC (SiO_2 F_{254}) *n*-hexane–EtOAc 1:3] and compound **5** [DBLE-21-8-16-12, 9.2 mg, R_f 0.60 on the TLC (SiO_2 F_{254}) in *n*-hexane–EtOAc 1:3].

Compounds **1**, **2**, and **3** were identified as stigmasterol, β-sitosterol, and daucosterol, respectively, from the comparison of collected spectroscopic data with that of authentic samples and literature [7–9]. FAB-MS, ^{1}H NMR, ^{13}C NMR, and 2D NMR (gCOSY, gHSQC, and gHMBC) were used to identify compounds **4** and **5**.

Stigmast-5-en-3β,7β-diol (4), white powder, mp 157–158°C, $[\alpha]_D^{25}$ –4° (*c* 0.25, $CHCl_3$); positive FAB-MS: *m/z* 431 $[M + H]^+$. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 5.26 (1H, br.s, H-6), 3.83 (1H, br.d, J = 7.6, H-7), 3.55 (1H, m, H-3), 1.02 (3H, s, H-19), 0.90 (3H, d, J = 6.4, H-21), 0.85 (3H, t, J = 6.6, H-29), 0.81 (3H, d, J = 7.6, H-26), 0.79 (3H, d, J = 7.2, H-27), 0.67 (3H, s, H-18). ^{13}C NMR spectrum (100 MHz, $CDCl_3$, δ, ppm): 143.37 (C-5), 125.54 (C-6), 73.36 (C-7), 71.44 (C-3), 55.97 (C-14), 55.39 (C-17), 48.29 (C-9), 45.88 (C-24), 42.96 (C-13), 41.75 (C-4), 40.95 (C-12), 39.60 (C-8), 36.98 (C-1), 36.48 (C-10), 36.15 (C-20), 31.98 (C-22), 31.67 (C-2), 29.75 (C-23), 28.61 (C-16), 26.45 (C-15), 26.16 (C-25), 22.76 (C-28), 21.15 (C-11), 19.89 (C-27), 19.23 (C-26), 19.09 (C-21), 18.9 (C-19), 12.06 (C-29), 11.91 (C-18).

Graduate School of Biotechnology, Institute of Life Sciences & Resources, Kyung Hee University, Yongin 446-701, Korea, fax: 82 31 204 8116, e-mail: nibaek@khu.ac.kr. Published in Khimiya Prirodnykh Soedinenii, No. 5, pp. 744–745, September–October, 2011. Original article submitted May 19, 2010.

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Stigmast-5-en-3β,7α-diol (5), white powder, mp 219–220°C, $[\alpha]_D^{25}$ –45° (*c* 0.25, $CHCl_3$); positive FAB-MS: *m/z* 431 $[M + H]^+$. ^1H NMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 5.58 (1H, d-like, J = 4.8, H-6), 3.82 (1H, br.s, H-7), 3.59 (1H, m, H-3), 0.97 (3H, s, H-19), 0.90 (3H, d, J = 6.4, H-21), 0.84 (3H, t, J = 6.8, H-29), 0.81 (3H, d, J = 8.0, H-26), 0.79 (3H, d, J = 8.0, H-27), 0.66 (3H, s, H-18). ^{13}C NMR spectrum (100 MHz, $CDCl_3$, δ, ppm): 146.13 (C-5), 123.79 (C-6), 71.33 (C-3), 65.36 (C-7), 49.48 (C-14), 55.73 (C-17), 45.85 (C-24), 42.29 (C-9), 42.18 (C-13), 42.04 (C-4), 39.21 (C-12), 37.56 (C-8), 37.44 (C-1), 37.05 (C-10), 36.15 (C-20), 33.74 (C-22), 31.42 (C-2), 29.76 (C-23), 28.19 (C-16), 25.95 (C-15), 24.32 (C-25), 23.02 (C-28), 20.74 (C-11), 19.85 (C-27), 19.03 (C-26), 18.84 (C-21), 18.30 (C-19), 12.06 (C-29), 11.71 (C-18).

Leafy culms of *D. bipinnata* contained stigmasterol (**1**), β-sitosterol (**2**), daucosterol (**3**), stigmast-5-en-3β,7β-diol (**4**), and stigmast-5-en-3β,7α-diol (**5**). All of these sterols were reported for the first time from the plant of the monotypic genus *Desmostachya*.

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