

## SUPPLEMENTARY DATA

**Characteristics of the constituents from the roots of *Polygonum multiflorum*:** The constituents were purified from the roots of *Polygonum multiflorum* and analyzed, as described under Materials and Methods.

Compound **1** showed the following characteristics:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , ppm):  $\delta$  12.25 (1H, s, 8-OH), 12.05 (1H, s, 1-OH), 7.55 (1H, d,  $J = 1.2$  Hz, H-4), 7.29 (1H, d,  $J = 2.4$  Hz, H-5), 7.01 (1H, d,  $J = 1.2$  Hz, H-2), 6.61 (1H, d,  $J = 2.4$  Hz, H-7), 3.86 (3H, s,  $-\text{OCH}_3$ ), and 2.38 (3H, s,  $\text{CH}_3$ ); and  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , ppm):  $\delta$  190.9 (C-9), 182.1 (C-10), 166.6 (C-6), 165.3 (C-8), 162.6 (C-1), 148.5 (C-3), 135.3 (C-10a), 133.3 (C-4a), 124.6 (C-2), 121.4 (C-4), 113.7 (C-9a), 110.3 (C-8a), 108.3 (C-5), 106.9 (C-7), 56.2 ( $-\text{OCH}_3$ ), and 22.3 ( $\text{CH}_3$ ). This compound was identified as physcion based on the 2D heteronuclear correlation of the  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra, which were in agreement with published data [19].

Compound **2** showed the following characteristics:  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , ppm):  $\delta$  12.05 (1H, s, 8-OH), 11.97 (1H, s, 1-OH), 11.38 (s, 1H, 6-OH), 7.44 (1H, d,  $J = 1.2$  Hz, H-4), 7.12 (1H, d,  $J = 1.2$  Hz, H-2), 7.08 (1H, d,  $J = 2.4$  Hz, H-5), 6.57 (1H, d,  $J = 2.4$  Hz, H-7), and 2.39 (3H, s,  $-\text{CH}_3$ ); and  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , ppm):  $\delta$  190.2 (C-9), 181.8 (C-10), 166.1 (C-6), 164.9 (C-8), 161.9 (C-1), 148.7 (C-3), 135.5 (C-10a), 133.2 (C-4a), 124.6 (C-2), 120.9 (C-4), 113.8 (C-9a), 109.4 (C-8a), 109.3 (C-5), 108.4 (C-7), and 22.0 ( $-\text{CH}_3$ ). Correlation analysis of the  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra using heteronuclear single quantum correlation (HSQC) and heteronuclear multiple bond connectivity (HMBC) suggested that the isolated compound was emodin. The spectral data matched published data [19–20].

Compound **3** showed the following characteristics:  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , ppm):  $\delta$  7.48 (1H, s, H-4), 7.36 (1H, d,  $J = 2.8$  Hz, H-5), 7.18 (2H, d,  $J = 2.8$  Hz, H-7), 5.18 (1H, d,  $J = 8.0$  Hz, H-1'), 3.96 (3H, s,  $-\text{OCH}_3$ ), 2.41 (3H, s,  $-\text{CH}_3$ ), and 3.16–3.65 (6H, m, H-2' - H-6'); and  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , ppm):  $\delta$  187.0 (C-9), 182.4 (C-10), 165.2 (C-6), 162.2 (C-1), 161.2 (C-8), 147.6 (C-3), 136.8 (C-10a), 132.5 (C-4a), 124.7 (C-2), 119.9 (C-4), 114.9 (C-9a, C-8a), 107.8 (C-7), 106.9 (C-5), 101.1 (C-1'), 21.9 ( $-\text{CH}_3$ ), 77.9 (C-5'), 77.1 (C-3'), 73.7 (C-2'), 70.2 (C-4'), 61.2 (C-6'), and 56.6 ( $-\text{OCH}_3$ ). This compound was determined to be physcion-8-*O*- $\beta$ -D-glucopyranoside on the basis of the  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR analyses and comparison with published data [19].

Compound **4** showed the following characteristics:  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , ppm):  $\delta$  9.19 (1H, s, 5-OH), 8.94 (1H, s, 7-OH), 8.87 (1H, s, 3'-OH), 8.83 (4'-OH), 6.71 (1H, d,  $J = 2.0$  Hz, H-2'), 6.68 (1H, d,  $J = 7.9$  Hz, H-5'), 6.56 (1H, dd,  $J = 7.9, 1.8$  Hz, H-6'), 5.77 (1H, d,  $J = 2.4$  Hz, H-6), 5.70 (1H, d,  $J = 2.4$  Hz, H-8), 4.40 (1H, d,  $J = 7.6$  Hz, H-2), 3.81 (1H, ddd,  $J = 8.5, 7.9, 5.5$  Hz, H-3), 2.68 (1H, dd,  $J = 16.5, 5.5$  Hz, H-4), and 2.34 (1H, dd,  $J = 16.5, 8.5$  Hz, H-4); and  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , ppm): 156.9 (C-5), 156.6 (C-7), 155.8 (C-9), 145.3 (C-4', C-3'), 131.0 (C-1'), 118.9 (C-6'), 115.5 (C-2'), 115.0 (C-5'), 99.5 (C-10), 95.7 (H-6), 94.3 (H-8), 81.5 (H-2), 66.8 (C-3), 28.3 (C-4). This compound was identified as catechin based on comparison with published data [21–22].

Compound **5** showed the following characteristics:  $[\alpha]_D^{20} -60.8$  (c 0.354,  $\text{DMSO}$ );  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , ppm):  $\delta$  11.27 (br, s,  $-\text{OH}$ ), 7.46 (1H, d,  $J = 1.2$  Hz, H-4), 7.29 (1H, d,  $J = 2.4$  Hz, H-5), 7.17 (1H, d,  $J = 1.2$  Hz, H-2), 6.99 (1H, d,  $J = 2.4$  Hz, H-7), 5.05 (1H, d,  $J = 7.6$  Hz, H-1'), 2.41 (3H, s,  $\text{CH}_3$ ), and 3.29–3.53 (6H, m, H-2' - H-6');  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , ppm):  $\delta$  186.3 (C-9), 182.0 (C-10), 164.0 (C-6), 161.6 (C-1), 160.9 (C-8), 146.8 (C-3), 136.4 (C-10a), 131.9 (C-4a), 124.1 (C-2), 119.2 (C-4), 114.3 (C-9a), 113.2 (C-8a), 108.1 (C-5 and C-7), 100.5 (C-1'), 21.3 ( $-\text{CH}_3$ ), 77.2 (C-5'), 76.3 (C-3'), 73.1 (C-2'), 69.3 (C-4'), and 60.4 (C-6'). This compound was identified as emodin-8-*O*- $\beta$ -D-glucopyranoside, which was supported by previously reported data [19].

Compound **6** showed the following characteristics: mp: 154–160 °C;  $[\alpha]_D^{20} +24.9$  (c 0.487, MeOH); FAB-MS  $m/z$ : 407  $[M+H]^+$ ; high-resolution FAB-MS  $m/z$  407.1332  $[M+H]^+$  (calculated for  $C_{20}H_{23}O_9$ ; 407.1342);  $^1H$  NMR (400 MHz,  $CD_3OD$ , ppm): d 7.72 (1H, d,  $J = 16.8$  Hz, H-8), 7.43 (2H, d,  $J = 8.4$  Hz, H-2', H-6'), 6.93 (1H, d,  $J = 16.8$  Hz, H-7), 6.77 (2H, d,  $J = 8.4$  Hz, H-3', H-5'), 6.61 (1H, d,  $J = 2.3$  Hz, H-6), 6.23 (1H, d,  $J = 2.3$  Hz, H-4), 4.56 (1H, d,  $J = 7.8$  Hz, H-1''), 3.80 (2H, m, H-6''), 3.56-3.54 (2H, overlapped, H-2'', H-4''), 3.45 (1H, m, H-3''), and 3.30 (1H, m, H-5'');  $^{13}C$  NMR (100 MHz,  $CD_3OD$ , ppm):  $\delta$  157.0 (C-4'), 154.6 (C-5), 150.7 (C-3), 136.6 (C-2), 132.4 (C-1'), 129.5 (C-8), 128.7 (C-1), 127.8 (C-2', C-6'), 120.3 (C-7), 115.1 (C-3', C-5'), 106.9 (C-1''), 102.2 (C-4), 101.3 (C-6), 76.8 (C-5''), 76.6 (C-3''), 74.1 (C-2''), 69.4 (C-4''), and 60.7 (C-6''). This compound was identified as (*E*)-2,3,5,4'-tetrahydroxystillbene-2-*O*- $\beta$ -D-glucopyranoside (THSG) according to published data [23].