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FLAVONOIDS FROM THE AERIAL PART OF *Scutellaria schachristanica*

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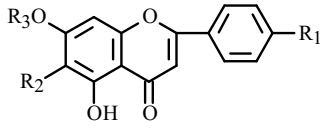
Plants of the genus *Scutellaria* L. (Lamiaceae) are broadly distributed in nature and are rich sources of flavonoids. Therefore, its individual species have been investigated by many researchers [1]. Flavonoids, the most numerous class of natural phenolic compounds such as chalcones, flavones, flavanones, isoflavones, biflavones, and lignoflavones, which exhibit P-vitamin, inhibiting, cytotoxic, antimetastatic, antibacterial, and other types of activity, have been isolated from representatives of this plant genus [1].

We studied for the first time the aerial part of *S. schachristanica* Zuz. collected in Samarkand Oblast of the Republic of Uzbekistan during flowering. Dried and ground plant (1000 g) was extracted at room temperature by EtOH (×6, 70%). The combined alcohol extract was condensed in vacuo to 0.75 L and diluted with water to 1.5 L. The aqueous alcohol extract was shaken successively with petroleum ether (6 × 0.5 L), $CHCl_3$ (6 × 0.5 L), and EtOAc (10 × 0.5 L). Solvents were removed to produce petroleum-ether (10.5 g), $CHCl_3$ (12.0 g), and EtOAc (20 g) fractions.

The EtOAc extract (20 g) was chromatographed over a column (2.5 × 150 cm) of silica gel (450 g) with gradient elution by $CHCl_3$ and $CHCl_3$:CH_3OH. Elution of the column with this system in ratios 97:3, 95:5, 90:10, and 85:15 isolated six compounds (**1**–**6**) of flavonoid character.

A comparison of spectral data (UV with added NaOAc; IR, PMR, ^{13}C NMR) with the literature and direct comparison with authentic samples identified chrysin (**1**) [2], apigenin (**2**) [3], hispidulin (**3**) [4], scutellarin (**4**) [5], cosmosiin (**5**) [6], and scutellarein-7-*O*-*β*-D-glucopyranoside (**6**) [5].



1 - 6

1: $R_1 = R_2 = R_3 = H$; **2:** $R_1 = OH$, $R_2 = R_3 = H$
3: $R_1 = OH$, $R_2 = OMe$, $R_3 = H$; **4:** $R_1 = R_2 = OH$, $R_3 = H$
5: $R_1 = OH$, $R_2 = H$, $R_3 = Glc$; **6:** $R_1 = R_2 = OH$, $R_3 = Glc$

Chrysin (5,7-dihydroxyflavone) (1). $C_{15}H_{14}O_4$, mp 289–292°C. PMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 6.45 (1H, d, J = 2.0, H-6), 6.86 (1H, d, J = 2.0, H-8), 6.98 (1H, s, H-3), 7.57 (2H, m, H-3′,5′), 8.20 (2H, dd, J = 1.2, 7.9, H-2′,6′), 12.77 (1H, s, 5-OH).

Apigenin (5,7,4′-trihydroxyflavone) (2). Yellow crystals, $C_{15}H_{10}O_5$, mp >340°C. UV spectrum (MeOH, λ_{max}, nm): 270, 330. IR spectrum (ν, cm^{-1}): 3117 (OH), 1669 (C=O), 1605, 1506 (C=C). PMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 6.14 (1H, d, J = 2.5, H-6), 6.43 (1H, d, J = 2.5, H-8), 6.73 (1H, s, H-3), 6.87 (2H, d, J = 8.8, H-3′,5′), 7.87 (2H, d, J = 8.8, H-2′,6′), 10.37 (1H, br.s, 4′-OH), 10.8 (1H, br.s, 7-OH), 12.91 (1H, s, 5-OH).

Hispidulin (5,7,4′-trihydroxy-6-methoxyflavone) (3). $C_{16}H_{12}O_6$, mp 286–289°C. PMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 6.21 (1H, s, H-8), 6.68 (1H, s, H-3), 7.55 (2H, dd, J = 1.6, 7.8, H-3′,5′), 7.97 (2H, dd, J = 1.6, 7.8, H-2′,6′), 3.88 (3H, OMe), 10.35 (1H, br.s, 4′-OH), 12.62 (1H, s, 5-OH).

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Scutellarin (5,6,7,4′-tetrahydroxyflavone) (4). $C_{15}H_{10}O_6$, mp >340°C. UV spectrum (MeOH, λ_{max}, nm): 279, 338. IR spectrum (ν, cm^{-1}): 3300 (OH), 1672 (C=O), 1603, 1508 (C=C). PMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz): 6.58 (1H, s, H-8), 6.76 (1H, s, H-3), 6.91 (2H, d, J = 8.8, H-3′,5′), 7.94 (2H, d, J = 8.8, H-2′,6′), 12.30 (1H, s, 5-OH).

Cosmosiin (apigenin-7-*O*-glycoside) (5). $C_{21}H_{20}O_{10}$, mp 227–229°C. UV spectrum (MeOH, λ_{max}, nm): 270, 337; +NaOAc 268, 339. PMR spectrum (400 MHz, DMSO-d_6, δ, ppm, J/Hz): 3.5–4.2 (6H, sugar), 5.55 (1H, d, J = 7.8, glucose H-1″), 6.13 (1H, d, J = 2.2, H-6), 6.42 (1H, d, J = 2.2, H-8), 6.72 (1H, s, H-3), 6.88 (2H, dd, J = 1.96, 8.8, H-3′,5′), 7.88 (2H, dd, J = 1.96, 8.8, H-2′,6′), 12.90 (1H, s, 5-OH).

Scutellarein-7-*O*-β-D-glucopyranoside (6). $C_{21}H_{20}O_{11}$, mp 194–196°C. UV spectrum (EtOH, λ_{max}, nm): 225, 279, 309, 338; +NaOAc 279, 309, 338. IR spectrum (ν, cm^{-1}): 3450–3200 (OH), 1664 (C=O), 1607, 1503 (C=C), 1440, 1386, 1320, 1242, 1187, 1134, 1106, 1076, 1044, 991, 708. PMR spectrum (400 MHz, DMSO-d_6, δ, ppm, J/Hz): 3.15-3.73 (sugar protons), 4.92 (1H, d, J = 7.3, glucose H-1″), 6.62 (1H, s, H-8), 6.81 (1H, s, H-3), 6.95 (2H, d, J = 8.9, H-3′,5′), 7.96 (2H, d, J = 8.8, H-2′,6′), 8.78 (1H, s, 6-OH), 10.45 (1H, s, 4′-OH), 12.35 (1H, s, 5-OH).

^{13}C NMR spectrum (100 MHz, DMSO-d_6, δ, ppm): 164.18 (C-2) 102.74 (C-3), 182.6 (C-4), 147.08 (C-5), 127.04 (C-6), 151.27 (C-7), 98.71 (C-8), 152.41 (C-9), 105.21 (C-10), 121.36 (C-1′), 128.71 (C-2′), 116.11 (C-3′), 161.39 (C-4′), 116.11 (C-5′), 128.71 (C-6′), 101.31 (C-1″), 73.27 (C-2″), 75.82 (C-3″), 69.79 (C-4″), 77.33 (C-5″), 60.75 (C-6″).

Chrysin, apigenin, hispidulin, scutellarin, cosmosiin, and scutellarein-7-*O*-β-D-glucopyranoside were isolated for the first time from *S. schachristanica*.

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