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CHEMICAL COMPONENTS OF THE AERIAL PART OF *Scutellaria schachristanica*

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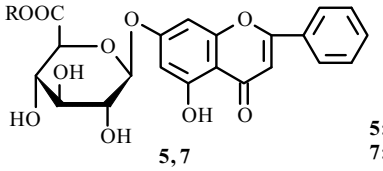
In continuation of research on the EtOAc extract of *Scutellaria schachristanica* [1], rechromatography of fractions obtained by elution using $CHCl_3$:MeOH (9:1 and 4:1) in a gradient of $CHCl_3$ and $CHCl_3$:MeOH isolated another seven compounds (**1**–**7**) in addition to those isolated earlier.

Spectral data (UV with added NaOAc, NaOH, CH_3COONa/H_3BO_3, $AlCl_3$, $ZrOCl_2$; IR, PMR, and ^{13}C NMR), a comparison with the literature, and direct comparison with authentic samples identified these compounds as 5,7-dihydroxy-8-methoxyflavone (wogonin) (**1**); 3,5-dihydroxy-7-methoxyflavone (**2**); 5,7-dihydroxy-6-methoxyflavone (oroxylin) (**3**); 5,7-dihydroxy-3-methoxyflavone (**4**); chrysin-7-*O*-glucuronide (**5**); saccharose (**6**); and chrysin-7-*O*-methylglucuronide (**7**) [2–4].



5,7

5: R = H
7: R = CH_3

5,7-Dihydroxy-8-methoxyflavone (wogonin) (1), $C_{16}H_{12}O_5$, mp 196–197°C. UV spectrum (MeOH, λ_{max}, nm): 246, 277, 315; +CH_3COONa: 292, 395; +NaOH: 296, 402; +CH_3COONa/H_3BO_3: 276, 315; +$ZrOCl_2$: 295, 336, 417. IR spectrum (ν, cm^{-1}): 3462-3230 (OH), 2925 (OCH_3), 1661 (C=O), 1614, 1585 (C=C).

PMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz, 0 = HMDS): 3.88 (3H, s, OCH_3), 6.72 (1H, s, H-3), 6.93 (1H, s, H-6), 7.47 (3H, m, H-3′,4′,5′), 7.95 (2H, d, J = 8.0, H-2′,6′), 12.99 (1H, s, 5-OH).

3,5-Dihydroxy-7-methoxyflavone (2), $C_{16}H_{12}O_5$, mp 230°C. UV spectrum (MeOH, λ_{max}, nm): 279, 309, 328; +CH_3COONa: 279, 307, 326. IR spectrum (ν, cm^{-1}): 3460–3220 (OH), 2912 (OCH_3), 1664 (C=O), 1607, 1505 (C=C).

PMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz, 0 = HMDS): 3.99 (3H, s, OCH_3), 6.39 (1H, s, H-8), 6.63 (1H, s, H-6), 7.50 (3H, m, H-3′,4′,5′), 7.85 (2H, d, J = 8.0, H-2′,6′), 12.98 (1H, s, 5-OH).

^{13}C NMR spectrum (100 MHz, $CDCl_3$, δ): 162.66 (C-2), 152.54 (C-3), 182.20 (C-4), 161.30 (C-5), 99.27 (C-6), 163.63 (C-7), 94.80 (C-8), 157.35 (C-9), 106.11 (C-10), 130.59 (C-1′), 126.58 (C-2′), 129.62 (C-3′), 132.42 (C-4′), 129.62 (C-5′), 126.58 (C-6′), 62.40 (OCH_3).

5,7-Dihydroxy-6-methoxyflavone (oroxylin) (3), $C_{16}H_{12}O_5$, mp 215–217°C. UV spectrum (MeOH, λ_{max}, nm): 271, 320; +CH_3COONa: 374; +NaOH: 378; +CH_3COONa/H_3BO_3: 321; +$ZrOCl_2$: 368. IR spectrum (ν, cm^{-1}): 3480–3290 (OH), 2933 (OCH_3), 1685 (C=O), 1605, 1510 (C=C).

PMR spectrum (400 MHz, $CDCl_3$, δ, ppm, J/Hz, 0 = HMDS): 3.93 (3H, s, OCH_3), 6.37 (1H, s, H-8), 6.62 (1H, s, H-3), 7.49 (3H, m, H-3′,4′,5′), 7.87 (2H, d, J = 8.2, H-2′,6′), 12.45 (1H, s, 5-OH).

5,7-Dihydroxy-3-methoxyflavone (4), $C_{16}H_{12}O_5$, mp 120°C. UV spectrum (MeOH, λ_{max}, nm): 276, 324; +CH_3COONa: 378. IR spectrum (ν, cm^{-1}): 3400–3220 (OH), 1679 (C=O), 1607, 1510 (C=C).

PMR spectrum (400 MHz, $CDCl_3$ + DMSO-d_6, δ, ppm, J/Hz, 0 = HMDS): 3.89 (3H, s, OCH_3), 6.33 (1H, s, H-8), 6.60 (1H, s, H-6), 7.49 (3H, m, H-3′,4′,5′), 7.88 (2H, dd, J = 1.4, 7.5, H-2′,6′), 10.00 (1H, 7-OH), 12.35 (1H, s, 5-OH).

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The location of the methoxyl was determined by double resonance.

Chrysin-7-*O*-glucuronide (5), $C_{21}H_{18}O_{12}$, mp 218–220°C. UV spectrum (MeOH, λ_{max}, nm): 272, 307; +CH_3COONa: 270, 309; +$AlCl_3$: 252, 283, 330, 379. IR spectrum (ν, cm^{-1}): 3530–3320 (OH), 1726 (ester C=O), 1668 (γ-pyrone C=O).

PMR spectrum (400 MHz, DMSO-d_6, δ, ppm, J/Hz, 0 = HMDS): 3.84–5.19 (4H, H-2″,3″,4″,5″), 5.45 (1H, br.s, H-1″), 6.41 (1H, s, H-6), 6.82 (1H, s, H-8), 6.98 (1H, s, H-3), 7.54–7.58 (3H, m, H-3′,4′,5′), 8.03 (2H, d, J = 6.6, H-2′,6′), 12.75 (1H, br.s, 5-OH).

^{13}C NMR spectrum (100 MHz, DMSO, δ): 163.69 (C-2), 105.49 (C-3), 182.32 (C-4), 160.82 (C-5), 99.86 (C-6), 163.25 (C-7), 96.07 (C-8), 157.20 (C-9), 105.76 (C-10), 130.61 (C-1′), 126.52 (C-2′), 129.22 (C-3′), 132.23 (C-4′), 129.22 (C-5′), 126.52 (C-6′), 99.65 (C-1″), 72.96 (C-2″), 75.25 (C-3″), 71.91 (C-4″), 76.30 (C-5″), 172.79 (C-6″).

Saccharose (6), $C_{12}H_{22}O_{11}$, mp 188–190°C. PMR spectrum (400 MHz, DMSO-d_6, δ, ppm, J/Hz, 0 = HMDS): 5.07 (1H, d, J = 6.0, H-1), 4.43 (1H, dd, J = 1.4, 8.0, H-2), 4.35 (1H, m, H-3), 4.27 (1H, m, H-4), 3.83 (1H, m, H-5), 5.15 (2H, dd, J = 3.71, 7.62, H-6), 4.69 (1H, d, J = 5.6, H-1′), 4.73 (2H, m, H-2′), 3.62 (1H, m, H-3′), 3.48 (1H, m, H-4′), 3.44 (1H, m, H-5′), 3.10–3.18 (2H, H-6′).

^{13}C NMR spectrum (100 MHz, DMSO, δ, ppm): 103.98 (C-1), 72.90 (C-2), 74.21 (C-3), 70.00 (C-4), 77.61 (C-5), 60.73 (C-6), 95.60 (C-1′), 62.48 (C-2′), 82.94 (C-3′), 71.91 (C-4′), 91.77 (C-5′), 61.82 (C-6′).

Chrysin-7-*O*-methylglucuronide (7), $C_{22}H_{20}O_{10}$, mp 184–186°C. UV spectrum (MeOH, λ_{max}, nm): 271, 306; +CH_3COONa: 272, 307. IR spectrum (ν, cm^{-1}): 3340 (OH), 1725 (ester C=O), 1669 (γ-pyrone C=O).

PMR spectrum (400 MHz, DMSO-d_6, δ, ppm, J/Hz, 0 = HMDS): 3.61 (3H, $COOCH_3$), 6.45 (1H, d, J = 2.0, H-6), 6.86 (1H, d, J = 2.0, H-8), 7.01 (1H, s, H-3), 7.55–7.57 (3H, m, H-3′,4′,5′), 8.05 (2H, dd, J = 1.24, 8.0, H-2′,6′), 4.17 (1H, d, J = 9.2, H-1″), 5.27–5.53 (4H, H-2″,3″,4″,5″), 12.77 (1H, s, 5-OH).

^{13}C NMR spectrum (100 MHz, DMSO, δ, ppm): 164.66 (C-2), 105.51 (C-3), 182.56 (C-4), 161.20 (C-5), 99.51 (C-6), 163.79 (C-7), 94.78 (C-8), 157.15 (C-9), 105.76 (C-10), 130.59 (C-1′), 126.53 (C-2′), 129.19 (C-3′), 132.25 (C-4′), 129.19 (C-5′), 126.53 (C-6′), 99.06 (C-1″), 72.72 (C-2″), 75.16 (C-3″), 71.32 (C-4″), 77.98 (C-5″), 171.14 (C-6″), 52.00 (OCH_3).

Compounds **1–7** were isolated for the first time from the aerial part of *S. schachristanica*.

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