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Chemistry of Natural Compounds

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BIOLOGICALLY ACTIVE COMPOUNDS FROM *Climacoptera obtusifolia*

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and M. Iqbal Choudhary²

Arid soils cover 34% of Kazakhstan. A multitude of halophytes grow on them. The chemistry of halophytes is of significant scientific and practical interest. Mainly salt-accumulating plants of the family Chenopodiaceae, which is represented in Kazakhstan by 47 genera and 218 species [1–3], exhibit halophilicity. These include plants of the genus *Climacoptera*, of which 14 species grow in Kazakhstan [4–7].

Herein we communicate results for the chemical composition of *C. obtusifolia* collected during flowering in Almaty Region. An analysis of the constituents detected flavonoids (1.4%), saponins (2.3%), amino acids (2.7%), phenolic acids (1.8%), carbohydrates (2.5%), and coumarins (0.1%).

Biologically active compounds from this plant were studied by extracting ground raw material with EtOH (70%) in a raw material–extractant ratio of 1:6–8 for 3 d at room temperature. The aqueous EtOH extract was concentrated. The concentrate was worked up successively with CHCl₃, EtOAc, and *n*-BuOH with subsequent condensing of each fraction. Column chromatography over silica gel of the CHCl₃ fraction isolated 1–4 upon elution by CHCl₃–hexane (9:1 and 8:2). Biologically active compounds were isolated from the *n*-BuOH extract using absorption-distributive chromatography over a nanosorbent produced by carbonization of plant raw material (rice husks) at the Institute of Combustion Problems, Al-Farabi Kazakh Nat. Univ. [7]. The eluents were H₂O and aqueous EtOH in various ratios. Thus, compound 5 was isolated pure from the *n*-BuOH fraction.

The isolated compounds were identified based on physicochemical data and comparisons with the literature as stigmasteryl (1), C₂₉H₂₈O, FAB-MS *m/z* 412 [7] and dehydrodiconiferylaldehyde (2), C₂₀H₂₁O₆, EI-MS *m/z* [M]⁺ 356, white amorphous compound, [α]_D²⁵ +20.0° (*c* 0.1, MeOH), mp 205°C (dec.), *R*_f 0.5 (CHCl₃–MeOH, 9.3:0.7).

The IR spectrum of 2 exhibited absorption bands for CHO stretching vibrations (1670 cm⁻¹) and skeletal benzene ring vibrations (1608, 1505). ¹H NMR spectrum (300 MHz, CDCl₃, δ, ppm, J/Hz): 6.90 (s, H-2), 6.90 (s, H-5), 6.90 (s, H-6), 5.65 (d, J = 7.9, H-7), 3.70 (m, H-8), 3.96 (s, H-9), 7.05 (d, J = 1.3, H-2'), 7.13 (d, J = 1.3, H-6'), 7.40 (d, J = 17.5, H-7'), 6.61 (dd, J = 17.5, 8.5, H-8'), 9.65 (d, J = 8.5, H-9'), 3.88 (s, OMe), 3.94 (s, OMe), 5.70 (s, 4-OH), 9.65 (d, J = 8.5, 4-CHO) [8].

3-[2-(4-Hydroxy-3-methoxyphenyl)-3-hydroxymethyl-7-methoxy-2,3-dihydro-1-benzofuran-5-yl]propan-1-ol (3), C₂₀H₂₅O₆, [M]⁺ 360, white amorphous compound, [α]_D²⁵ +5.5° (*c* 0.18, MeOH), mp 209°C (dec.), *R*_f 0.5 (CHCl₃–MeOH, 9.3:0.7). ¹H NMR spectrum (300 MHz, CDCl₃, δ, ppm, J/Hz): 6.93 (d, J = 1.83, H-2), 6.86 (d, J = 8.09, H-5), 6.90 (dd, J = 8.09, 1.83, H-6), 5.54 (d, J = 7.48, H-7), 3.59 (m, H-8), 3.94 (dd, J = 10.91, 4.42, H-9a), 3.88 (dd, J = 10.91, 6.02, H-9b), 6.67 (s, H-2'), 6.65 (s, H-6'), 2.66 (t, H-7'), 1.87 (m, H-8'), 3.68 (t, J = 6.41, H-9'), 3.88 (s, OMe), 3.94 (s, OMe), 5.70 (s, 4-OH), 3.87 (s, 9-OH) [9].

5,4'-Dihydroxy-6,7,3'-trimethoxyflavone (4), C₁₈H₁₆O₇, mp 201–203°C, [M]⁺ 344. ¹H NMR spectrum (400 MHz, CD₃OD, δ, ppm, J/Hz): 7.60 (1H, dd, J = 8.2, 1.8, H-6'), 7.9 (1H, d, J = 1.8, H-2'), 6.8 (1H, d, J = 8.2, H-5'), 6.3 (1H, s, H-3), 6.43 (1H, s, H-8), 3.7–3.9 (9H, s, OCH₃), 12.60 (1H, s, 5-OH) [10].

Hyperin (5), C₂₂H₂₂O₁₂, mp 232–235°C, [α]_D²⁰ –71.5° (*c* 0.5, EtOH). UV spectrum (EtOH, λ_{max}, nm): 361, 298 (sh.), 259; (+NaAc) 370, 270; (+AlCl₃) 420, 280; (+NaAc + H₃BO₃) 380, 290; (+NaOC₂H₅) 410, 280. IR spectrum (mineral oil, ν, cm⁻¹): 3400–3200 (OH), 1670, 1620, 1615 (C=O), 1520, 1470 (C=C). ¹H NMR spectrum (400 MHz, CD₃OD, δ, ppm, J/Hz): 5.4 (d, J = 7, H-1''), 6.12 (d, J = 2, H-6), 6.43 (d, J = 2, H-8), 6.85 (d, J = 8.5, H-5'), 7.2 (d, J = 2.5, H-3'), 7.53 (d, J = 2.5, H-2'), 7.85 (dd, J = 8.5, 2, H-6') [11].

Compounds 2–4 were isolated for the first time from plants of the genus *Climacoptera*.

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