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FLAVONOIDS OF *Lavandula spica* FLOWERS

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Flowers of common lavender, *Lavandula spica* L. (Lamiaceae), possess a broad spectrum of biological activity (antiseptic, cholegogic, sedative, diuretic). However, this valuable plant has not been widely used for medicinal purposes in the Russian Federation. Only the bactericidal preparations Livian and Lavender Alcohol that are based on the essential oil prepared from fresh lavender flowers are produced at present in the RF [1-3] whereas this plant is widely used abroad as a sedative [4, 5].

The goal of our work was to study the flavonoid composition of lavender flowers growing in Morocco.

We used flowers of common lavender collected in Morocco in a valley in the Atlas Mountains (2006) and dried in the open air in shade.

Lavender flowers (200 g) were exhaustively extracted with ethanol (70%) and macerated at the same time (24 h) followed by heat extraction at 85-90°C. The aqueous alcohol extracts were evaporated in vacuo to a thick residue (~50 mL). The condensed extract was dried over silica gel L 40/100. The resulting powder (extract and silica gel) was placed on a layer of silica gel pretreated with $CHCl_3$. The chromatography column was eluted with $CHCl_3$ and $CHCl_3$:EtOH of various ratios (97:3, 95:5, 93:7, 90:10, 88:12, 85:15, 80:20, 70:30). The separation was monitored by TLC.

Fractions containing flavonoids were combined (compounds **1** and **2** separately) and placed on Wolem polyamide for further purification. The dry powder (extract and polyamide) was transferred to a chromatography column (sorbent height 4.0 cm, diameter 5 cm) that was eluted with water and aqueous ethanol (20, 40, 70, and 96%). The purification over the polyamide columns produced compounds **1** (70% EtOH eluent) and **2** (40% EtOH eluent), which were further purified by recrystallization from aqueous alcohol.

The structures of **1** and **2** were elucidated using PMR, UV spectroscopy, mass spectrometry, and chemical transformations.

Flavonoids **1** and **2** were cleaved by β-glucosidase (Fluka, Hungary) into glucose and aglycons, which were identified by TLC as apigenin (5,7,4′-trihydroxyflavone) and luteolin (5,7,3′,4′-tetrahydroxyflavone), respectively.

The PMR spectrum of **1** contained two 2H doublets at 7.95 and 7.02 ppm with spin—spin coupling constants 9 Hz that were assigned to protons H-2′, H-6′ and H-3′, H-5′, respectively; two 1H doublets at 6.81 ppm and 6.43 ppm with J = 2.5 Hz that were characteristic of protons in ring A of a flavonoid (H-8 and H-6); and a singlet for H-3 at 6.69 ppm (flavonoid compound). Furthermore, the spectrum had a singlet for a 5-OH of a flavonoid, which in combination with the results of enzymatic hydrolysis and UV spectroscopy data (lack of a bathochromic shift of the short-wavelength absorption band in the presence of sodium acetate) placed a carbohydrate on the 7-OH group with the glucose bonded as a β-D-glucopyranosyl moiety (characteristic doublet of an anomeric proton at 5.15 ppm with J = 7.5 Hz).

The combined results from chemical transformations and spectral data suggest that **1** has the structure 5,7,4′-trihydroxyflavone 7-*O*-β-D-glucopyranoside (cosmosiin).

The chemical structure of **2** was studied analogously. Based on UV, NMR, mass spectra, and chemical transformations, it was identified as luteolin 7-*O*-β-D-glucopyranoside (cinaroside).

Cosmosiin (apigenin-7-*O*-β-D-glucopyranoside) (1), light yellow crystals, $C_{21}H_{20}O_{10}$, aglycon $[M]^+$ 270 (100%), mp 225-227°C (aqueous alcohol). UV spectrum (EtOH, λ_{max}, nm): 270, 335; +NaOAc, 269, 378. PMR spectrum [200 MHz, $(CD_3)_2CO$, δ, ppm, J/Hz]: 3.3-4.0 (6H, glucose), 5.15 (1H, d, J = 7.2, glucopyranose H-1″), 6.43 (1H, d, J = 2, H-6), 6.81 (1H, d, J = 2.5, H-8), 6.89 (1H, s, H-3), 7.02 (2H, d, J = 9, H-3′, H-5′), 7.95 (2H, d, J = 9, H-2′, H-6′), 12.50 (1H, s, 5-OH).

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Cinaroside (luteolin-7-*O*-β-D-glucopyranoside) (2), light yellow crystals, $C_{21}H_{20}O_{11}$, aglycon $[M]^+$ 286 (100%), mp 232-234°C (aqueous alcohol). UV spectrum (EtOH, λ_{max}, nm): 257, 266sh, 352; +NaOAc, 258, 268sh, 380. PMR spectrum [200 MHz, $(CD_3)_2CO$, δ, ppm, J/Hz]: 3.3-3.9 (6H, glucose), 5.09 (1H, d, J = 7.2, glucopyranose H-1″), 6.43 (1H, d, J = 2, H-6), 6.59 (1H, s, H-3), 6.80 (d, J = 2.5, H-8), 6.87 (1H, d, J = 9, H-5′), 7.36 (1H, d, J = 2.5, H-2′), 7.38 (1H, dd, J = 2, 9, H-6′).

Compounds **1** and **2** were isolated for the first time from lavender flowers. Regarding flavonoids in general, the presence in lavender flowers of luteolin (5,7,3′,4′-tetrahydroxyflavone) has been reported in the foreign literature [6]. However, in our opinion this claim requires confirmation because luteolin was not observed in lavender flowers during our investigations.

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