POLYPHENOLIC COMPOUNDS OF Scabiosa caucasica

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In Scabiosa caucasica M. B. (Caucasian scabious), family Dipsacaceae, growing in the environs of Kislovodsk, we have found nine compounds of phenolic nature. Seven of them have been isolated by chromatography on cellulose and by gel filtration through Sephadex of type G-50. A comparison of the chemical composition of this species with the composition of the scabiouses that we have studied previously [1] showed that this species, as well, is characterized by the presence of quercetin 7-β-D-glucopyranoside (mp 245-246°C, from methanol; λ_{max} 372, 257 nm) and luteolin 7-β-D-glucopyranoside (mp 255-257°C; λ_{max} 350, 264, sh., 255 nm).

Substance (III), $C_{28}H_{32}O_{15}$, has mp 275-277°C (from pyridine, λ_{max} 342, 255, 265 nm. A study of this substance in the UV region with diagnostic additives showed the presence in it a free hydroxy group on C-5 and the absence of free hydroxy groups from C-7 and in the lateral phenyl radical. Quantitative acid hydrolysis showed the presence of two sugar residues (yield of aglycone 48.8%). On the basis of the results of UV spectroscopy, alkaline degradation, and comparison with known samples, the aglycone was identified as diosmetin, and the carbohydrate component as rutinose. A comparison of the physicochemical properties of substance (III) with the pale yellow diosmetin 7-rutinoside isolated previously from scabious showed that they were identical.

Substances (IV) and (V), were obtained from the freshly gathered herb by extraction with water. The concentrated aqueous extract was chromatographed on a column of Kapron powder. The ethyl acetate extraction of the acidified eluates gave substance (IV), $C_9H_8O_4$, mp 195-197°C (from hot water), which was identified by its physicochemical properties as caffeic acid [2].

Substance (V) was obtained from a concentrated alcoholic eluate by exhaustive extraction with acidified diethyl ether. It had the composition $C_{18}H_{18}O_9$ and melted at 204-206°C, $[\alpha]_D^{20}$ $-33°$ [c 0.1; methanol–water (4:1)]. The formation of an acetyl derivative showed that the substance contains five hydroxy groups. On acid hydrolysis it decomposed into caffeic and quinic acids, and it did not form a lactone [3, 4] on being heated with conc. acetic acid. The physicochemical properties of compound (V) were identical with those of 3-caffeoylquinic (chlorogenic) acid.

Substances (VI) and (VII) were isolated from the freshly-gathered flowers by extraction with acetone followed by precipitation of the flavonoids with benzene–chloroform (1:1). The combined substances were separated by chromatography on a column of cellulose.

Substance (VI), $C_{15}H_{10}O_5$, has mp 349-351°C, λ_{max} 270, 336 nm, R_f 0.85 [benzene–ethyl acetate–acetic acid (24:73:2)]. The IR spectrum of this flavonoid coincided with that of apigenin when superposed upon it.

Substance (VII), $C_{27}H_{30}O_{14}$, mp 240-242°C. UV spectrum: λ_{max} 262, 334 nm; $\lambda_{max}^{AlCl_3}$ 278, 300, 345, 380 nm (free hydroxy group on C-5; $\Delta\lambda$ +46 nm); $\lambda_{max}^{C_2H_5ONa}$ 270, 304, 390 nm (free OH group on C_4'). No bathochromy was observed on the addition of sodium acetate. Acid hydrolysis in methanol–conc. hydrochloric acid–water (2:1:1) for 3.5 h gave apigenin, glucose, and rhamnose. To determine the structure of the carbohydrate component, apigenin 7-O-β-neohesperidoside (rhoifoline) was synthesized independently by Seshadri's method [5] from naringin (naringenin 7-O-β-neohesperidoside), and the identity of substance (VII) with rhoifoline was shown.

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LITERATURE CITED

1. G. N. Zemtsova and V. A. Bandyukova, Khim. Prirodn. Soedin., 4, 247 (1968).
2. V. A. Bandyukova, G. N. Zemtsova, N. V. Sergeeva, and V. I. Frolova, Khim. Prirodn. Soedin., 6, 388 (1970).
3. H. Fischer and G. Dangschat, Chem. Ber., 65, 1009 (1932).
4. H. Fischer and G. Dangschat, Chem. Ber., 65, 1037 (1932).
5. T. R. Seshadri and N. Narasimhachari, Proc. Ind. Acad. Sci., 30A, 151 (1949).