COUMARINS OF Peucedanum baicalense

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The composition of the roots and fruit of Peucedanum baicalense Redow. C. Koch. has been studied previously by paper chromatography [1, 2]. On the basis of a chromatographic comparison of an extract of the roots with authentic samples of coumarins, it was concluded that the plant contained peucedanin [1] and peucedanin and imperatorin [2].

We have studied the roots of P. baicalense collected in September, 1972 in the Kulundinskaya steppe in the environs of the village of Novoegor'evskii (Altai territory). By the chromatography of a defatted acetone extract of the roots on silica gel L 40/100 μ using carbon tetrachloride and ethyl acetate with an increasing gradient of the latter as eluents and subsequent crystallization we isolated four individual compounds: (I) $C_{16}H_{14}O_4$, mp 104-106° C, R_f 0.45 [Silufol, petroleum ether−ethyl acetate (1 : 1), yellow fluorescence in UV light]; (II), $C_{17}H_{16}O_5$, mp 100-101 C, R_f 0.25, yellow fluorescence; (III), $C_{19}H_{20}O_5$, mp 104-105.5° C, $[\alpha]_D^{18}$ −47.5° (c 1.0; $CHCl_3$), R_f 0.23, violet fluorescence; and (IV), $C_{12}H_8O_5$, mp 221-222° C, R_f 0, yellow fluorescence. By preparative chromatography in a thin layer of silica gel in the petroleum ether−ethyl acetate (1 : 1) system we isolated a substance (V), $C_{12}H_8O_4$, mp 186-188° C from the mother liquors after the crystallization of (II).

According to its NMR spectrum (Varian HA-100D, 0 − HMDS, 20° C), substance (I) is a furocoumarin [chemical shifts in ppm (CCl_4): H_3 6.01, d, 9.5 Ha; H_4 7.90, d, 9.5 Hz; H_8 6.94, s; $H_{4'}$ 6.92, d, 3 Hz; $H_{5'}$ 7.45, d, 3 Hz] containing an isopentenyloxy group [$(CH_3)_2C{=}C$ 1.64, 1.74 s; $CH-CH_2-0$, 4.80, d, 7 Hz; $C{=}CH-CH_2-$ 5.44, t, 7 Hz]. A comparison of IR spectra and the melting point of a mixture of (I) with an authentic sample enabled this substance to be identified as isoimperatorin. Compound (II) is also a furocoumarin (δ, ppm ($CDCl_3$): H_3 6.17, d, 9.5 Hz; H_4 8.01, d, 9.5 Hz; $H_{4'}$ 6.90, d, 3 Hz; $H_{5'}$ 7.53, d, 3 Hz] containing a methoxy group (4.08 s), and an isopentenyloxy group [$(CH_3)_2C{=}C$ 1.61, 1.64; $CH-CH_2-O$ 4.76, d, 7 Hz; $CH_2-CH{=}C$ 5.53, t, 7 Hz]. The results of a comparison of the IR spectra of (II) and of an authentic sample of phellopterin and the absence of a depression of the melting point of a mixture showed their identity. Substance (III) is a linear hydroxydihydrofurocoumarin [δ, ppm (CCl_4): H_3 5.97, d, 9.5 Hz; H_4 7.38, d, 9.5 Hz; H_5 7.04, s; H_8 6.53, s; $(CH_3)_2C-O$ 1.49, 1.55; $CH-CH_2-Ar$ 3.16, d, 8 Hz; CH_2-CH-O (5.0, t, 8 Hz] acylated with angelic acid (characteristic multiplets at 1.6-1.9 ppm and 5.9 ppm); the substances had an IR spectrum identical with that of deltoin and gave no depression of the melting point in a mixture with an authentic sample. Substances (IV) and (V) were shown to be identical with authentic samples of 8-hydroxy-5-methoxypsoralen and bergapten, respectively, by their IR spectra and mixed melting points.

Thus, the roots of P. baicalense contain isoimperatorin, phellopterin, deltoin, 8-hydroxy-5-methoxypsoralen, and bergapten and do not contain the peucedanin and imperatorin that were identified by paper chromatography [1, 2].

LITERATURE CITED

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