ISOPEUCENIDIN FROM *Libanotis montana*

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From the roots of *Libanotis montana* Crantz, collected in the Moscow oblast by L. I. Sdobnina, by extraction with carbon tetrachloride followed by chromatography on silica gel in the petroleum ether–ethyl acetate system with an increasing concentration of the latter, we have isolated a colorless crystalline substance with the composition $C_{21}H_{22}O_7$, mp 132-134°C, $[\alpha]_D^{20}$ + 134° (c 0.89; ethanol), R_f 0.44 [Silufol;petroleum ether–ethyl acetate (1:1)]; M^+ 386.

The UV spectrum of the substance [λ_{max}^{EtOH} 217, 249, 259, 323 nm (log ε 4.45, 3.64, 3.45, 4.12, respectively)] shows that it is a derivative of 7-hydroxycoumarin.

The IR spectrum (Fig. 1 has the absorption bands of the C=O group of an α-pyrone ring and of an ester grouping (1730 cm^{-1}) and of the C=C groups of an aromatic system (1650, 1625, 1580 cm^{-1}).

The NMR spectrum ($CDCl_3$, 20°C, 0 – HMDS, Varian HA-100D) shows that the compound is a derivative of a 9-acyloxyoroselol { δ, ppm: 1.51, 1.62 s, 3H each [$(CH_3)_2$—C—]; 5.12, d, J = 6.1 Hz, 1H (CH—CH—O); 6.92 d, J = 6.1 Hz, 1H (AcO—CH—CH); 6.75, d, J = 8 Hz, 1H (H_6); 7.31 d, J = 8 Hz, 1H (H_5); 6.15, d, J = 10 Hz, 1H (H_3); 7.52, d, J = 10 Hz, 1H (H_4) }, acylated with acetic acid (1.91, s, 3H) and senecioic acid (1.82, 2.17, s, 3H each; 5.52, m, 1H).

Thus, the substance has structure (I) or (II).

Structure (I) corresponds to peucenidin [1], which was first ascribed structure (II) [2]; however, as was shown later [3], peucenidin is identical with 9-acetoxy-O-senecioyl-8,9-dihydrooroselol [4]. The compound isolated differs from peucenidin in its physicochemical constants (mp, IR spectrum), and in the NMR spectrum of a mixture of a sample of this substance with peucenidin separation of the H_3, H_8 signals and also the signals of the protons of the methyl groups of the acetic and senecioic acids is observed.

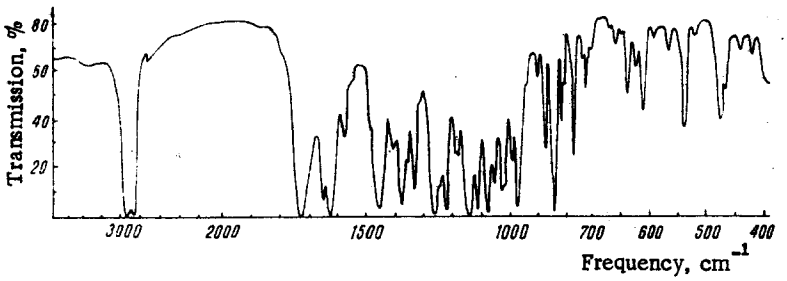

Fig. 1. IR spectrum of isopeucenidin (mull in paraffin oil).

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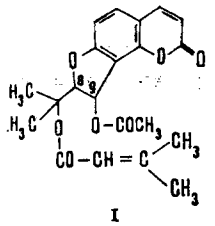
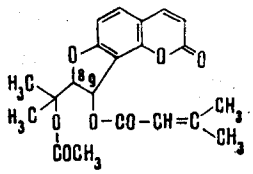


I



II

Consequently, the substance is the isomer of peucedinin isopeucedinin, and corresponds to structure (II).

LITERATURE CITED

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4. F. Bohlmann and M. Grenz, Chem. Ber., 102, 1673 (1969).