ISOGOSFEROL - A NEW FUROCOUMARIN FROM THE ROOTS OF Prangos lophoptera

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In a study of a chloroform extract from the roots of <u>Prangos lophoptera</u> Boiss, we have isolated a crystalline substance (I) with the composition $C_{16}H_{14}O_{5}$, mp $72-73.5^{\circ}C$ (from ether). This compound possesses the characteristic properties of coumarin derivatives and belongs to the group of 8-monosubstituted linear furocoumarins. The structure of (I) was shown on the basis of its chemical and spectral properties.

Thus, in the NMR spectrum of (I) (Fig. 1a) in the region of aromatic protons there are doublets with chemical shifts of δ 6.35 and 7.75 (J = 10 Hz) (1 H each) and 6.81 and 7.68 ppm (J = 2.5 Hz) (1 H each), corresponding to protons 3 and 4 of the coumarin nucleus and protons 4' and 5' of the furan ring. A singlet at 7.37 ppm (1 H) is due to the proton in position 5. On the basis of this, substance (I) can be assigned to the 8-monosubstituted furocoumarins with a substituent having the composition $C_5H_9O_2$. In the region of aliphatic protons there are the signals of the protons of a methyl group on a double bond (1.81 ppm, singlet, 3 H), a hydroxy group (1.87 ppm, singlet, 1 H), and a methylene group on a double bond (4.99 and 5.06 ppm, singlets, 1 H each). A multiplet in the range from 4.30 to 4.68 (3 H) is due to the protons in the $-O-CH_2-CH_2$ grouping. These facts show that (I) has the structure of 8-(2*hydroxy-3*-methyl-butenyloxy)-furo-2*,3*: 7,6-coumarin and is an isomer of gosferol [1].

The acetylation of (I) with acetic anhydride in pyridine formed a monoacetate (II), $C_{18}H_{16}O_6$, with mp 67-68°C (from petroleum ether), the NMR spectrum (Fig. 1b) of which showed the signal from the COCH₃ group at 2.05 ppm (singlet, 3 H) and a paramagnetic shift of the signal of the methine proton, which was located at 5.58 ppm (quartet, 1 H, $J_1 = 4$ Hz, $J_2 = 8.5$ Hz).

The treatment of (I) with 10% sulfuric acid gave a substance (III) with the composition $C_{16}H_{14}O_5$, mp 134-135.5°C (from a 1:1 mixture of chloroform and petroleum ether), which was shown to be identical with a known furocoumarin which we obtained previously from (-)-heraclenin and prangenin hydrate [2].

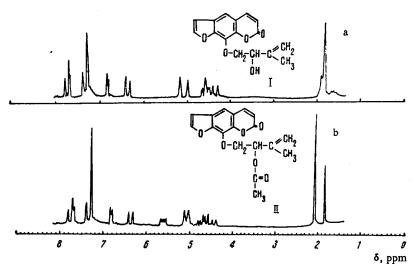


Fig. 1. NMR spectra of isogosferol (a) and isogosferol acetate (b).

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The NMR spectra were taken on a Varian HA-100D instrument with HMDS as 0, and the melting points were determined on a Kofler block.

LITERATURE CITED

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