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PRANFEROL FROM THE ROOTS OF PRANGOS FERULACEA

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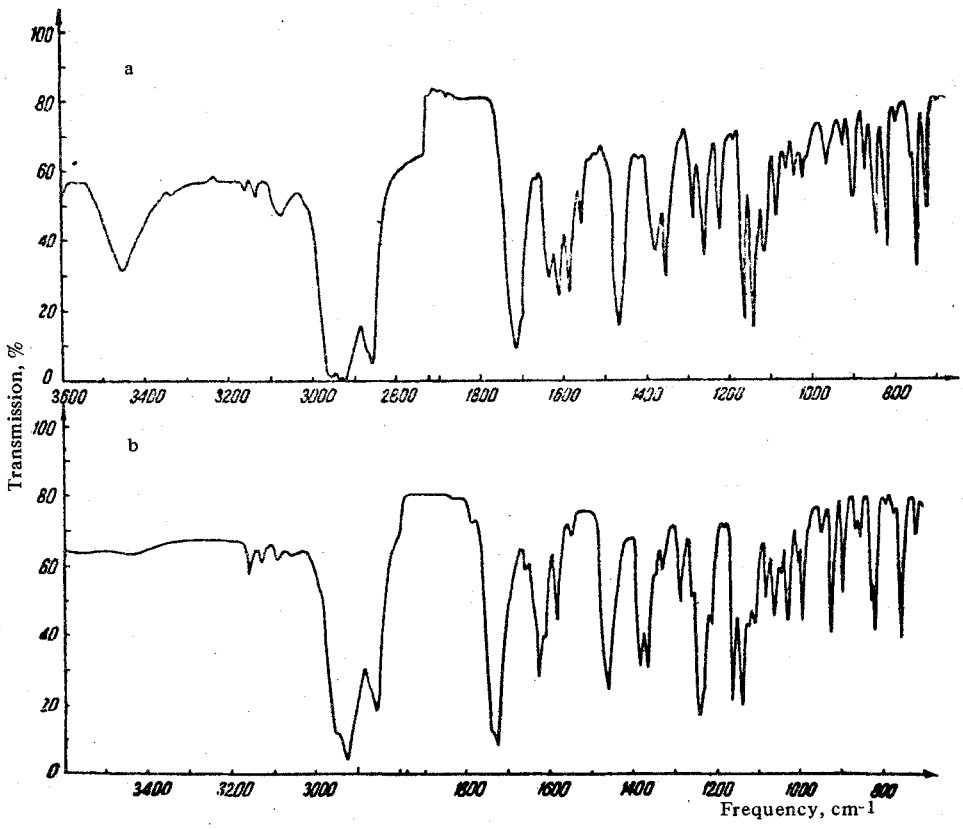
The present paper gives the results of a study of the structure of a coumarin derivative (I) $C_{16}H_{16}O_5$ from the roots of Prangos ferulacea (L.) Lindl., growing in Armenia.

The UV spectrum of (I) has characteristic maxima at 222, 250, 258, 266, and 310 mμ (log ε 4.19, 4.24, 4.09, 4.16, and 4.04, respectively), showing that it is a furocoumarin.



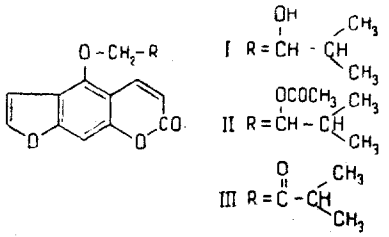
IR absorption spectra of (±)-pranferol (a) and its acetate (b).

The IR spectrum of (I) has absorption bands at 3445 cm^{-1} (OH), 1715 (C=O of a δ-lactone), 1630, 1610, 1585, and 1555 cm^{-1} (aromatic ring), and 748 and 760 cm^{-1} (furan ring) (figure, a). The IR spectrum of (I) is extremely similar to that of pranferol, the structure of which we have determined previously [1]. These results show that substance (I) is a 5-monosubstituted alkoxyfurocoumarin.

Acetylation of (I) with acetic anhydride in pyridine gave a monoacetyl derivative (II). The IR spectrum of the latter lacks the band of a hydroxy group and, in addition to the band of a C=O group of an α-pyrone (1725 cm^{-1}), there is the band of the C=O group of an ester (1740 cm^{-1}) (figure, b).

Oxidation of (I) with chromic anhydride in glacial acetic acid led to a substance (III) which was identified by a mixed melting point and by the similarity of the IR spectra as a known furocoumarin—isooxypeucedanin.

Results obtained enable us to propose for (I) the structure 5-(2"-hydroxy-3"-methylbutoxy)furo-2',3' : 7,6-coumarin. This structure corresponds to that of pranferol [1]. Nevertheless, the melting points of (I) and its acetate differ markedly from those for pranferol (mp 111° C) and its acetyl derivative (mp 112.5° C). Moreover, a mixture of (I) with an authentic sample of pranferol gave a depression of the melting point. On the basis of the above facts, it has been established that substance (I) is an optical isomer of pranferol.



I $R = CH(OH)-CH(CH_3)_2$

II $R = CH(OCOCH_3)-CH(CH_3)_2$

III $R = C(=O)-CH(CH_3)_2$

Experimental

Isolation of (±)-pranferol. A chloroform extract (158 g) from the roots (1.72 kg) was chromatographed on alumina (1.5 kg, activity grade 2.5). Elution was carried out with petroleum ether (for fractions 1–4), mixtures of chloroform and petroleum ether (1 : 4 for fractions 5–7; 1 : 2 for fractions 8–15; and 1 : 1 for fractions 16–27), and chloroform (for fractions 28–44). The volume of each fraction was 250 ml. After distillation of the solvent, the chloroform fractions 32–34 yielded (±)-pranferol (I) with mp 133° C (from ethanol), $[\alpha]_D^{20}$ ±0° (chloroform, acetone), R_f 0.34 [Al_2O_3, activity grade 2, ethyl acetate–benzene (1 : 1)]. Found, %: C 66.38; 66.41; H 5.38; 5.43. Calculated for $C_{16}H_{16}O_5$, %: C 66.66; H 5.55.

Acetylation of (±)-pranferol. A mixture of 0.069 g of (±)-pranferol, 3 ml of acetic anhydride, and 1 ml of pyridine was heated in the water bath for 2 hr. Then it was diluted with water and treated in the usual way. This gave 0.061 g of the monoacetyl derivative (II) with mp 119–120° C (from petroleum ether), R_f 0.62 [Al_2O_3, activity grade 2, ethyl acetate–benzene (1 : 4)]. Found, %: C 65.51; H 5.30. Calculated for $C_{18}H_{18}O_6$, %: C 65.45; H 5.45.

Oxidation of (±)-pranferol. A solution of 0.0489 g of (±)-pranferol in 0.6 ml of glacial acetic acid was treated with 0.034 g of chromic anhydride in 8 ml of 50% glacial acetic acid and the mixture was left for 2 days. From the reaction products was isolated a substance (III) with mp 146.5° C and R_f 0.66 (Al_2O_3, activity grade 2, ethyl acetate–benzene, 1 : 2).

The IR spectra were taken on a UR-10 infrared spectrophotometer (mull in paraffin oil). The microanalyses were performed by E. A. Sokolova.

Conclusions

From the roots of Prangos ferulacea (L.) Lindl. growing in Armenia an optically inactive furocoumarin $C_{16}H_{16}O_5$, an isomer of pranferol, has been isolated.

REFERENCE

1. G. A. Kuznetsova, A. Z. Abyshev, M. E. Perel'son, Yu. N. Sheinker, and G. Yu. Pek, KhPS [Chemistry of Natural Compounds], 2, 310, 1966.

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