SECORIN – A NEW DIHYDROFUROCOUMARIN FROM THE ROOTS OF Seseli coronatum

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From an acetone extract of the roots of Seseli coronatum Ledeb., collected by M. G. Pimenov in the environs of the village of Priozernyi (East Kazakhstan oblast), by chromatography on silica gel L 40/100 in the petroleum ether – ethyl acetate (3:1) system we have isolated a new coumarin derivative, secorin, $C_{23}H_{20}O_6$, with mp 212-213°C (from ethyl acetate), $[\alpha]^{20}_{D}$ −220° (c 1.0; ethanol), M^+ 392.

The UV spectrum of this substance in ethanol [λ_{max}, nm (log ε): 218 infl. (4.69), 247 infl. (4.16), 258 (4.13), 302 infl. (4.60), 3.19 (4.70)] shows that it is a 7-hydroxycoumarin derivative.

The NMR spectrum of secorin (Varian HA-100 D, $CDCl_3$, 0 – HMDS, 25°C) showed signals (δ, ppm) at 1.54 and 1.57 (s, 3H each, two $CH_3-\overset{|}{C}-OCOR$); at 3.23 (d, 2H, J = 8 Hz, $Ar-C\underline{H}_2-CH$); at 5.06 [t, 1H, J = 8 Hz, $-\overset{|}{\underset{|}{C}}-CH(OAr)-CH_2-Ar$]; at 6.17 (d, 1H, J = 10 Hz; H_3); and at 7.54 (d, 1H, J = 10 Hz, H_4). This shows that one of the fragments of the secorin molecule is a dihydrofurocoumarin residue [1]; the presence in the NMR spectrum (CD_3OD, 0 – HMDS, 25°C) of secorin of one-proton singlets at 7.34 ppm (H_5) and 6.69 ppm (H_8) shows that the secorin molecule is based on a dihydrofurocoumarin of the linear type – marmezin or nodakenetin. This conclusion is also confirmed by the presence in the mass spectrum of secorin of a peak with m/e 246, which is characteristic for derivatives of this type, such as esters of marmezin.

In addition to the band of a lactone carbonyl (1720 cm^{-1}), the IR spectrum of secorin (Fig. 1) has a band at 1690 cm^{-1}. This indicates that secorin consists of an ester of a dihydrofurocoumarin and an acid $C_9H_8O_3$ containing a double bond in the α,β position; this is also indicated by the presence in the mass spectrum of the compound of a strong peak with m/e 147 ($C_8H_7O-C{\equiv}O^+$), which is characteristic for such esters. The structure of the acyl residue follows from the IR and NMR spectra of secorin. An absorption band at 3350 cm^{-1} in the IR spectrum (see Fig. 1) shows that there is a hydroxyl in the acyl residue. In the

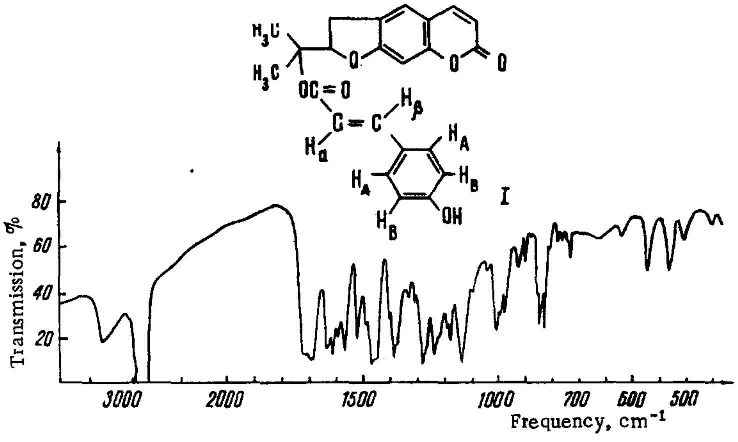

Fig. 1. IR spectrum of secorin (mull in paraffin oil).

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NMR spectrum (CD_3OD) there are the signals characteristic for a trans-p-hydroxycinnamic acid residue; two one-proton doublets at δ 5.98 ppm (H_α) and 7.05 ppm (H_β), J = 15.8 Hz (trans-CH = CH−), and two two-proton doublets at δ 6.65 ppm (H_A) and 7.11 ppm (H_B), J = 8.8 Hz (protons of a benzene ring).

The sign and large angle of the optical rotation of secorin enable it to be considered, with a fair degree of probability, to be a derivative of nodakenetin and not of marmezin.

Thus, secorin (I) is nodakenetin trans-p-hydroxycinnamate.

LITERATURE CITED

1. M. E. Perel'son, Yu. N. Sheinker, A. A. Savina, and G. P. Syrova, Khim. Prirodn. Soedin., 712 (1971).