SMIRNIORIN—A NEW COUMARIN FROM THE ROOTS OF SMIRNIOPSIS AUCHERI

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By extraction with methanol and subsequent chromatography on alumina, we have isolated from the roots of Smirniopsis aucheri Boiss. a new coumarin $C_{18}H_{18}O_7$ with mp 143–145° C (from aqueous ethanol), $[\alpha]_D^{20}$ −138° (c 0.96; ethanol), mol. wt. 346 (mass spectrometry), which we have called smirniorin.

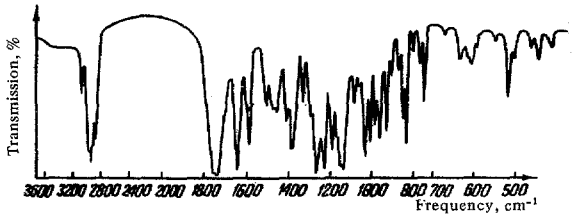


Fig. 1. IR spectrum of smirniorin (mull in paraffin oil).

Smirniorin's IR spectrum (Fig. 1) and its UV spectrum [λ_{max}, mμ: 220, 246, 257, 300 (inflection), 323; log ε 4.33, 3.57, 3.50, 3.99, 4.22] show that it belongs to the coumarin group.

The saponification of smirniorin gave acetic acid, which was identified by paper chromatography.

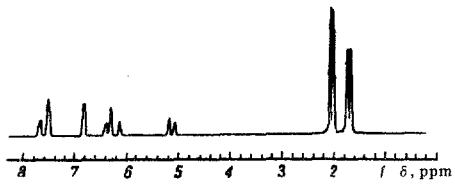
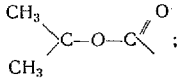
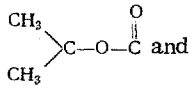
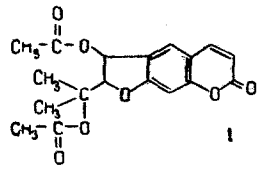


Fig. 2. NMR spectrum of smirniorin (60 MHz, O—TMS).

In the NMR spectrum of smirniorin (Fig. 2) the singlet with δ 1.66 and 1.72 ppm is due to the two nonequivalent methyl groups in the fragment  ; and the singlet with δ 2.02 and 2.05 ppm to two methyl groups of acetyl radicals. The doublets with δ 7.60 and 6.22 ppm (J = 10 Hz) relate to the $H_{(4)}$ and $H_{(3)}$ protons, a singlet with δ 7.52 of the $H_{(5)}$ proton being superposed on the $H_{(4)}$ signal. The singlet with δ 6.80 is due to the $H_{(8)}$ proton. Consequently, smirniorin is a 6,7-substituted coumarin. If we take into account the presence of  and CH_3CO— groupings, it is a dihydrofurocoumarin with two acetyl residues, which occupy a position in harmony with the doublets δ 5.4 and 6.37, J = 6.5 Hz (the latter is superposed on the $H_{(3)}$ signal). The doublet depends on two interacting protons in the —CH—OAr and —C—OCH—Ar groupings. Thus, smirniorin may be ascribed structure I—4'-acetoxy-5'-(1-acetoxy-1-methylethyl)-4',5'-dihydrofuro-2',3':7,6-coumarin



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