CONFERIN – NEW COUMARIN FROM THE ROOTS OF Ferula conocaula

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UDC 547.9:582.89

From the roots of Ferula conocaula Korov collected in the mountains of Mogol-Tau (Western Tadzhikstan) we have isolated a new terpenoid coumarin – conferin, $C_{26}H_{30}O_6$, with mp 141-142°C [diethyl ether–petroleum ether, $[\alpha]_D^{20}-124°$ (c 1.0; ethanol], M^+ 438. On the basis of the following facts, its most probable structure is considered to be that shown by formula (I).

The UV spectrum of conferin, [λ_{max}^{EtOH} 216, 243, 252, 296 infl., 324 nm (log ε 4.35; 3.86; 3.68; 4.07; 4.32, resp.) λ_{min} 260 nm (log ε 3.46)], is typical for umbelliferone derivatives. The IR spectrum of the compound (Fig. 1) – 1731 cm^{-1} (C=O of an α-pyrone and of an ester), 1715 cm^{-1} (C=O), 1655, 1615, 1564, and 1518 cm^{-1} (C=C bond of aromatic and heteroaromatic rings) – confirms that conferin is a coumarin derivative and shows the presence of keto and acyloxy groups in the terpenoid part of the molecule of the substance.

NMR spectrum of conferin ($CDCl_3$; 20°; 0 – HMDS; Varian HA-100D), δ, ppm: 1.02; 1.10; 1.20, singlets (3 CH_3–C–); 1.70, s., $W_{1/2}$=4.2 Hz ($\underline{CH_3}$–C=C–H); 2.04, s. (CH_3–COO–); 4.10, m (Ar–O–$\underline{CH_2}$–CH–) 5.41, s., $W_{1/2}$=6.0 Hz ($\underline{H}$–C=C–CH_3); 5.45, m., $\Sigma J \simeq 15$ Hz ($\underline{H}$–C–OOCCH_3); 6.21, d, J=9.5 Hz, (C_3–H) 6.78, m (C_6–H, C_8–H); 7.32, d, J=9.0 Hz, (C_5–H); 7.57, d., J=9.5 Hz (C_4–H). In the NMR spectrum of conferin the signals from the C_3'–H and C_4'–H are superposed on one another, and therefore their multiplicity was determined from the spectrum obtained with the addition of a diamagnetic shift complex [praseodymium (III) tris (1, 1, 1, 2, 2, 3, 3-heptafluoro-heptafluoro-7,7-dimethyloctane-4,6-dionate) monohydrate].

The acetoxy group was assigned to position 4' on the basis of a number of considerations. According to the value of the chemical shift of the proton geminal to the acetoxy group, the latter is adjacent to a C=O or –C=O bond. The half-width of the signal of the vinyl proton in the NMR spectrum of the analogous

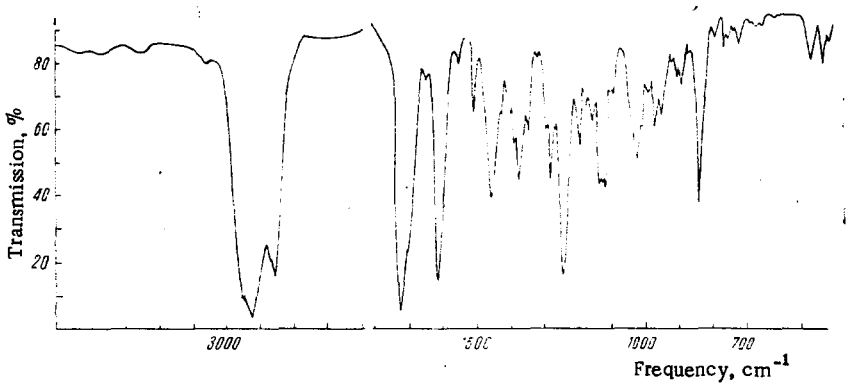
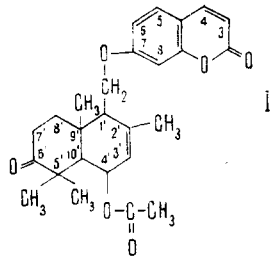


Fig. 1. IR spectrum of conferin (mull in paraffin oil).

All-Union Scientific-Research Institute of Medicinal Plants. Translated from Khimiya Prirodnykh Soedinenii, No. 5, pp. 660-661, September-October, 1974. Original article submitted May 5, 1974.

signal in the spectra of conferone and conferol ($W_{1/2}$ = 10 Hz) [1, 2]. This permits the assumption that the acetoxy group is most probably present in position 4'.



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