CONFERDIONE – A NEW COUMARIN FROM *Ferula conocaula*

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Continuing an investigation of *Ferula conocaula* Korov [1], growing in the mountains of Mogol-Tau (Southern Tadzhikstan), we have isolated from the fruit and roots of this plant a new terpenoid coumarin, conferdione (I), $C_{24}H_{26}O_5$, M^+ 394, mp 150-152°C (diethyl ether–petroleum ether), $[\alpha]_D^{20}$ –51.9° (c 0.2; ethanol).

It follows from the UV spectrum of (I) [$\lambda_{max}^{C_2H_5OH}$ 216, 235, 296, 322 nm (log ε 4.29, 418, 3.98, 4.23, respectively) λ_{min} 264 nm (log ε 3.51)] that it belongs to the 7-hydroxycoumarin derivatives. The absorption maximum at 235 nm shows the presence in the substance of a $-C=C-C=O$ grouping not conjugated with the coumarin nucleus. This is also confirmed by the IR spectrum of (I) (Fig. 1) which contains, in addition to bands of the C=O group of an α-pyrone (1725 cm^{-1}) and the band of an isolated keto group at 1710 cm^{-1}, a band at 1670 cm^{-1}. The empirical formula of (I) and the presence of two keto groups and one double bond, and also the NMR spectrum of the compound (see Table 1) show that conferdione is an ether of umbelliferone and a terpenoid alcohol of the iresane type. By means of double resonance it was shown that the compound contains the structural fragment $Ar-O-CH_2-CH-C(CH_3)=CH-$. In actual fact, irradiation of the olefinic proton (5.91 ppm) led to an increase in the peak intensity and to a decrease in the half-width of the signal of the methyl groups on the double bond (1.94 ppm, $W_{1/2}$=2.0 Hz). When the multiplet from the protons of the $Ar-O-CH_2=$group (4.21 ppm) was irradiated, the form of the signal at 2.64 ppm due to the proton at C_1' changed, and when an additional frequency corresponding to the resonance of this proton

TABLE 1. Characteristics of the NMR Spectrum of Conferdione ($CDCl_3$, 20°C, 0 – HMDS, HA-100D)

Chemical shift, ppm	Intensity	Multiplicity, J, Hz	Assignment
1,24	3H	s	$3CH_3-C-$
1,27	3H	s	
1,39	3H	s	
1,94	3H	ur $W_{1/2}$=4,0	2′–CH_3
2,47	1H	s	10′–H
2,64	1H	m	1′–H
4,21	2H	m	1′–CH_2–O–Ar
5,91	1H	ur $W_{1/2}$ = 6,0	3′–H
6,22	1H	d 9,5	3–H
6,78	2H	m	6–H; 8–H
7,34	1H	d 9,0	5–H
7,57	1H	d 9,5	4–H

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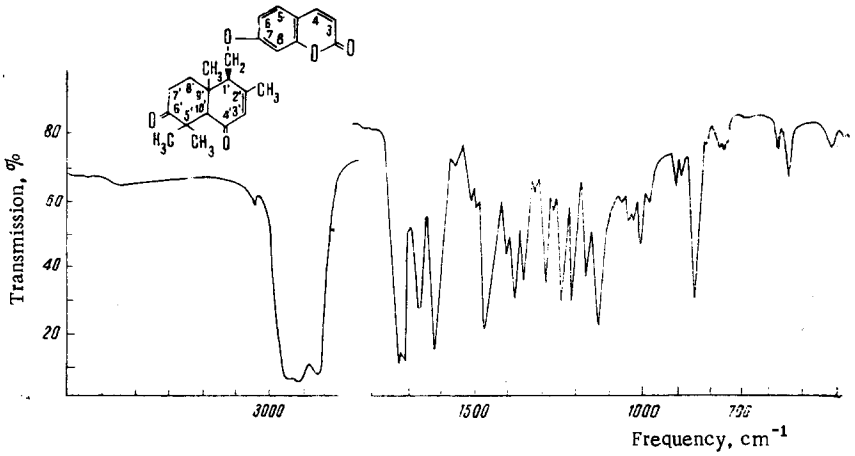

Fig. 1. IR spectrum of conferdione (mull in paraffin oil).

was superposed the multiplet at 4.21 ppm fused and its peak intensity increased, with a simultaneous contraction of the signal at 1.92 ppm (J = 2.2 Hz). The downfield shift of the signals of the methyl groups on the double bond and of the olefinic proton as compared with the corresponding signals of substances having similar structures (conferol, conferone, etc.) shows the conjugation of the double bond with the keto group. The position of the signals of the proton of the gem-dimethyl grouping shows that there is a carbonyl group in the α position to it. The results of a comparison of the nature of the splitting of the signal of the aryloxymethylene grouping with the corresponding signals of known compounds shows that the methylene group in conferdione is equatorial as in conferone and conferol [2]. The results obtained permit the assumption that conferdione most probably has the structure shown in Fig. 1.

LITERATURE CITED

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2. M. E. Perel'son, A. A. Kir'yanov, Yu. E. Sklyar, and V. V. Vandyshev, Khim. Prirodn. Soedin., 726 (1973).