CONFERONE – A NEW TERPENOID COUMARIN FROM THE FRUIT OF Ferula conocaula

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UDC 547.9:582.89

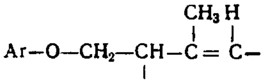
From the fruit of Ferula conocaula Korov., collected in the mountains of Mogoltau (Northern Tadzhikistan), by chloroform extraction and subsequent chromatography on alumina we have isolated a new terpenoid coumarin with the composition $C_{24}H_{28}O_4$ (M^+ 380), mp 142-142.5°C (from petroleum ether–ethyl acetate), $[\alpha]_D^{20}$ −51.0° (c 1.3; ethanol), and have called it conferone.

The UV spectra of the compound λ_{max}^{EtOH} 216, 242, 252, 325 nm (log ε 4.26, 3.71, 3.58, 4.31) is characteristic for coumarin derivatives with an O-alkyl substituent in position 7.

The IR spectrum of conferone (Fig. 1) shows, in addition to the bands specific for coumarin derivatives [1721 cm^{-1} (C=O of an α-pyrone ring), 1610, 1566, and 1508 cm^{-1} (C=C)] a ketone band (1710 cm^{-1}).

The NMR spectrum of the coumarin (taken on a Varian HA-100D instrument, $CDCl_3$, O – HMDS) showed that it is a terpenoid ether of umbelliferone (C_3–H, δ 6.16 ppm, d, J = 9.4 Hz; C_4–H, δ 7.55 ppm, d, J = 9.4 Hz; C_5–H, δ 7.29 ppm, d, J = 9.2 Hz; C_6–H, δ 6.77 ppm, q, J_{ortho} = 9.2 Hz, J_{meta} = 2.5 Hz; C_8–H, δ 6.75 ppm, d, J = 2.5 Hz).

The terpenoid residue $C_{15}H_{23}O$, contains three methyl groups attached to saturated quaternary carbon atoms (1.02, 1.06, and 1.08 ppm, 3H each), a methyl group at a double bond (1.65 ppm, broadened signal, $W_{1/2}$ 5 Hz, 3H), and an olefinic proton (5.54 ppm, broadened signal, $W_{1/2}$ 10 Hz). The terpenoid residue is attached to the hydroxy group of umbelliferone through a methylene group (4.09 ppm, 2H, J_{gem} = 10.0 Hz, J_{1vic} = 4.0 Hz, J_{2vic} = 4.9 Hz). The nature of the splitting of the signal of this group shows that it is attached to a secondary atom. It was shown by the double-resonance method that the terpenoid part of conferone contains the



$Ar{-}O{-}CH_2{-}\underset{|}{CH}{-}\overset{CH_3}{C}{=}\overset{H}{C}{-}$

fragment.

It follows from the empirical formula of the compound and the presence of one C=O and one C=C bond that the terpenoid residue has a bicyclic structure. When conferone was deuterated in an alkaline medium, two hydrogen atoms were replaced by deuterium (NMR spectrum). This shows that the carbonyl is located between a quaternary carbon atom and a methylene group.

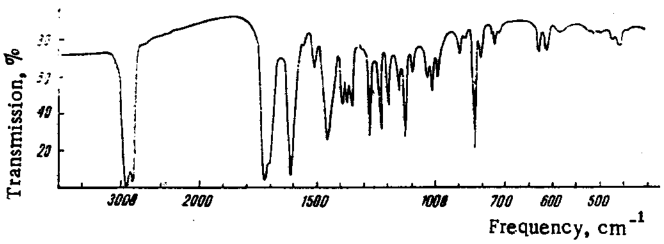
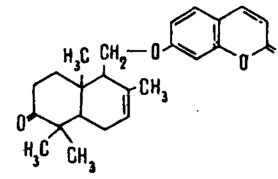


Fig. 1. IR spectrum of conferone (mull in paraffin oil.



The facts obtained permit us to put forward the structure shown above for conferone.

All-Union Scientific-Research Institute of Medicinal Plants. Translated from Khimiya Prirodnykh Soedinenii, No. 5, pp. 669-670, September-October, 1972. Original article submitted April 19, 1972.