ISOSAMARCANDIN FROM Ferula microloba

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From a neutral ethereal extract of the roots of Ferula microloba Boiss (Turkmen SSR), by chromatography on silica gel, we have isolated an optically active crystalline substance with mp 221°C, composition $C_{24}H_{32}O_5$, $[\alpha]_D^{20}$ +26.75° (c 0.4; ethanol), R_f 0.06 [TLC, benzene–chloroform–ethyl acetate (5 : 4 : 1) system], mol. wt. 400 (mass spectrometrically).

The UV spectrum [λ_{max}^{EtOH} 218, 243, 253, 295, 326 nm (log ε 4.14; 3.63; 3.53; 3.93; 4.19)] corresponds to that of a 7-O-alkylcoumarin.

IR spectrum, cm^{-1}: 3440, 3380 (OH), 1720 (α-pyrone carbonyl), 1620, 1510, 1460 (aromatic ring), 1390, 1365, and 1200 (gem-dimethyl group).

The nature of the fragmentation of this compound is typical for terpenoid coumarins. The umbelliferone part of the molecule consists of peaks with m/e (%) 162 (100) and 163 (43), and the terpenoid part of peaks with m/e 221 (8) $[M^+-161-18]$, 220 (49) $[M^+-162-18]$, 203 (37) [220−17], 187 (8) [220−18−15], 177 (6) [220−43]. In the region of high mass, information is given by several peaks with m/e 349 $[M^+-2H_2O-CH_3]$, 382 $[M^+-H_2O]$, and 385 $[M^+-CH_3]$.

The NMR spectrum of the compound (Varian, HA-100 D, $CDCl_3$, 0 – HMDS) shows the singlets of four methyl groups at 0.73 ppm; 0.88; 0.95 $\left(CH_3-\overset{|}{\underset{|}{C}}-\right)$ 1.17 $\left(CH_3-\overset{|}{\underset{|}{C}}-OH\right)$, a broadened signal at 3.2 ppm, $\frac{1}{2}\ \Sigma=$ 16 Hz ($H-\overset{|}{\underset{|}{C}}-OH$ axial proton), and the signals of $(Ar-O-CH_2-)$ methylene protons in the form of two quartets with their centers at 4.1 and 4.32 ppm, J_{gem} = 10.5 Hz; J_{vic} = 6 Hz. In the 6.1-7.6 ppm region are found the signals of the five protons of a 7-hydroxy-substituted coumarin ring.

On the basis of its melting point, $[\alpha]_D$ value, and its physicochemical properties, the structure of the compound corresponds to that isosamarcandin, which has previously been obtained synthetically [1].

This is the first time that isosamarcandin has been isolated from natural sources.

LITERATURE CITED

1. N. P. Kir'yalov and T. V. Bukreeva, Khim. Prirodn. Soedin., 643 (1972).

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