SAMARCANDIN ACETATE FROM THE ROOTS OF *Ferula pseudooreoselinum*

N. P. Kir'yalov and T. V. Bukreeva

UDC 547.314

In addition to the isosamarcandin angelate described previously [1], from the neutral fraction of the resin of the roots of Ferula pseudooreoselinum (Rgl. et Schmahl) K. Pol., by chromatography on neutral Al_2O_3 (activity grade II) with elution by chloroform and subsequent chromatography of the coumarin fraction (R_f 0.16) on inactive Al_2O_3 with elution by diethyl ether–petroleum ether (2 : 1), after prolonged crystallization from diethyl ether we have isolated a coumarin $C_{26}H_{24}O_6$, mp 152-153°C (from aqueous ethanol), $[\alpha]_D^{20}$ + 29.4° (c 1; ethanol); ethanol, M^+ 442 (mass spectrometry). This coumarin has not been found in plants previously.

UV spectrum:. $\nu_{max}^{ethanol}$ 325, 252, 242, 218 nm (log ε 4.19, 3.36, 3.56, 4.27).

IR spectrum: λ_{max} (cm^{-1}) 3560 and 3490 (OH group), 1720 (C = O of a lactone and C = O of an acetyl group), 1618, 1510 (C = C of a conjugated aromatic system), and 1260 (C–O of an acetyl group) (paraffin oil) (Fig. 1).

NMR spectrum: δ $CCDl_3$, 7.56 and 6.18 ppm (doublets, each 1H, J = 9 Hz) corresponding to H-4 and H-3; 7.3 ppm (doublet, 1H, J = 7 Hz) corresponding to H-5; 6.84 (singlet, 1H) corresponding to H-8; 6.79 ppm (quartet, 1H, J_1 = 7 Hz, J_2 = 2 Hz) corresponding to H-6; 4.6 ppm (broadened singlet, 1H) corresponding to C_3–H, equatorial at an acetyl residue; 4.36 and 4.10 (two quartets, each 1H, J_1 = 11 Hz, J_2 = 4 Hz and J_1 = 11 Hz, J_2 = 6 Hz) corresponding to O–CH_2–C_9; 2.0 ppm (singlet, 3H) corresponding to CH_3 of an acetyl group; 1.18 ppm (singlet, 3H) corresponding to CH_3–C_8; 0.88 ppm (singlet, 3H) and 0.81 ppm (singlet, 6H) corresponding to CH_3–C_{10} and $(CH_3)_2$–C_4. On the basis of these facts we came to the conclusion that the substance is an acetate.

The saponification of the coumarin under investigation gave a substance with mp 175-177°C which was identified by its melting point and IR spectrum as samarcandin [2].

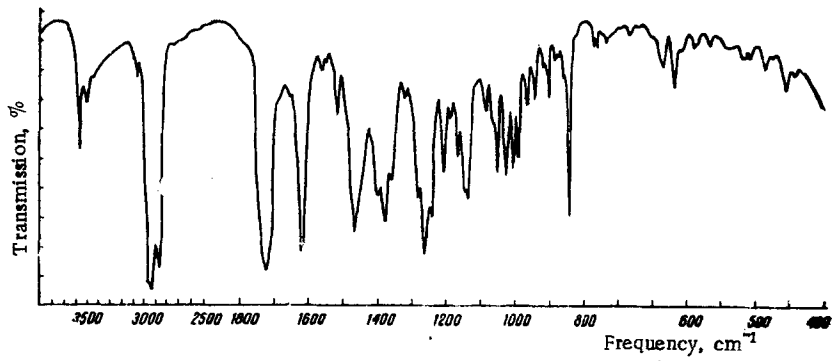
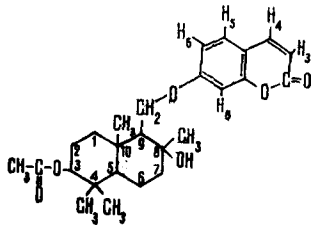


Fig. 1. IR spectrum of samarcandin acetate (paraffin oil).

V. L. Komarov Botanic Institute, Academy of Sciences of the USSR. Translated from Khimiya Prirodnykh Soedinenii, No. 6, pp. 798-799, November-December, 1972. Original article submitted June 6, 1972.

It follows from the chemical and spectral results that the coumarin under study is samarcandin 3-acetate [2].



The acetate with mp 152-153°C obtained by the acetylation of samarcandin gave no depression of the melting point with the isolated natural coumarin, and their IR spectra were identical.

LITERATURE CITED

1. N. P. Kir'yalov and T. V. Bukreeva, Khim. Prirodn. Soedin., 643 (1972).
2. N. P. Kir'yalov and S. D. Movchan, Khim. Prirodn. Soedin., 73 (1968).