STRUCTURE OF THALFLAVIDINE

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Studying the alkaloids of the roots of Thalictrum flavum L., we have isolated yellowish acicular crystals of an optically inactive base $C_{22}H_{21}NO_6$ with mp 219-220°C (methanol).

In the IR spectrum of the base there are absorption bands at 950 and 1060 cm^{-1} (CH_2O_2) and 1730 cm^{-1} ($C=O$). Its UV spectrum has four absorption maxima, at 254, 263, 296, and 400 nm (log ε 4.38, 4.49, 3.94, and 3.60), which are characteristic for phenanthrene derivatives [1].

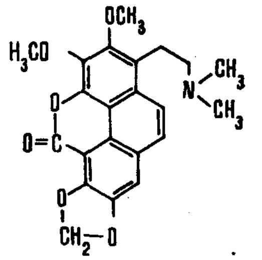
The NMR spectrum of the base shows the signals of protons at (τ scale) 7.70 ppm (singlet, 6H) [$N(CH_3)_2$], two three-proton singlets at 6.18 and 5.96 ppm from two methoxy groups, and a two-proton singlet at 3.71 ppm from a methylenedioxy group.

The base that we isolated proved to be new, and we have called it thalflavidine. On the basis of a study of spectral characteristics and a comparison of them with literature information, thalflavidine can be assigned to the dimethylaminoethylphenanthrene derivatives [1, 2].

The absorption at 1730 cm^{-1} in the IR spectrum of the base shows the presence of an α-pyrone system in it. The presence of the signal of the protons of the methylenedioxy group in the weak field of the NMR spectrum of thalflavidine (normal values 3.95-4.10 ppm) is due to the action of the carbonyl group and, consequently, the methylenedioxy group is located at C_6-C_7. Doublets at 2.44 ppm (J = 9 Hz), and 2.19 ppm (J = 9 Hz) belong to the two ortho-interacting C_9 and C_{10} protons. A multiplet at 7.50 ppm is due to a methylene group connected with an aromatic ring, and one at 6.74 ppm is due to nitrogen. A singlet at 2.56 ppm is due to the aromatic proton at C_8.

In the mass spectrum of thalflavidine (taken on an MKh-1303 instrument, 40 V, 0.4 mA, 120°C) there are peaks with m/e 395 (M^+), 337 $(M-58)^+$, 322, 279, 58 (100%) $CH_2={}^+N(CH_3)_2$.

On the basis of these facts, the following most probable structure can be suggested for thalflavidine:



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2. N. M. Mollov, Le Nyat Thuan, and P. P. Panov, Dokl. Bolgarskoi AN, 24, No. 8, 1047 (1971).

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