UDC 547.974/945

NMR SPECTRUM OF PRANGOSINE

S. T. Akramov, Kh. S. Mukhamedova, M. R. Yagudaev, and S. Yu. Yunusov

Khimiya Prirodnykh Soedinenii, Vol. 3, No. 4, pp. 287–288, 1967

A new alkaloid prangosine $C_{14}H_{13}O_3N$ has previously been isolated from Prangos pabularia [1, 2].

The results of a study of the oxidation, acetylation, and Hofmann degradation of this substance and its UV and IR spectra have permitted structure (I) to be proposed.

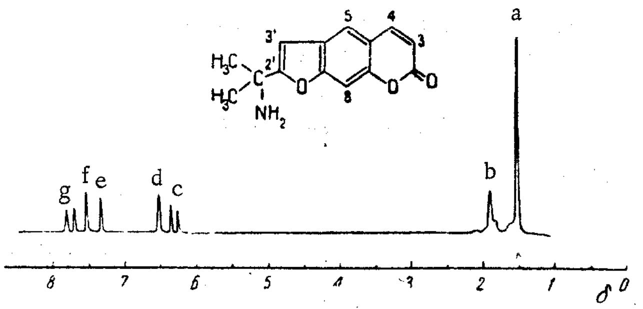
However, the position of the isopropylamine group and the arrangement of the furan nucleus in prangosine have not been rigidly demostrated.

The results of a study of the NMR spectrum of prangosine unambiguously confirm its structure as a 2'-monosubstituted furocoumarin and the linear arrangement of the furan nucleus in it.

As shown in the figure (spectrum recorded on a JNM-4H-100/100 MHz instrument in $CDCl_3$ solution, chemical shifts calculated in parts per million of the field with respect to tetramethylsilane, as internal standard, taken as 0), there are the doublets c($\delta = 6.22$; J = 10 Hz) and g ($\delta = 7.77$; J = 10 Hz) relating to the protons of positions 3 and 4 of the lactone ring, the singlets f ($\delta = 7.45$) and e ($\delta = 7.25$) relating to the protons in positions 8 and 5 of the coumarin ring, and the singlet d ($\delta = 6.44$) which is due to the proton in the 3' position of the furan ring [3].

If the furan nucleus were nonlinear, two systems of the type of c and g, i.e., four doublets, would be expected in the NMR spectrum of prangosine.

In our case there were the doublets c and g, the intensity of each of them being equal to one proton unit. The position of the signal at $\delta = 6.44$ shows that the lateral aminoisopropyl group is located in position 2' of the furan nucleus, as in anhydromarmesin, in which the signal of the 3'-proton is at 6.58 ppm [3]. At the same time, it is known that a proton in position 2' of the furan ring in furocoumarins shifts to a weaker field than that in position 3'. For example, the signals of the 2'-protons in psoralen and xanthotoxin are at 7.80 and 7.83, respectively [3].



The signal h ($\delta = 1.86$) with an intensity of two proton units relates to the protons of the NH_2 group and the singlet a (1.50) with an intensity of six proton units to the protons of the two CH_3 groups.

Thus, an analysis of the NMR spectrum of prangosine enables its structure to be established unambiguously as a 2'-monosubstituted furocoumarin with a linear arrangement of the furan nucleus with respect to the coumarin nucleus.

REFERENCES

1. S. Yu. Yunusov, S. T. Akramov, and G. P. Sidyakin, DAN UzSSR, no. 7, 23, 1957.
2. Kh. S. Mukhamedova, S. T. Akramov, and S. Yu. Yunusov, KhPS [Chemistry of Natural Compounds], 117, 1967.
3. Yu. N. Sheinker, G. Yu. Pek, and M. E. Perel'son, DAN SSSR, 158, 1382, 1964.

18 March 1967

Institute of the Chemistry of Plant Substances
AS UzSSR