MASS AND NMR SPECTRA OF HEMIPRANGOSINE AND N-DIMETHYLPRANGOSINE

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We have previously proposed structural formulas for hemiprangosine (I) and N-dimethylprangosine (II) on the basis of their chemical properties and their IR and UV spectra [1].

The mass spectrum of hemiprangosine has the peak of a molecular ion (M^+) with m/e 226, the peaks of ions with m/e 198, 183, and 155, and others. In the spectra of prangosine, N-dimethylprangosine (II), and hemiprangosine (I), the peaks of the molecular ions are the maximum peaks. The fragmentation of compound (I) under the action of electron impact takes place similarly to the fragmentation of prangosine and of (II) (beginning with m/e 226) [2]. The transitions m/e 226 → 198 and 198 → 193 are confirmed by metastable peaks of ions with m/e 173 and 169.

The NMR spectrum of (I) was taken on a JNM-4H-100 MHz instrument in $CDCl_3$ solution, the chemical shifts being calculated in parts per million relative to TMS as internal standard taken as zero. It showed doublets at δ 6.23 and 7.65 ppm, ascribed to the protons of a lactone ring, two one-proton singlets at δ 7.28 and 7.50 ppm from the protons of a benzene ring, a singlet with δ 6.56 from a furan proton, a three-proton singlet from methyl protons at δ 2.06 ppm, and two one-proton singlets at δ 5.76 and 5.18 ppm from two protons of a methylidene group.

The NMR spectrum of (II) differs from that of prangosine [3] by the fact that at δ 2.2 ppm there is a six-proton singlet from the protons of two methyl groups.

Thus, the results of the mass and NMR spectra of compounds (I) and (II) confirm the structures of prangosine and the products of its transformation that were proposed previously [1].

LITERATURE CITED

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