

A MASS SPECTROMETRIC STUDY OF PEDICULARINE AND ITS METHYL ESTER

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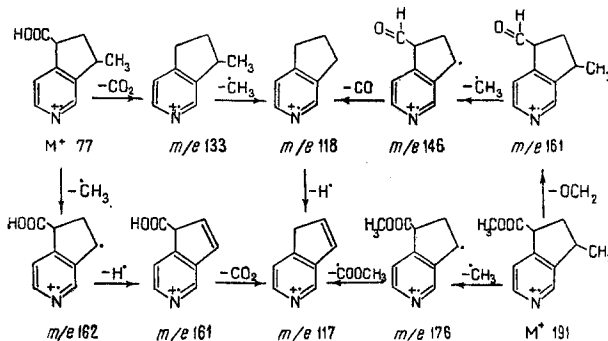
The mass spectrum of pedicularine (I) [1] has the peaks of ions with m/e 177 (52%), 162 (100%), 133 (40%), 118 (68%), 117 (52%), 91 (34%) and 77 (14%). The fragmentation of the molecular ion (M^+ , 177) takes place mainly in two directions.

First direction: A methyl group is eliminated from the molecular ion with m/e 177, and the maximum ion with m/e 162 appears, which loses a hydrogen atom and gives an ion with m/e 161. A molecule of CO_2 splits out from the latter forming an ion with m/e 117.

Second direction: Fragmentation begins with the splitting out of CO_2 from the molecular ion; an ion with m/e 133 is formed which is converted by the elimination of a methyl radical into an ion with m/e 118.

The mass spectrum of the methyl ester of pedicularine (II) has peaks of ions with m/e 191 (100%), 176 (88%), 161 (22%), 146 (20%), 118 (39%), 117 (22%), 91 (13%), and 77 (11%). The molecular ion forms the maximum peak (M^+ , 191) and is converted by the loss of a methyl radical into an ion with m/e 176. Then the ion with m/e 176 loses a CH_3OOC group, being converted into a fragment with m/e 117. Another fragmentation route begins with the splitting out of an OCH_2 group from the molecular ion (M^+ , 191) and the formation of an ion with m/e 161, which, by losing a CH_3 group, is converted into an ion with m/e 146. The ejection of a CO group from the ion with m/e 146 leads to an ion with m/e 118. Then the ion with m/e 118 loses a hydrogen atom and is converted into a fragment with m/e 117.

The further fragmentation of I and II takes place similarly to that of indicaine and plantagonine [2].



The mass spectra were taken on an MKh-1303 instrument at 95° C with an ionization energy of 40 eV.

REFERENCES

1. A. Abdusamatov, S. Khakimdzhanov, and S. Yu. Yunusov, KhPS [Chemistry of Natural Compounds], 5, 457, 1969.
2. A. Abdusamatov and S. Yu. Yunusov, KhPS [Chemistry of Natural Compounds], 4, 392, 1968.

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