# STRUCTURE OF PEDICULARIDINE

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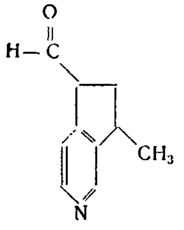
By the treatment of the combined alkaline ethereal alkaloids of Pedicularis olgae Rgl. with acetone we have isolated a new alkaloid $C_{10}H_{11}ON$, mp 211-212°C (from ethanol), $[\alpha]_D^{20} + 67.7°$ (c 1.2; methanol), $R_f$ 0.70 [TLC, silica gel, ethanol–chloroform–butyl acetate (3 : 2 : 1) system], mol. wt. 161 (mass spectrometry), which we have called pedicularidine (I) [1].

The UV spectrum of the base has two absorption maxima, at 236 and 270 nm (log ε 3.36 and 3.32, respectively), showing the presence of a pyridine ring in the alkaloid. The IR spectrum of (I) shows absorption bands at 2960 $cm^{-1}$ (C-methyl and methylene groups), 1700 $cm^{-1}$ ($-C=O$ of an aldehyde group), and 1600 $cm^{-1}$ (pyridine). The mass spectrum of (I) (MKh-1303 instrument, energy of the ionizing electrons 40 eV, 85°C) shows the peaks of ions with m/e: $M^+$ 161 (100%), 160 (16%), 133 (4%), 132 (15%), 118 (16%), 117 (19%), 91 (10%), and 77 (6%). The fragmentation pathways of the molecular ion are similar to those for indicaine [2].

When (I) was oxidized with silver oxide in an alkaline medium, an amino acid $C_{10}H_{11}O_2N$ (II) with mp 203-204°C (from methanol), $[\alpha]_D^{20} + 52.85°$ (c 1.4; ethanol), mol. wt. 177 (mass spectrometry) was formed. In the UV spectrum of (II), as in that of pedicularine, there are two maxima, at 265, 272 nm (log ε 3.12, 3.15). In the IR spectrum of (II) there is an absorption band at 1710 $cm^{-1}$ ($-C=O$ of a carboxy group). The methylation of (II) gave its methyl ester $C_{11}H_{13}O_2N$ (III) with mp 82-83°C (ether), mol. wt. 191 (mass spectrometry). The IR spectra of this compound had an absorption band at 1730 $cm^{-1}$ ($-C=O$ of an ester).

The IR spectra of (II) and (III) proved to be similar to the spectra of pedicularine and its methyl ester [3, 4], respectively. A mixture of the product of the oxidation of pedicularidine with pedicularine melted at 205-207°C.

On the basis of the facts presented, we propose structural formula (I) for pedicularidine.



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