PHYSOCHLAINE – A NEW ALKALOID FROM Physochlaina alaica

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The combined alkaloids from the roots of Physochlaina alaica E. Korot., collected in the period of the withering of the epigeal part, were separated into benzene-, chloroform-, and water-soluble fractions. From the benzene fraction, apart from previously-known compounds [1], by chromatography on a column of silica gel with elution by ether we isolated bases $C_{17}H_{19}NO_3$ (I) with mp 79-80°C and $C_{17}H_{21}NO_2$ (II) with mp 62-63°C (ether).

The chloroform-soluble fraction was treated with hot benzene, giving 6-hydroxyhyoscyamine [1]. The benzene-insoluble chloroform- and water-soluble fractions of the combined alkaloids were chromatographed on a column of silica gel. Elution with chloroform–methanol (9:1) gave the new bases $C_{17}H_{23}NO_4$ (III) with mp 68-69°C and physochlaine (IV).

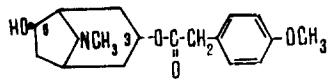
On the basis of its IR, UV, mass, and NMR spectra, and also the absence of a depression of the melting point of a mixture with an authentic sample, substance (II) was identified as apoatropine [2, 3].

Physochlaine, $C_{17}H_{23}NO_4$, mp 75-76°C (hexane), $[\alpha]_D^{20} \pm 0°$ (c 3.4; methanol), R_f 0.44 [in a thin layer of silica gel in the methanol–benzene–ammonia (9:1:0.1) system]; M^+ 305.

The IR spectrum of (IV) shows absorption bands at (cm^{-1}) 825 (para-disubstituted benzene ring), 1730 (ester carbonyl group) and 3280-3420 (broad) (hydroxy group). Physochlaine forms a monoacetyl derivative (NMR spectrum: 2.00 ppm, 3 H, singlet, $CDCl_3$).

The IR spectrum shows absorption maxima at 230 and 283 nm (log ε 3.85, 3.55) which are characteristic for a disubstituted benzene ring. In the NMR spectrum of (IV) (CF_3COOH, δ scale) there are the signals of the protons of a $N-CH_3$ group at 2.52 ppm (3 H, singlet), an aromatic methoxy group at 3.50 ppm (3 H, singlet), a one-proton triplet at 4.78 ppm (C_3H), and the signals of four aromatic protons in the range from 6.30 to 6.55 ppm. The mass spectrum of physochlaine has the peaks of ions with m/e 305 (M^+), 261, 156, 140, 96, 95, 94, 83, 82, 81, which are characteristic of the tropane alkaloids [4]. The formation of an ion with m/e 261 with the elimination of hydroxyethylene shows that in (IV) the hydroxy group is located at C_6. This is also confirmed by the results of the hydrolysis of the base to tropane-3α,6β-diol [5, 6].

Consequently, physochlaine has the structure of 3α-(p-methoxyphenylacetoxy)tropan-6β-ol.



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