NEW ALKALOIDS FROM Peganum harmala

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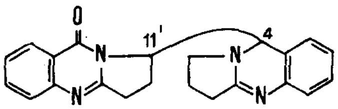
After the separation of the bases described previously [1, 2], we continued the separation of the mother liquors and obtained four individual substances.

Base (I), mp 169-170°C (ethanol), $[\alpha]_D$ ±0°, picrate 177-178°C. The UV and mass spectra of (I) and of peganidine [3] coincide, and their IR spectra are very similar but have some differences. The results of a comparison of the NMR spectra of the two bases are given in Table 1.

Substance (I) and peganidine are probably racemic diastereoisomers. We have called compound (I) isopeganidine; deoxypeganidine [2] was obtained from it by a known method [4].

Base (II), mp 221-223°C (acetone), UV spectrum $\lambda_{max}^{ethanol}$, nm: 226, 277, 305 (inflection), 317 (inflection) (log ε 4.48, 4.14, 4.05, 3.89). IR spectrum, cm^{-1}: 1590, 1620, 1660 (double bonds, amide carbonyl). The mass spectrum had the peak of the molecular ion with m/e 356, and a strong peak with m/e 171 (100%) and a peak with m/e 185 (3%). Consequently, (II) is a biomolecular base consisting of fragments of deoxypeganine and deoxyvasicinone; it has been called dipegine. In the NMR spectrum of (II) in the region of aromatic protons there is a single-proton doublet and two multiplets with intensities of 7 proton units. The absence of a two-proton singlet in the 4.5 ppm region (δ scale) shows that in the deoxypeganine fragment position 4 is substituted. This is confirmed by the oxidation of dipegine with potassium permanganate. Deoxyvasicinone was isolated from the reaction products. These results, and also the ease of cleavage of the bond on electron impact show that the most probable position for the bridge in dipegine is 4-11', and that the structure of (II) can be represented by the formula



Bases (III) and (IV) were isolated by the vacuum distillation of the liquid part of the combined bases (15 mm Hg). Two fractions were obtained with bp 126-134°C and 144-150°C. Both fractions gave a picrate with mp 201-202°C. From the mother liquor a second picrate was obtained with mp 187°C. The picrates were identified by direct comparison with those of quinoline and quinaldine.

Thus, from the mixture of bases of Peganum harmala we have obtained another four substances: isopeganine and dipegine – new alkaloids – and quinoline and quinaldine, which have been found in the family Zygophyllaceae for the first time.

TABLE 1

Compound	Aromatic protons (4H)	C_9 C_4 (2H)	C_{10} (2H)	C_{11} (2H)	C_{12} (2H)	C_{14} (3H)
Peganidine	6,86	5,02	2,4 2,04	3,35 3,73	3,07	1,86
Isopeganidine	6,86	5,05	2,45 2,05	3,47	2,95	1,82

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