

## ISOLATION OF BETAINE FROM *Chenopodium botrys*

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*Chenopodium botrys* L. (Jerusalem oak) has long been used as an antiasthmatic, antiplasmatic, and anticatarrh agent. Recently, additional information has been obtained on its use in the treatment of hyper-tonia.

Previously [1], one of the authors isolated from the epigeal part of Jerusalem oak 0.12% of total alkaloids, which were separated into four bases characterized by their temperatures and empirical formulas.

The present paper gives the results of the isolation from this plant of another nitrogenous base - betaine.

We investigated the epigeal part of Jerusalem oak collected in the fruit-bearing phase in the valley of the R. Issyk, Alma-Ata oblast. The comminuted air-dry raw material (40.0 g) was moistened with 10 ml of 10%  $\text{NH}_4\text{OH}$ , covered with 250 ml of methanol, and steeped for a day with periodic stirring. The extraction was repeated three times, the extract was concentrated to 100 ml, 20 ml of methanol was added, and the precipitate that deposited was filtered off. The filtrate was chromatographed on a column containing 20 g of air-dry alumina and eluted with methanol. The eluent was collected in 10-ml fractions which were analyzed by TLC [type KSK silica gel, acetone-methanol (2:8)]. The fractions containing the substances with similar  $R_f$  values were combined. By recrystallization from n-butanol a substance was isolated with mp  $292^\circ\text{C}$  (decomp.) and  $R_f$  0.37 in an amount of 1.52% of the weight of the air-dry raw material. A large amount of this substance was obtained from the extract of 30 kg of air-dry raw material by five extractions with ethanol under factory conditions. The substance isolated gave positive reactions for alkaloids. The action of ethereal HCl on an alcoholic solution gave the hydrochloride. The molecular weight determined for the hydrochloride by potentiometric titration was 151.

On the basis of its physicochemical constants, the hypothesis was put forward that the substance isolated was betaine with the structure  $(\text{CH}_3)_3\text{N}^+-\text{CH}_2-\text{C}\begin{matrix} \text{O}^- \\ \diagup \\ \text{O} \end{matrix}$ . Its elementary composition and its spectra confirmed this conclusion. The IR spectrum of this substance has bands characteristic for a carboxylate ( $1400$  and  $1635\text{ cm}^{-1}$ ), while on passing to the hydrochloride as a result of the formation of a carboxy group the  $1635\text{-cm}^{-1}$  band shifted to  $1730\text{ cm}^{-1}$ .

In the NMR spectrum, taken in  $\text{D}_2\text{O}$ , there were two singlets at 3.40 and 4.02 ppm, relating to methyl and methylene groups. The ratio of the signals was close to 4.5 ( $392\text{ mm}^2/85\text{ mm}^2$ ). In the mass spectrum taken at an ionizing voltage of 40 V there were the molecular peak  $\text{M}^+$  with  $m/e$  117 and the  $\text{M}-1$  peak, of equal intensity, corresponding to the detachment of hydrogen and a series of peaks corresponding to the cleavage of the  $\alpha$  and  $\beta$  bonds with respect to the nitrogen with the loss of one or more hydrogens of which the strongest were those with  $m/e$  58, 57, 56, and 55, and 72 and 71. The high intensity of such peaks is due to the presence of quaternary nitrogen in the fragments. This is the first time that betaine has been isolated from Jerusalem oak. In addition to betaine, we obtained preparatively a second nitrogenous base with  $R_f$  0.057. Chromatographically, this base was found in the stems, inflorescences, and roots of *Chenopodium botrys* L. in all phases of development.

### LITERATURE CITED

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