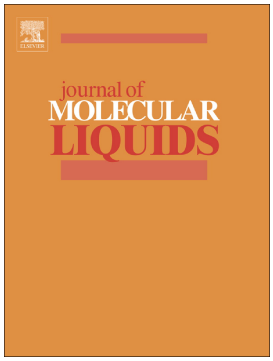

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Marina V. Fedotova, Sergey E. Kruchinin

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Hydration and Ion-Binding of Glycine Betaine: How They May Be Involved into Protection of Proteins under Abiotic Stresses

Marina V. Fedotova* and Sergey E. Kruchinin

G.A. Krestov Institute of Solution Chemistry, the Russian Academy of Sciences, Akademicheskaya st., 1, Ivanovo, 153045 Russia

* To whom correspondence should be addressed. Email address: hebrus@mail.ru (M. V. Fedotova)

Abstract

Glycine betaine (GB) is a widespread natural osmolyte, which accumulates in the cell cytoplasm to protect structure and function of various proteins and enzymes under osmotic, salinity, or temperature stresses. It is assumed that the hydration of GB is playing an important role in the protective mechanism. However, the details of GB interactions with water surroundings are far from being fully understood. In this contribution, the hydration structure of GB under effects of concentration, temperature, and NaCl/KCl additions, as well as ion-binding of this zwitterionic compound was studied to gain information on the functioning of GB in particular and of osmolytes in general. The data were obtained by the integral equation method in the framework of the 1D- and 3D-RISM (Reference Interaction Site Model) approaches. An attempt was made to link the structural features of hydration and ion-binding of GB to its biological role. It was found that under osmolyte concentration effect, as well as under temperature and salinity stresses, GB molecules are strongly hydrated, revealing the strong ability of the osmolyte to bind a significant amount of water. These results are a confirmation for the stabilizing effect of GB on proteins under abiotic stresses via an indirect mechanism. Moreover, the salt additions stimulate the formation of direct ion-molecular associates between the charged groups of GB and inorganic ions as a result of ion-specific interactions. In our opinion, the ability of GB to retain the inorganic ions around itself is directly related to the protection of proteins from salting-out.

Keywords: Biomolecule; Osmolyte; Glycine betaine; Hydration; Ion-binding; 1D- and 3D-RISM integral equation methods