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ORIGINAL ARTICLE

Taurine as a water structure breaker and protein stabilizer

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Abstract The enhancing effect on the water structure has been confirmed for most of the osmolytes exhibiting both stabilizing and destabilizing properties in regard to proteins. The presented work concerns osmolytes, which should be classified as "structure breaking" solutes: taurine and *N,N,N*-trimethyltaurine (TMT). Here, we combine FTIR spectroscopy, DSC calorimetry and DFT calculations to gain an insight into the interactions between osmolytes and two proteins: lysozyme and ubiquitin. Despite high structural similarity, both osmolytes exert different influence on protein stability: taurine is a stabilizer, TMT is a denaturant. We show also that taurine amino group interacts directly with the side chains of proteins, whereas TMT does not interact with proteins at all. Although two solutes weaken on average the structure of the surrounding water, their hydration spheres are different. Taurine is surrounded by two populations of water molecules: bonded with weak H-bonds around sulfonate group, and strongly bonded around amino group. The strong hydrogen-bonded network of water molecules around the amino group of taurine further improves properties of enhanced protein hydration sphere and stabilizes the native protein form. Direct interactions of this group with surface side chains provide a proper orientation of taurine and prevents the SO_3^- group from negative influence. The weakened SO_3^- hydration sphere of TMT breaks up the hydrogen-bonded network of water around the protein and destabilizes it. However, TMT at low concentration stabilize both proteins to a small extent. This effect can be attributed to an actual osmophobic effect which is overcome if the concentration increases.

Keywords Taurine · Hydration · Protein interactions · DSC calorimetry · FTIR spectroscopy · DFT calculations

Introduction

Many organisms living in harsh environmental conditions developed different mechanisms to overcome the effects of adverse surrounding. One of them is an accumulation of small organic compounds commonly called osmolytes (Yancey 2001, 2004; Yancey et al. 2002; Auton et al. 2011; Singh et al. 2011; Panuszko et al. 2009, 2016; Bruździak et al. 2012, 2016) which, besides the osmotic pressure regulatory function, have an impact on macromolecules' stability. Considering the chemical structure, this group of molecules includes: polyols, amino acids, amines, urea and its derivatives, etc. This article is devoted to taurine and its influence on water structure and protein stability.

Taurine is a β-amino acid, however, instead of the carboxylic group it has the sulfonate one. This functional group is more acidic than the carboxylate one and this property [$pK_a < 0$–1.5, various values are available in literature (Madura et al. 1997)] makes taurine almost completely zwitterionic (NH_3^+–CH_2–CH_2–SO_3^-) over the physiological pH range. Taurine can be found in many animal tissues,

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