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WATER EFFECTS ON SACCHARIDE MATRICES STUDIED THROUGH MD AND FTIR

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Introduction

Saccharides, and in particular trehalose, are known for their high efficiency in protecting biostructures against adverse environmental conditions [1], although the preservation mechanism is still debated. Experiments and simulations on carboxy-myoglobin (MbCO) have shown that the protein dynamics is highly inhibited in a low-water trehalose host medium, the inhibition being markedly dependent on the amount of residual water. Trehalose effects have been related to its hydrogen-bonding (HB) properties, which have been studied by Infrared Spectroscopy (FTIR) and Molecular Dynamics simulations (MD) [2,3,4].

FTIR, through the study of the water association band and of the CO stretching band, pointed out the existence of a reciprocal protein-matrix coupling modulated by water content. In these systems different classes of water molecules could be distinguished, whose ratio is altered by chaotropic and kosmotropic solutes [3,5].

MD simulations pointed out that water molecules shared between protein and sugar could modulate the *strength* of the constraints imposed by the surrounding matrix on the protein, thus affecting its internal dynamics (atomic fluctuactions on ps/ns time scale) [4].

A deeper understanding of the role of water molecules in the dynamics of these system could shed light on trehalose peculiarity.

Experimental

Here we report on MD study of model systems constituted by a MbCO molecule embedded in a highly viscous (amorphous) trehalose-water matrix (830 trehalose molecules and 1909 water molecules, 89% w/w). NAMD code was used with CHARMM22 parameters. The system was equilibrated in the NPT ensemble with the Nosé-Hoover Langevin piston pressure control and then left to evolve in the NVT ensemble up to 5 ns. Runs were performed at various temperatures in the range 50-400K. For each temperature parallel simulations with either free or fixed water molecules (unable to either translate or translate *and* rotate) were performed in order to elucidate the