Coupling between Protein and Solvent Dynamics

TANER E. DIRAMA, GUSTAVO A. CARRI, Department of Polymer Science, The University of Akron, Akron, OH 44325-3909 — Trehalose and glycerol are commonly used to preserve biopolymers like proteins against denaturation and its consequent loss of activity. The molecular mechanism behind the preservation ability of such bio-protective agents is not fully understood at present. In this talk, we present a Molecular Dynamics simulation study of the short time (<1 ns) dynamics of lysozyme in trehalose and glycerol. The analysis of the dynamic structure factor and incoherent scattering function shows that the dynamics of lysozyme follows the one of the solvent. However, the effectiveness of this coupling decreases as we move away from the surface of the protein. In addition, we find that trehalose provides a better suppression of the dynamics than glycerol at temperatures above 250 K whereas glycerol is more effective at low temperatures, in agreement with experimental observations. Our hydrogen bonding analysis shows that trehalose forms stronger hydrogen bonds with lysozyme at high temperatures while glycerol has more robust hydrogen bonds at low temperatures. This correlation between hydrogen bond behavior and the dynamics suggests that hydrogen bonding between the protein and the solvent plays an important role in the suppression of the dynamics.

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