Abstract Submitted for the MAR08 Meeting of The American Physical Society

Dynamics of Lysozyme in Trehalose solutions PAVAN GHATTY, The University of Akron, EDWARD C. UBERBACHER, Oak Ridge National Laboratory — Anhydrobiosis in Tardigrades and Nematodes has been a topic of constant interest and intrigue in the scientific community. An increase in the concentration of Trehalose has been attributed to the ability of some organisms to survive extreme conditions of temperature, pressure and pH. Although there exist many experimental studies attributing this effect to Trehalose, the molecular details governing the interaction between Trehalose and proteins remains unclear. We have conducted a 20ns study of Lysozyme in varying concentrations of Trehalose in water. Strong and weak hydrogen bonds and hydrophobic interactions between water, Trehalose and protein seem to dictate the interactions in the system. We have observed a hydrogen bonded network of Trehalose around the protein entrapping a layer of water between itself and protein. Lysozyme remains in a near-native conformation throughout the simulation giving hints on the ability of Trehalose in preserving the structure of protiens.

Pavan Ghatty The University of Akron

Date submitted: 26 Dec 2007 Electronic form version 1.4