

Abstract Submitted
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Dynamics of Lysozyme in a Glycerol-Water system PAVAN GHATTY, GUSTAVO CARRI, The University of Akron — Bio-preservation of proteins is of great commercial and academic interest. A variety of sugars have been found to be effective in preserving the structure of proteins. This has been attributed and in some cases proved to their ability to form strong hydrogen bonds with proteins thus restricting their motion. The work presented here explores the hypothesis that glycerol, a tri-alcohol curbs the motion of protein.

We have carried out a 10ns Molecular Dynamics simulation to study the phenomenon. The structure of Lysozyme (PDB code 193L) has been studied in three solutions of 10, 20 and 30 % by weight of glycerol in water.

Glycerol molecules in all three solutions have shown a tendency to agglomerate around the protein. Strong hydrogen bonding has also been observed between glycerol molecules and the protein. With increasing time, the $g(r)$ of glycerol molecules around proteins shows two peaks with increasing prominence suggesting the movement of glycerol cluster to positions closer to the protein surface.

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