National Institute of Technology Rourkela

Synopsis Seminar

Seminar Title	: MOLECULAR DYNAMICS STUDIES OF PROTEINS IN AQUEOUS SOLUTION OF AMINO ACIDS AND WATER-ALCOHOLS MIXED SOLVENTS
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Abstract	: Preservation of a protein&rsquos three-dimensional native structure is crucial for structural biology, pharmaceuticals, and biomedical applications. Improper preservation can lead to loss of activity, aggregation, or immunogenicity. Proteins require carefully controlled environments to preserve their native structure. Conversely, disruption of protein structure is an important strategy to prevent Virus entry through host cell. Specific solvents and additives play a great role in regulating both phenomena. Thus, protein-solvent interactions have become a highly active and important field of research. The prime objectives of this thesis are to investigate the role and governing factors of protein conformational stabilities in the presence of two different sets of cosolvents, i.e., mixtures of different amino acids (AAs) solutions and water-alcohol(s) mixtures at various temperatures. The thesis consists of eight chapters. **Chapter 1** briefly describes current research on protein stability, focusing on the effects of aqueous environments and the presence of AAs as additives and alcohols as cosolvents. It also explores how solvents and key molecular factors contribute to maintaining protein structural integrity. To meet the objectives of the thesis, methodologies such as atomistic molecular dynamics (MD) simulations, molecular docking, and replica exchange MD (REMD) simulation techniques were adopted. **Chapter 2** discusses the methodologies briefly. **Chapters 3 &ndash 7** describe the work carried out. In **Chapter 3**, the influence of aqueous proline solutions with varying concentrations in modulating protein ubiquitin conformations at ambient and elevated temperatures was investigated. The study revealed the dual role of proline. **Chapter 4** deals with the effects of different hydrophobic AAs such as ala, val, ile, phe, on the protein ubiquitin. The relative stability of the protein in these AAs was quantified, and the solvation properties were explored. In **Chapter 5,** the comparative study based on REMD-generated trajectories on the stability of another protein, chymotrypsin inhibitor 2, in a wide range of temperatures was investigated in basic and acidic AA solutions, such as arg and glu, respectively. Further, the effects of the mixture of these AAs were explored. While **Chapter 6** elucidates the impact of various monohydric alcohols ethanol, iso-propanol, and n-propanol in their aqueous solutions (binary) and the mixtures of alcohols (ternary), on the conformations and solvation properties of the receptor binding domain (RBD) of SARS-CoV-2 at two different temperatures, **Chapter 7** discusses the impact of one of the potential ternary mixtures as identified from the previous chapter to influence the RBD-human ACE2 interactions at two different temperatures. The study reveals the rupture of the binding zone of both proteins in the presence of the ternary water-ethanol-isopropanol mixtures. This could be one of the possible reasons for reduced contamination of the virus spread. In the last chapter, **Chapter 8**, the chapter-wise conclusions and future scope of the thesis have been discussed.