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Preferential melting of secondary structures during protein unfolding in different solvents: Competition between hydrophobic solvation and hydrogen bonding BIMAN BAGCHI, SUSMITA ROY, RIKHIA GHOSH, Indian Institute of Science, Bangalore, India — Aqueous binary mixtures such as water-DMSO, water-urea, and water-ethanol are known to serve as denaturants of a host of proteins, although the detailed mechanism is often not known. Here we combine studies on several proteins in multiple binary mixtures to obtain a unified understanding of the phenomenon. We compare with experiments to support the simulation findings. The proteins considered include (i) chicken villin head piece (HP-36), (ii) immunoglobulin binding protein G (GB1), (iii) myoglobin and (iv) lysozyme. We find that for amphiphilic solvents like DMSO, the hydrophobic groups and the strong hydrogen bonding ability of the $>S=O$ oxygen atom act together to facilitate the unfolding. However, the hydrophilic solvents like urea, due to the presence of more hydrophilic ends (C=O and two NH_2) has a high propensity of forming hydrogen bonds with the side-chain residues and backbone of beta-sheet than the same of alpha helix. Such diversity among the unfolding pathways of a given protein in different chemical environments is especially characterized by the preferential solvation of a particular secondary structure.

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