



Abstract The Lysozyme Interaction with ZnONP Induces Structural Heterogeneity: A Thermodynamic-Based Approach ⁺

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Protein is an important biomolecule that needs to maintain 3D (three-dimensional) dynamic structure in respective physiological conditions in order for homeostasis to be maintained in an organism. This 3D structure is majorly governed by non-covalent intramolecular interactions. These interactions are highly subjected to changes in the local physicochemical environments of proteins. Any changes in the environment perturb the protein 3D conformation, leading to partial unfolding, consequently rendering the protein non-functional or the functional efficiency goes down. In recent years, various domains of biological sciences have increasingly embraced nanoparticles, primarily driven by its diverse array of physicochemical properties and applications. Protein adsorption onto nanoparticle surfaces affects the interaction that governs a 3D structure, resulting in conformational rearrangement and altered functional efficacy. The induced changes are very important to explaining the proper functioning of proteins in the presence of nanoparticles, regardless of whether it is being used as a platform for biological applications. In this line, lysozyme, a well-studied globular protein model, interaction with the ZnONP in different pH conditions is explored using various biophysical techniques. Lysozymes exhibit different conformations at varying pH levels, affecting their interaction interface with ZnONP. This altered protein conformation significantly influences the nature of interactions and ultimately impacts its thermodynamic attributes with ZnONP. Once the lysozyme interacts with the ZnONP interface, it sequesters the protein monomeric population into predominantly two population fractions, where the stable bulk monomeric population remains in equilibrium with relatively less thermodynamically stable monomeric lysozymes present in corona of ZnONP in the complex. However, changes in the conformation do not affect the secondary structure or the functional efficacy of the protein, thereby leaving the protein functional and adequately preserving its efficacy.

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