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Title Study of supramolecular interactions between proteins and lanthanide complexes

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The determination of the 3-D structure of any protein is essential for understanding its function. X-ray crystallography is the most used technique for the structure determination of biomacromolecules. Despite the availability of various experimental and computational methods for structure refinement, continuous improvement remains essential. Enter the crystallophore—a game-changing innovation. It is a lanthanide complex that acts as a molecular adhesive, enhancing the crystallization capacity of multiple proteins. This tiny molecule nestles between protein units, actively contributing to the crystal lattice. Due to the anomalous nature of f-block elements, it also acts as a very good phasing agent for X-ray crystallography. To boost performance, additional functional groups have been grafted onto the original compound. These modifications yield either fluorescent properties or more elegantly shaped crystals. Our focus lies on the understanding of the role of the crystallophore in the nucleation process through MD simulations and crystallization assays. We aim to unravel its interaction pattern with a model lysozyme protein, to understand the molecular basis of its nucleating properties. Additionally, we delve into other variants of the crystallophore, particularly to control and tune the size of protein crystals. We shall also study the impact of amino acid mutations in proteins on the efficiency of the crystallization process through the analysis of variants of the lysozyme protein.

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