Simulating walls of castle: understanding intricate protein lipid interactions during cellular process

Recognition of biomolecules is a fundamental control mechanism in eukaryotic cells. The precise targeting and versatility of these interactions such as, protein-protein, protein-ligand, and protein-membrane is the hallmark of several cellular processes that culminates into key biological functions. Therefore, an understanding of these processes on atomistic level would have significant biological and medical impacts. We use computational methods, in particular biomolecular simulations and structural bioinformatics, to understand the following processes (a) mechanism of peripheral membrane proteins and structural changes associated with their membrane localization (b) identifying structural scaffolds that targeted multiple binding partners in autophagy (c) structural and dynamical information of bacterial membrane interaction with small molecules. In this talk, I will provide a brief introduction to multi-scale computational approaches, and how they enable us to study biologically interesting problems. I will later converge to reveal our findings on the above mentioned themes.