# Structural and Dynamical Organization of Biomolecules: What are the Molecular Rules?

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Emergent properties of living systems evolve through a cascade of ordering events, executed by the constituent biomolecules. The fundamental molecular units of life, such as, DNA, RNA and proteins inside a cell have their own unique ways to organize themselves in order to actively perform cellular functions; cells can then come together to emerge as tissues, which can then work together and emerge as organs, organ systems, and finally organisms. In today's talk, I will discuss my efforts to understand the single molecular and collective behavior of biomolecules, leading to their structural and dynamical organization.

In the first part of my talk, I will discuss the highlights of my PhD work; I will briefly describe our work on identifying the fundamental hydrophobic, native contacts in two different proteins, HP36[1] and Myoglobin[2] which determine their tertiary structures and corresponding free energy landscape of unfolding. I will also discuss the experimental efforts to validate our *in-sillico* observation of remarkable structural transformation of Myoglobin in aqueous ethanol solution.

In the second part of my talk, I will first introduce the audience to the novelty of bottoms-up, coarse-grained computational approaches in order to develop understanding on collective behavior of living systems[3]. The emergent phenomena occurring in cellular systems are always accompanied by changes in cell shape, and therefore remodeling of their physical envelope, the bilayer membrane. However, due to the inherent complexity of these cellular processes, it often remains unclear what drives formation of such unique membrane morphologies and the associated events. Coarse-grained methodologies serve as one of the best strategies to approach this problem. I will describe our efforts to model two important cellular events which involve membrane remodeling — membrane budding[4] and membrane division[5]. We found that each of these events can be uniquely controlled by controlling the lipid distribution between the two leaflets of the membrane. Small changes in such transbilayer asymmetry generate substantially different mechanical tensions locally, which in turn control the preferred membrane curvature and morphology. Our results challenge the popular believe that membrane remodeling can only be achieved by complex cellular machinery and demonstrate alternative, non-trivial mechanisms of membrane remodeling, arising from the physical principles of membrane curvature elasticity which can be adopted in synthetic experimental procedures to execute remodeling of nanovesicles or liposomes.

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