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Using computational biophysics to understand protein evolution and function

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Understanding how proteins evolve and function is vital for human health (e.g., developing better drugs, predicting the outbreak of disease, etc.). In spite of its importance, little is known about the underlying molecular mechanisms behind these biological processes. Computational biophysics has emerged as a useful tool in this area due to its unique ability to obtain a detailed, atomistic view of proteins and how they interact. I will give two examples from our studies where computational biophysics has provided valuable insight: (i) Protein evolution in viruses. Our results suggest that the amino acid changes that occur during high temperature evolution of a virus decrease the binding free energy of the capsid, i.e., these changes increase capsid stability. (ii) Determining realistic structural ensembles for intrinsically disordered proteins. Most methods for determining protein structure rely on the protein folding into a single conformation, and thus are not suitable for disordered proteins. I will describe a new approach that combines experiment and simulation to generate structures for disordered proteins.