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Using computational biophysics to study protein structure, function and evolution

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Understanding how proteins evolve and function is vital for developing better drugs and for predicting and controlling the outbreak of disease. Yet, the biophysical implications of protein evolution are often not well understood. Computational biophysics has emerged as a useful tool in this area due to its unique ability to obtain an atomically detailed view of proteins and how they interact with other biomolecules. I will give examples from our studies where computational biophysics has provided valuable insight into protein evolution, and has been used to determine and analyze structural ensembles for intrinsically disordered proteins.