Molecular Simulation Studies of Pressure Effects on Proteins

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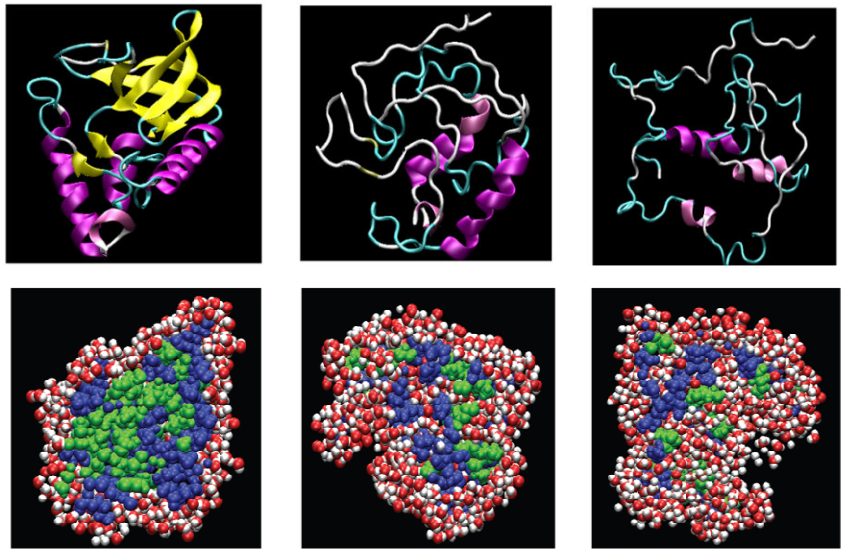
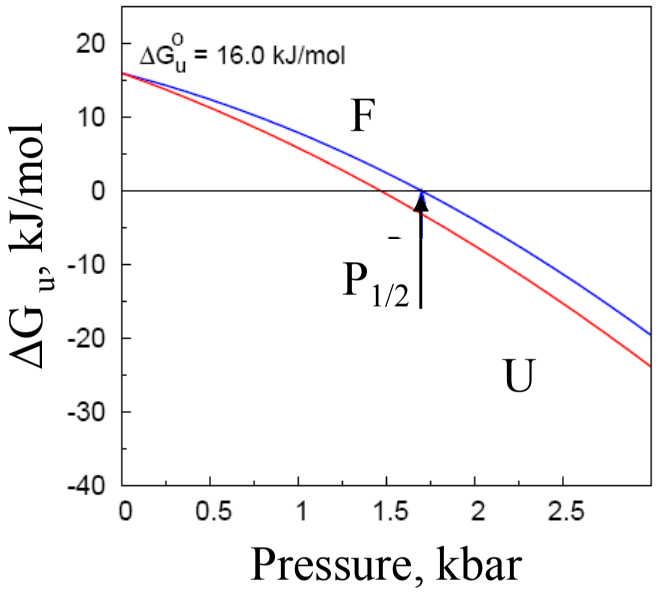
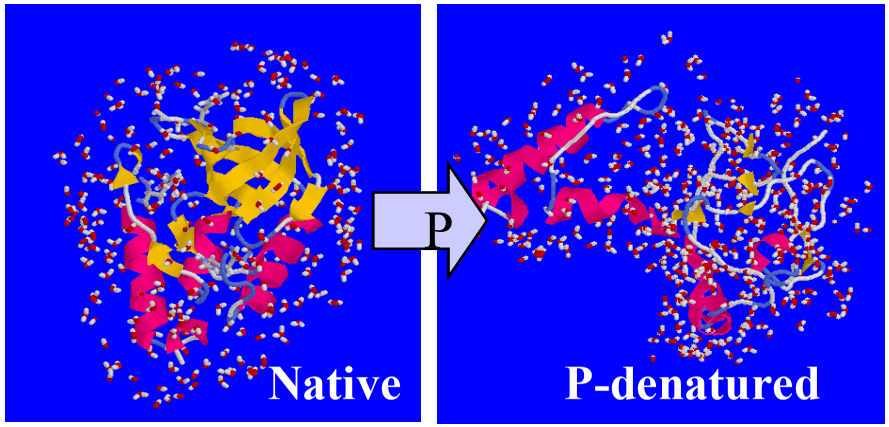


Brute force simulations of pressure unfolding of proteins are limited by length and timescales involved. We generated ensembles of partially to fully unfolded proteins using water insertions into protein interior.

Our method allows us to obtain partial molar volumes of folded and unfolded proteins, integration of which provides the free energy of unfolding at different pressures. Our results for Staph Nuclease are in good agreement with experimental data.





We are currently extending this work to study fundamental water-mediated (e.g., hydrophobic) interactions as well as other proteins and protein-protein complexes.