

All-Atom Simulations of Disordered and Flexible Proteins

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Molecular dynamics (MD) simulations are a useful tool to investigate the structure and dynamics of proteins because they can provide an all-atom view of their complex conformational landscapes. Using MD simulations, we can identify highly populated conformational states and determine the effects of perturbations (e.g. mutation, ligand binding, solution conditions) on their populations. I will present recent and ongoing simulation studies of disordered and flexible proteins, including the cancer protein STAT5B.