

Molecular simulation methods for ensemble-based drug design

Our group develops computational methodologies to enable rational modulation of protein dynamics for ligand design purposes. In this talk I will present molecular simulation methodologies we have used to characterise cryptic ligand binding sites in proteins. I will also discuss our efforts to develop robust alchemical free energy protocols and software for predicting protein-ligand binding energetics. I will present results obtained on diverse proteins that were the subject of retrospective studies, blinded predictions, and joint computational/experimental efforts.