

Protein interactions and dynamics

Abstract

The lecture will showcase how NMR and molecular dynamics simulations can provide insight into fundamental problems of protein biochemistry and biophysics. How can an electron-transfer protein use the same binding site to interact with different protein partners in order to receive, respectively deliver, an electron? How can we determine the thermodynamics of transitions to minor conformational species with very low populations (~1%)? Are structural changes required to propagate a molecular response to ligand binding through a protein molecule? How can exchanging water molecules and fluctuating intermolecular interactions contribute to sequence-specific recognition of DNA by proteins? At the end, methodologies will be presented that are capable of speeding up NMR analyses by orders of magnitude.

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