LAUFER CENTER
FOR PHYSICAL AND QUANTITATIVE BIOLOGY

Stony Brook University

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Seminar

Exploiting active site solvation structure and thermodynamics for drug discovery and design

Understanding the underlying physics of the binding of small-molecule drugs to protein active sites is a key objective of computational chemistry and biology. The displacement and reorganization of water molecules from the active site upon the binding of a ligand is a principal, and often dominant, source of binding free energy. We will discuss how we use statistical mechanics and molecular dynamics simulations to help characterize the solvation of protein active sites and how this information may be incorporated into computational tools aimed at aiding early-stage drug discovery and design efforts.

Friday, November 22, 2019

2:30 PM

Laufer Center Lecture Hall 101

Host: Rob Rizzo

Refreshments following the seminar in Laufer Hub 110

For a disability related accommodation, call 631-632-5400