Center for Soft Matter and Biological Physics

Discussion Meeting

Prof. David Minh

(Chemistry, Illinois Institute of Technology)

"New Computational Tools for Designing Compounds Active Against Biological Macromolecules"

Friday, July 12, 2019

1:30pm - 2:30pm

210 Robeson Hall

Most pharmaceuticals are small organic molecules that work via noncovalent interactions with biological macromolecules. Although drugs have saved or improved countless lives, drug discovery remains an inexact science that involves much trial and error. The main focus of my research group is the development of computer modeling tools to quickly characterize non-covalent protein-ligand interactions. Most of our tools are based on implicit ligand theory, a theoretical framework that I derived to predict how tightly molecules bind and how they influence the population of conformations accessed by their targets. At this point, we have established that our methods are able to reproduce results of more computationally expensive approaches. We are working on making them more efficient and feasible to use with large libraries of chemical compounds. We have also advanced the theory of end-point binding free energy methods, in which binding affinity is predicted based on molecular simulations of the bound complex.