

EXPAND

Simulating Protein Dynamics

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What you will do:

Molecular dynamics can be used in the drug development pipeline to analyze protein conformations and inform what type and size of drug is appropriate to bind to, and thus inhibit, the protein in question. **This project will teach the basics of molecular dynamics.** We will start by selecting a protein and defining what we want to analyze. Then we will go through the steps of preparing the structure, running a simulation, and analyzing the simulation. Within these confines, the student will get the freedom to make their own decisions based on what they feel is appropriate: they will select the protein they want to analyze, and decide on what analysis they want to do on this protein. This will increase their engagement and interest in the project. I have done these steps with several rotation students I mentored, mentees in my own labs, and experimental collaborators wishing to learn molecular dynamics, all of whom did not have previous experience in computer simulations. Furthermore, I completed these steps in my recent publication “Multiscale simulations examining glycan shield effects on drug binding to influenza neuraminidase” in the Biophysical Journal¹, so I am very familiar with them.

Skills you will acquire:

- Understanding of molecular dynamics
- Ability to use and implement modern tools to simulate protein dynamics
- Familiarity with the command line
- Capability to perform rigorous data analysis

1. <https://doi.org/10.1016/j.bpj.2020.10.024>