Virtual Screening for High Specificity Inhibitors of SSH-2
Dual Specificity Phosphatases or DSPs are characterized for their ability to dephosphorylate phospho-tyrosine and phospho-serine/threonine.

Finding specific inhibitors of DSPs like SSH-2 have potential in drugs to combat Alzheimer's and certain cancers.

The top 1% of the highest ranked inhibitors of SSH-2 are docked against other DSPs to determine specificity.

However, some DSPs were only recently modeled, such as by past PRIME students, and require loop optimization and energy minimization to improve their structure.
A list of previously generated models was worked through to determine best candidates for screening.

First two DSPs suitable for modeling optimization were DUSP 19 and PRL-2.

Loop optimization has been successful, though significant improvement as a result has not been observed.

Accuracy of the models were judged by MolProbity, an online structural model assessment program.

Olivia is running dock for DUSP19. I should have PRL-2 docking by tomorrow.
Future plans included looking into ways to display and utilize Modeller’s DOPE score function to determine best locations for loop minimization.

- We attempted to write script to generate scores, but had problems with python not recognizing Modeller module. Reinstallation may be required.
- We are still trying to determine the best method to optimize models. Options include loop modeling then energy minimization or vice versa.
- As docking gets underway, we will begin to look more into ways to determine specific inhibitors through pharmacophore generation and comparison.
Cultural Exploration!