

Identification of Unknown Protein Function

Jaron Deacon & Ashley Ringer McDonald

Dept. of Chemistry & Biochemistry

California Polytechnic Institute

San Luis Obispo, CA

Abstract:

The Protein Data Bank currently contains around 3500 proteins with known three-dimensional structure, but unknown function. In previous work, sequence alignment techniques and structural alignment techniques have been used to identify proteins of known function that have with structural similarity to proteins of unknown function. These structural alignment techniques identified possible enzyme classes for thirteen structures of unknown function. In this work, we aim to further characterize these structures through a ligand docking analysis. A database of possible ligands was assembled from the protein databank. Docking analysis was performed using AutoDock Vina via the PyRx interface. Identification of ligands with high binding affinities for the proteins of unknown function will help identify possible substrates for these enzymes.