**Abstract**

This project is to apply three docking tools (Zdock, Cluspro and Hex) to two CAPRI targets (T50 and T53) and improve accuracy by combining tools and assess the performance using a few complementary tools (RosettaDock and RMSD). First, we select PDBs of T50 and T53. After pre-processing for docking, we create decoys using Zdock, Cluspro and Hex, and then score and optimize them by RosettaDock. Next, we can compare the results between before docking and after docking. Then we can get some performances about the tools we use and conclusions about the methods. Ultimately, we visualize top model from each decoy group.

**Introduction**

Protein-protein docking is used to predict the structure of a protein complex in its parents. It is very useful in drug creation and disease prevention. First, for each target, we generate decoys from three servers (Zdock, Cluspro and Hex) and normalize the results using RosettaDock’s prediction scoring and get the ranking. We focus on RMSD of predicted interface to do the evaluation and get the similarity between predicted residue-residue interface sequence and native sequence. Next, we optimize them with Rosetta using top-score 10 decoys. We use Zdock and Rosetta to score to score the optimized decoys. Then we plot decoys from un-optimized and optimized groups to visualize evaluations and use Chimera to show predicted docking as well as the top10 before and after optimization.

**Cluspro**

ClusPro is a web server which uses an automated rigid-body docking and discrimination algorithm that rapidly filters docked conformations, and ranks them based on their clustering properties**.**

After signing up for an account and logging into the server, we can choose a docking job and have a receptor and ligand by uploading the PDB files of T50 and T53. Then we can optionally choose what chains to use in docking. After that, you can view the queue status for the decoys completed. It can generate You can choose the number of top models as you need.