

Title: “Benchmarking Predictive Protein Docking Algorithms
Student: Jonathan Williford
Advisor: Dr. A. Welch

For my research I have been comparing the two predictive docking: FTDock with RPScore and ZDOCK 2.3 (that uses PSC+DE+ELEC for scoring). There are two sets of protein test cases I've used for the evaluation, a set of protein dimers given to me by Dr. Daisuke Kihara and proteins listed in A Protein-Protein Docking Benchmark by Rong Chen, Julian Mintseris, Joe Janin, and Zhiping Weng.

I evaluated the proteins using 4 different scoring functions:

1. Overall RMSD
2. RMSD of the binding region
3. Number of Correctly Predicted Binding Residues / Number of Predicted Binding Residues
4. Number of Correctly Predicted Binding Residues / Number of Binding Residues in Known Protein Complex

These scoring functions were applied to what the algorithms said where the top 20 results. Of these 20 predictions, the best result for each of the scoring functions was recorded.