Docking Pre-processing

In our project, we choose T50 and T53 as our targets. In T50, the given initial file contains all receptor and ligand information, so we need spilt them into two pdb files so that we can dock them. Chain A and B are the structure of the receptor and Chain C is the structure of ligand. As for T53, CAPRI only provides the structure of receptor. We are given the sequence of the ligand, so we have to predict the structure before we can dock them. In our project, we predicted the structure of ligand of T53 by MuFold server.

Hex

Hex server is the first Fourier transform (FFT)-based protein docking server to be powered by graphics processors. Using two graphics processors simultaneously, a typical 6D docking run takes ∼15 s, which is up to two orders of magnitude faster than conventional FFT-based docking approaches using comparable resolution and scoring functions. The server requires two protein structures in PDB format to be uploaded, and it produces a ranked list of up to 1000 docking predictions. Knowledge of one or both protein binding sites may be used to focus and shorten the calculation when such information is available. The first 20 predictions may be accessed individually, and a single file of all predicted orientations may be downloaded as a compressed multi-model PDB file. The server is publicly available and does not require any registration or identification by the user.

Evaluation

After we generate decoys from three servers, we only pick up one best decoy as our evaluation target. We use TM-score and RMSD(overall) as our score functions. The following are two result tables:

T50(top one)

|  |  |  |  |
| --- | --- | --- | --- |
|  | Cluspro | ZDock | Hex |
| TM-Score | 1.0177(Impossible ?) | 0.1490 | 0.9941 |
| RMSD | 34.123 | 25.304 | 0.514 |

T53(top one)

|  |  |  |  |
| --- | --- | --- | --- |
|  | Cluspro | ZDock | Hex |
| TM-score | 0.7539 | 0.8420 | 0.2418 |
| RMSD | 16.898 | 16.637 | 8.712 |

Since the format of Cluspro server has some problems, it causes some issues when we calculate TM-score. So results may be generated again after we do some further work.

Also we still drew two histograms to compare the performance of three servers. But we also found none of three can do all great job on both two targets, so we need try more targets and run tests.

T50

T53