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 | 0.9941 | 0.1490 | 0.9941 |
| RMSD | 0.541 | 25.304 | 0.514 |

Table 1

T53(top one)

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

Table 2

After that, we used Rosettadock to optimize our decoys from three servers. Since the format of ZDock results is not acceptable for Rossettadock, we only optimize decoys of Hex and Cluspro. Table 3&4 show results (we only present the top structure). Very interesting, there is no improvement. We may figure out this problem in the further work.

T50(top one)

|  |  |  |
| --- | --- | --- |
|  | Cluspro | Hex |
| TM-Score | 0.9941 | 0.9941 |
| RMSD | 0.514 | 0.514 |

Table 3

T53(top one)

|  |  |  |
| --- | --- | --- |
|  | Cluspro | Hex |
| TM-Score | 0.2418 | 0.2418 |
| RMSD | 8.712 | 8.712 |

Table 4

Since overall rmsd can not reflect the quality of the complex very well, we tried to compare the interfaces of decoys with the one of native structure. The Table 5&6 show results. From these two tables, they indicate that good overall rmsd can’t promise a good interface structure sometimes.

T50

|  |  |  |  |
| --- | --- | --- | --- |
|  | Cluspro | ZDock | Hex |
| TM-Score | 0.1890 | 0..0291 | 0.1920 |
| RMSD | 0.328 | 20.319 | 0.334 |

Table 5

T53

|  |  |  |  |
| --- | --- | --- | --- |
|  | Cluspro | ZDock | Hex |
| TM-Score | 0.0592 | 0.0979 | 0.0557 |
| RMSD | 2.894 | 3.854 | 3.858 |

Table 6