Comparison of protein-protein docking prediction and optimization methods

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1 Abstract

2 Introduction

3 Methods

3.1 Pipeline

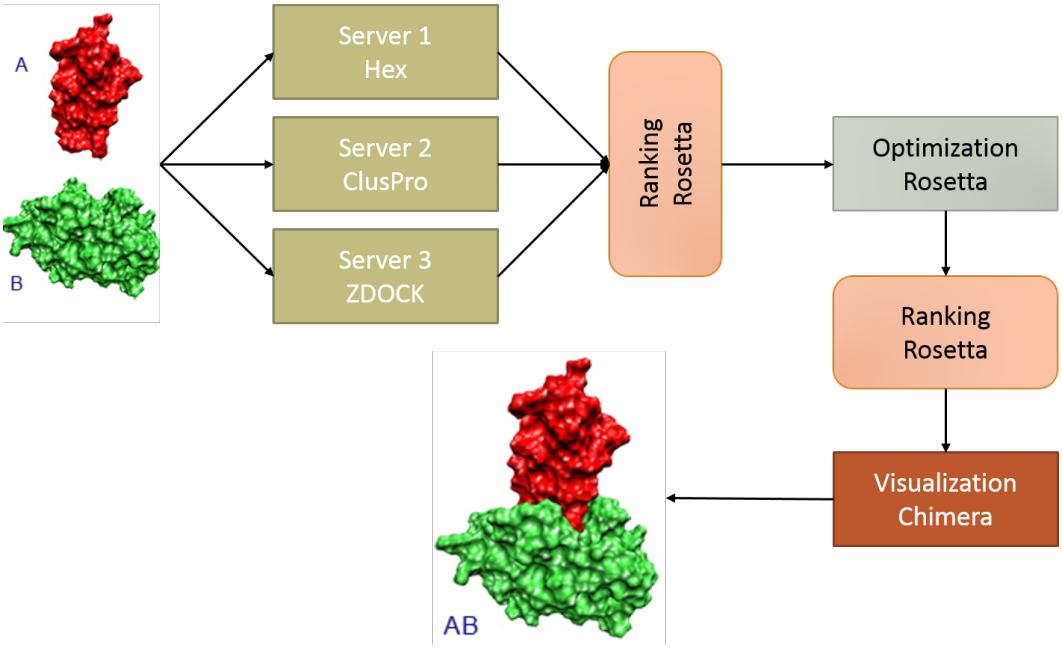

Figure 1: An overview of the comparison pipeline

1. Decoy Creation
2. Ranking
3. Optimization
4. Final Selection and Scoring

3.2 CAPRI Target Selection

We selected the following template-free targets from the CAPRI database to build a model for: T53, T50.

3.3 Pre-Processing

3.4 Decoy Creation

1. Hex
2. ClusPro
3. ZDOCK

3.5 Decoy Optimization

1. Decoy Ranking
2. Optimization

4 Results

4.1 Interface Creation

4.2 Scoring Methods - RMSD vs RosettaDock

1. Before Optimization
2. After Optimization

4.3 Visualization

5 Conclusion

6 Citations

We thank the following tools and papers: