**Rosettadock**

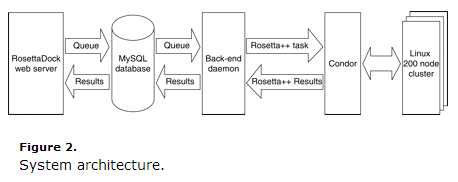
RosettaDock is a structure-prediction-based program, which searches the rigid-body and side-chain conformational space of two interacting proteins to find a minimum free-energy complex structure. RosettaDock has been highly successful in the blind prediction challenge of the Critical Assessment of PRedicted Interactions (CAPRI), producing several structures that were the most atomically accurate models submitted by any group in the CAPRI challenge.

Two limitations of RosettaDock have been that

1. the command-line interface can be difficult to use
2. it requires significant computational time to generate all-atom models, typically requiring a cluster of computers.

To make the computation available to a broader community, RosettaDock server (<http://rosettadock.graylab.jhu.edu>) has been developed, where the interface is simple and the computing resources are provided. Currently, the computing cost requires us to limit the public use to local searches near user-provided starting conformations [∼30 Å root mean-squared deviation (r.m.s.d). of Cα atoms]. Local searches are useful for refining top-ranked models from global searches by other docking methods or for searching for conformations given constraints provided by experimental data such as site-directed mutagenesis effects on binding affinity.

Rosettadock server identifies low-energy conformations of a protein-protein interaction near a given starting configuration by optimizing rigid-body orientation and side-chain conformations. The server requires two protein structures as inputs and a starting location for the search. RosettaDock generates 1000 independent structures, and the server returns pictures, coordinate files and detailed scoring information for the 10 top-scoring models. A plot of the total energy of each of the 1000 models created shows the presence or absence of an energetic binding funnel. RosettaDock has been validated on the docking benchmark set and through the Critical Assessment of PRedicted Interactions blind prediction challenge.



Results:

We are displaying three best results we got in each of the Docking tools:

**Cluspro T50 PDB:**

[**http://rosie.rosettacommons.org/docking2/viewjob/7529**](http://rosie.rosettacommons.org/docking2/viewjob/7529)

[**http://rosie.rosettacommons.org/docking2/viewjob/7533**](http://rosie.rosettacommons.org/docking2/viewjob/7533)

[**http://rosie.rosettacommons.org/docking2/viewjob/7534**](http://rosie.rosettacommons.org/docking2/viewjob/7534)

**Haddock T50 PDB:**

[**http://rosie.rosettacommons.org/docking2/viewjob/7537**](http://rosie.rosettacommons.org/docking2/viewjob/7537)

[**http://rosie.rosettacommons.org/docking2/viewjob/7542**](http://rosie.rosettacommons.org/docking2/viewjob/7542)

[**http://rosie.rosettacommons.org/docking2/viewjob/7545**](http://rosie.rosettacommons.org/docking2/viewjob/7545)

**Cluspro T53 PDB:**

[**http://rosie.rosettacommons.org/docking2/viewjob/7548**](http://rosie.rosettacommons.org/docking2/viewjob/7548)

[**http://rosie.rosettacommons.org/docking2/viewjob/7549**](http://rosie.rosettacommons.org/docking2/viewjob/7549)

[**http://rosie.rosettacommons.org/docking2/viewjob/7551**](http://rosie.rosettacommons.org/docking2/viewjob/7551)

**Haddock T53 PDB:**

**Still on queue in the server**

**References:**

1. Lyskov S., Gray J.J. "The RosettaDock server for local protein-protein docking" *Nucleic Acids Research* 36 (Web Server Issue), W233-W238 (2008).[**Online**](http://nar.oxfordjournals.org/cgi/content/abstract/36/suppl_2/W233)
2. Chaudhury S, Berrondo M, Weitzner BD, Muthu P, Bergman H, Gray JJ. "Benchmarking and analysis of protein docking performance in Rosetta v3.2" *PLoS One*. 2011;6(8):e22477. doi: 10.1371/journal.pone.0022477. Epub 2011 Aug 2. [**Online**](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3149062/)
3. Lyskov S, Chou FC, Conchúir SÓ, Der BS, Drew K, Kuroda D, Xu J, Weitzner BD, Renfrew PD, Sripakdeevong P, Borgo B, Havranek JJ, Kuhlman B, Kortemme T, Bonneau R, Gray JJ, Das R., "Serverification of Molecular Modeling Applications: The Rosetta Online Server That Includes Everyone (ROSIE)". PLoS One. 2013 May 22;8(5):e63906. doi: 10.1371/journal.pone.0063906. Print 2013. [Link](http://www.plosone.org/article/info:doi/10.1371/journal.pone.0063906)