

SymD server: a platform for detecting internally symmetric protein structures

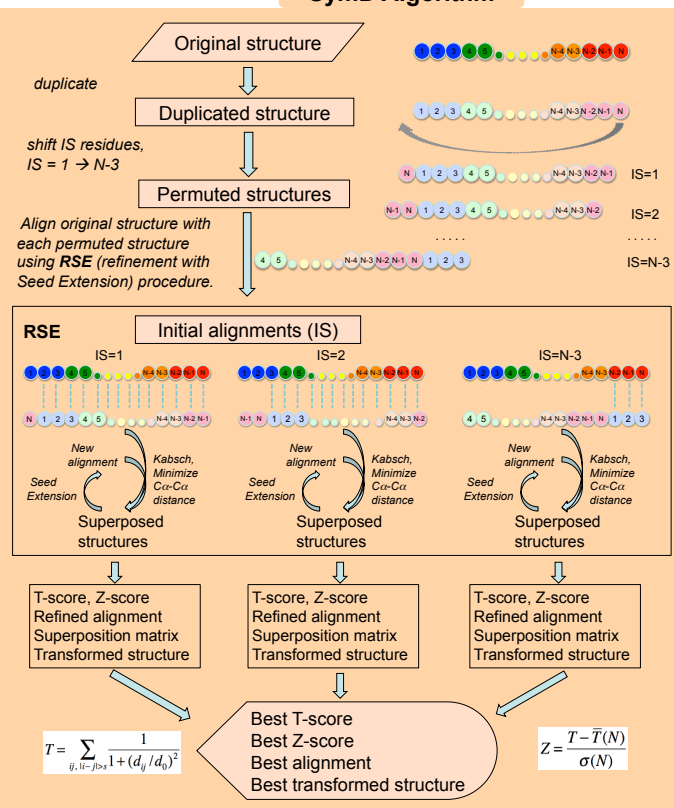
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Background

Many protein domains are made of repeating units of similar structures arranged in a beautifully symmetric manner. The mechanism of such an arrangement, the biological function, and the evolutionary history of symmetric proteins are largely unknown. To answer these questions, we first developed a program, called **Symmetry Detection (SymD)**, to detect internally symmetric protein structures. Here, we report on the development of the **SymD web server** (<http://symd.nci.nih.gov>), a dynamic platform based on **Galaxy** to determine if a protein is symmetric and to visualize the structure interactively.

SymD Algorithm



Framework

SymD web server uses the **Galaxy** framework, which is a common user interface that can integrate many different bioinformatics tools.

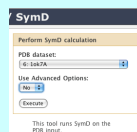
Input

Users may upload their own structure file or fetch from CATH, PDB or SCOP database.

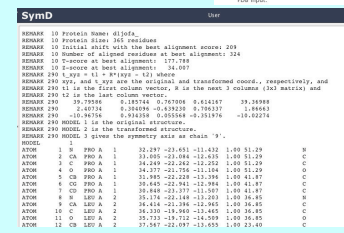
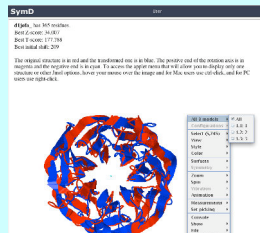
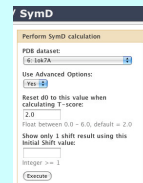
Execution and Output

Run SymD

To execute SymD, select "Perform SymD calculation" in the Tool Panel.



Advanced options allow users to adjust **d0** and to examine specific shift result.

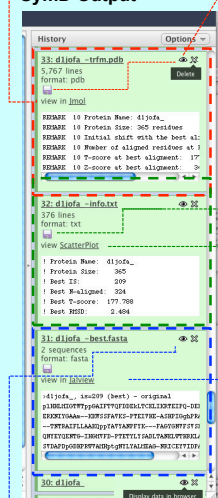


Jmol displays the original and the transformed structures and the symmetry axis

Structure Information

- Transformed pdb file gives:
 - transformation matrix
 - transformed structure
 - symmetry axis

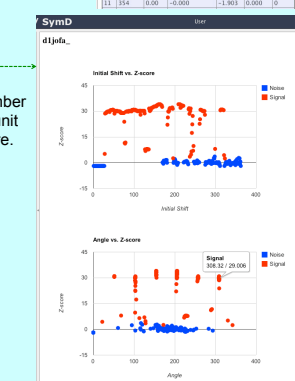
SymD Output



Info file gives the rotation angle, translation along the symmetry axis and the scores of each alignment

Scores

Scatter plots show the number of repeating unit in the structure.



Sequence Information

Sequence alignment between the original and the transformed structurein FASTA format file can be download for further analysis.

Jalview displays the sequence alignment.

Reference

- Kim, C., Basner, J., Lee, B. Detecting internally symmetric protein structures. *BMC Bioinformatics*. 2010; 11: 303.
- Kim C, Tai CH, Lee B. Iterative refinement of structure-based sequence alignments by Seed Extension. *BMC bioinformatics*. 2009;10:210.
- Tai CH, Vincent JJ, Kim C, Lee B. SE: an algorithm for deriving sequence alignment from a pair of superimposed structures. *BMC bioinformatics*. 2009;10(Suppl 1):54.
- Goecks, J., Nekrutenko, A, Taylor, J and The Galaxy Team. Galaxy: a comprehensive approach for supporting accessible, reproducible and transparent computational research in the life sciences. *Genome Biol*. 2010; 11:R86
- Blankenberg D, Von Kuster G, Coraor N, Ananda G, Lazarus R, Mangan M, Nekrutenko A, Taylor J. "Galaxy: a web-based genome analysis tool for experimentalists". *Current Protocols in Mol. Biol.* 2010, Chapter 19.