Due Date: December 19, 2017 (23:55)

CENG 465
Introduction to Bioinformatics

Fall 2017-2018

Assignment #3

Written Assignment on Protein Structure Alignment

Structural Similarities at the Fold and Superfamily levels

In this assignment your goal is to investigate structural similarities at the Fold and Superfamily levels of the SCOP (Structural Classification Of Proteins) hierarchy. Specifically, you will pick two pairs of domains from the SCOP database at http://scop.berkeley.edu with the following properties:

- Pick two different protein domains from the same fold but from two different superfamilies. The class of the protein domains should be one the 4 main classes: all alpha proteins (a), all beta proteins (b), alpha/beta (c), or alpha+beta (d). For example d1gy5a_ and d1nb3j_ are two protein domains from the same fold (fold d.17) but from two different superfamilies (d.17.4 and d.17.1). You are free to pick any pair of protein domains that satisfies these conditions.
- Pick another pair of protein domains this time from the same superfamily but from two different families. The class of the protein domains should be one the 4 main classes: all alpha proteins (a), all beta proteins (b), alpha/beta (c), or alpha+beta (d). For example d1gy5a_ and d1tp6a_ are two protein domains from the same superfamily (fold d.17.14) but from two different families (d.17.4.2 and d.17.4.12). You are free to pick any pair of protein domains that satisfies these conditions.

Compare structures of the the two pairs of domains you have selected using the RCSB PDB Protein Comparison Tool at http://www.rcsb.org/pdb/workbench/workbench.do using two different Pairwise Structure Alignment methods, each, as the structure alignment method. For example, you may select jCE and DALI and compare both pairs of domains you have selected with both of these tools separately.

Analyze your results and write a short report containing snapshots of the alignment results and alignment summaries. Some example questions you may address in your report are: 1) Are the structures more similar at the fold or superfamily level? 2) Which comparison tool is better (longer alignment, smaller RMSD) at finding structural similarities? 3) Are there similarities in the sequence as well (seq. identity etc.)? 4) Are there gaps in the structural alignment? You are free to address more issues if you find some interesting results.

Submission

Submit your report in PDF format via ODTU-Class before the deadline. Late submission is -20 pts per day.