Structural Bioinformatics 2003-04 Semester B
Assignment 5.
May 4

Write a program to perform a *pairwise rigid* structural alignment. The alignment should be based on Secondary Structure Element (SSE) superposition. There are two goals, the first is to compute the largest alignment between SSEs. The second goal is to compute the largest alignment between C_α atoms. Both alignments should be sequence order independent.

- Use the DSSP program for secondary structure assignment.
  /home/silly6/mol/software/dssp/mkdssps
- A set of transformations should be created based on the alignment of SSE pairs. Every possible SSE pair should be considered.
- Perform clustering of transformations.
- Report the best found SSE alignment as well as the best C_α alignment.
- Name your program *sse_align*. The program and the source code should be placed into username/SSEalign/.
  Input to the program:
  protalign *pdb1 pdb2*
  (assumes that pdb1.dssp and pdb2.dssp are in the current directory)

  First Output:
  SSE alignment-size : *3D transformation*

  Where 3D transformation should be applied on the pdb2 so it is aligned with pdb1. For example:
  12 : -1.51293 -0.500847 0.842489 35.1861 9.72255 18.5758

  SSE Match Table, where each row contains a pair of matched SSE's.
  For example:
  A.H.1 A.H.3
  A.H.2 A.H.2
  B.S.10 A.S.5

  Where A.H.2- helix from chain A with SSE ID 2 , A.S.5- strand from chain A with SSE ID 5.

  Second Output:
  Calpha alignment-size : *3D transformation*
  Calpha Match Table, where each row contains a pair of matched amino acids.
  For example:
  A.V.23 .V.4
  A.F.24 .P.5
  A.D.25 .D.6
  A.F.26 .L.7

  Where A.V.23 - residue 23 of type V (Valine) from chain A.

  In addition you should create two pdb files (for each transformation) which includes pdb1 and the transformed pdb2. The joined pdb files should be named *sse_aligned.pdb* and *calpha_aligned.pdb*.