

Structural Bioinformatics 2004-05 Semester B Assignment 5.

Due to 7 May

- Write a program that detects an (almost) largest structural alignment between two proteins. The alignment should be sequential as in Assignment 4 question 2. Input to the program is two protein structures in the PDB format.
- Consider only C_α atoms for both structures.
- Consider only transformations that align each pair of residues from both proteins, i.e. only $|pdb1| \cdot |pdb2|$ transformations. Notice, for each residue we can define a local coordinate system based on three atoms N , C_α and C .
- Name your program 'protalign'. The program and the source code should be placed into username/ProtAlign/.
Input to the program:
protalign *epsilon pdb1 pdb2*
Output:
{Size of the largest alignment} {3D transformation}
For example:
130 0.5 0.11 0.7 10.1 21.30 -10.1
In addition you should create a joined pdb file 'joined.pdb' that contains two superimposed structures. This file should contain all atoms (not only C_α atoms).
- Use GAMB++ library.
/home/silly6/mol/lib/gamb++
<http://bioinfo3d.cs.tau.ac.il/group/>
<http://bioinfo3d.cs.tau.ac.il/group/GAMB++/GAMB.html>