

Homework Assignment #5 (Due Thursday, May 12, 2005)

The course webpage <http://www.biostat.jhsph.edu/~iruczins/teaching/260.841/> contains some helpful material for this homework. If you use webservers to answer some of the questions below (which I assume you do), please include the relevant parts of the material that you received from the server.

1. Find the NMR structure file and the X-ray structure file of the immunoglobulin-binding domain of protein G in the PDB. Which organism is the protein from? How many NMR structures were determined? What is the resolution of the crystal structure? In your own words, describe the topology of the protein. What are its SCOP and CATH classifications? Name some pdb files of structurally similar proteins. In particular, find a protein similar in structure with less than 10% sequence identity, and determine its SCOP and CATH classifications.
2. For this exercise three Protein G like sequences are available on the course webpage.
 - The wild type TTYKLILNGKTLKGETTTEAVDAATAEKVFKQYANDNGVDGEWYDDATKTFTVTEK.
 - The wild type with the residues 23-33 substituted by the sequence AWTVEKAFKTF.
 - The wild type with the residues 42-52 substituted by the sequence AWTVEKAFKTF.

Predict the secondary structures of the three sequences using PHD (PredictProtein) and PSIPRED, and compare the predictions to the experimental results. (1-10 strand, 13-21 strand, 23-38 helix, 43-48 strand, 51-57 strand). Comment.

3. How many small proteins (length at most 70 amino acids), that are different in sequence (less than 5% identity in a pairwise sequence alignment) and have been crystallized at extremely high resolution ($\leq 1.0 \text{ \AA}$) can you find? A list of PDB file identifiers is fine.
4. The file decoy.pdb on the course website contains an ab initio prediction for a protein (the target) in the PDB. Find a list of possible targets using a 3D structure comparison algorithm. Looking at sequence alignments, which protein was the target?
5. Work through the Gale Rhodes' RASMOL and Swiss-PDB tutorial, linked on the course webpage. Nothing to be handed in here, but you get bonus points if you hand in a replicate of the figure in the "Making Images for Publications" section.