

Homework Assignment #5
(Due Tuesday, April 29, 2008)

The course webpage <http://www.biostat.jhsph.edu/~iruczins/teaching/260.655/> contains some helpful material for this homework. If you use web servers 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 PSIPRED and JPRED, 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 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. The protein structure with PDB identifier 1BAG contains a Greek key motif (residues 381-414). Use DeepView to create a figure suitable for publication which highlights that motif (use colors, ribbons, etc). The chapter *Making Images for Publications* in the Swiss-PDB tutorial from Gale Rhodes contains some helpful tips and tricks.