

Homework for Protein Bioinformatics 260.841 covering the 19th of April class

1. What is primary goal of 'Structural Genomics'?

2. Crystallography and NMR.
 - 2a. Which experimental technique is responsible for the majority of the structures deposited in the Protein Data Bank?

 - 2b. When x-rays interact with a protein, they can be scattered by the [protons, electrons, neutrons] of the protein atoms. [circle one choice].

 - 2c. Scattered x-rays form a diffraction spot (also called a reflection) when they have the same [intensity, spin, phase] . [circle one choice].

 - 2d. The location of a diffraction spot on the detector contains information about:

 - 2e. The intensity of a diffraction spot on the detector contains information about:

 - 2f. There are two properties associated with each diffraction spot that are necessary for determining a structure using x-ray crystallography. What are these two properties and which one is not recorded by x-ray detectors?

 - 2g. NMR structure determination involves perturbing the unpaired spins of atomic nuclei with a [magnetic field, electric field, force field]. [circle one choice].

 - 2h. What is the only element commonly found in proteins that contains an unpaired spin in its nucleus?

 - 2i. What are two other isotopes that are typically used as labels to introduce unpaired spins into protein samples for NMR?

 - 2j. Which experimental technique can tackle molecules greater than 40,000 Daltons in mass?

2k. Which experimental technique allows you to study molecules in solution?

2l. Which experimental technique typically generates a greater number of observables (data points) than the number of refinement parameters used to fit the structural model?

2m. Why is the ratio of observables to refinement parameters important?

3. Go to the website for the Protein Data Bank (<http://www.rcsb.org/pdb/>)
Search for structure '1AW0' (the '0' is a zero)

3a. What experimental technique was used to solve this protein structure?

3b. How many structures were deposited?

Click on the Download/Display button and open the PDB header.

3c. How many helices does this protein structure have?

3d. How many amino acids are there in this protein structure?

3e. What expression system was used to make the protein sample for this structure?

3f. At what pH was the data collected for this structure?

4. Search for structure '2SBL' at the Protein Data Bank

4a. What experimental technique was used to solve this protein structure?

4b. In what journal did the authors publish this structure?

Click on the Download/Display button and open the PDB header.

4c. What is the resolution of this structure?

4d. Would you consider this Low, High or Mid resolution?

4e. What is the R-factor of this structure?

4f. Is the R-factor acceptable for this resolution?

4g. How many beta-strands are in this protein?

4h. How many pi helices?

4i. Which amino acid in this protein has its main chain omega angle = 0° (CIS)?