

Bioinformatics 2 -- Homework 1

due 2/3/2012 (on paper)

Download the PDB files from the link "HW1 protein 1" and "HW1 protein 2" on the course web site. Display each using MOE (or JMOL).

For each protein:

(1) Divide the protein into domains to the best of your ability. Write the start and end position of each domain. These can be approximate sequence positions.

For each domain:

(2) Identify the class, and fold according to SCOP. Use descriptive terms (e.g. SCOP: alpha + beta. beta(3)-alpha; 2 layers: alpha/beta, etc etc. That is, don't use SCOP names or numbering.)

(3) Identify the class, and architecture according to the CATH database using descriptive terms (e.g. CATH: 3.15 alpha beta, super roll. In this case, please do use the CATH numbering.)

(4) Draw the TOPS cartoon. Number the SSEs sequentially (alpha and beta separately) in each shape.

(5) From the TOPS cartoon, draw a crude contact map, as described in the notes for lecture 3.