CS321: Numerical Methods in Comp Mol Bio

Homework 8

Due: Thursday, Nov 3 2005 at the begining of the section

Problem 1

The file 1NTF.ca holds the coordinates of the C_α atoms for the protein Cimex Nitrophorin, which is a protein in the saliva of the blood sucking bed bug (for real!).
a) Compute and plot the contact map for this protein and comment about secondary structures you identify in the contact map.
b) Go to the PDB website (http://www.rcsb.org/pdb/) and view the structure of this protein (the PDB ID for it is 1NTF). Compare your results from part a to the structure you see.

Problem 2

In CASP5 held at December 2002 many groups tried to predict the structure of the protein Cimex Nitrophorin.
The files T0142TS464.ca T0142TS419.ca T0142TS427.ca hold the coordinates of the C_α atoms of 3 of those predictions.
a) Compare each of these predictions with the experimental structure from Problem 1, using RMS distance.
b) Order these 3 predicted structures from best to worse.