

20.310 Section

09-12-06

Google → “protein data bank” → www.rcsb.org/pdb
Keyword → vinculin (found in focal adhesion complexes)

Resolution parameter: 1-2 Å is good for modeling

- find structures by NMR, electron diffraction, crystallography
 - data bank also provides sources for the protein structures → literature search
 - data file contains coordinate data for every atom in every amino acid
 - save data file as text file
 - save data file as .pdb file
- (data file is .pdb format with link available when searching for protein)

Protein Viewers

RasMol Version _____ (protein viewer)

Swiss-Pdb

- can use to view protein 3D structure
- can use to compare sequences of multiple Proteins
- can look at protein structure in ribbon form, ball-stick, space filling
- can highlight certain atoms by coloring them differently

look for cysteine amino acid and highlight it, this is where you might want to do some reactive chemistry

- can load multiple structures at once
 - useful to look at potential docking

determine distance between 2 amino acids either directly in Swiss-Pdb or by using coordinate data for N (on protein backbone)

distance between 2 vectors

$$\|b - a\| = \sqrt{(b_1 - a_1)^2 + (b_2 - a_2)^2 + (b_3 - a_3)^2}$$

length of a = $\|a\| = \sqrt{a \cdot a}$

$$a \cdot b = \|a\| \cdot \|b\| \cos \theta = a_1 b_1 + a_2 b_2 + a_3 b_3$$

Viewer for virus particles: Viper

Good amino acid for spectroscopy: tryptophan

- has aromatic ring
- absorbs in the UV