BT 210: BIOCHEMISTRY LAB

Exploring protein structure in three dimensions using SWISS-PDB Viewer DEEP VIEW and PDB structural data.

The function of any protein is closely related to its three dimensional structure. Ever since John Kendrew and his co-workers solved the three dimensional atomic structure of Myoglobin using X-ray crystallography in 1958, more than forty thousand macromolecular structures have been determined using techniques like X-ray crystallography NMR and occasionally theoretical modeling. These structures can be downloaded freely from the Protein Data Bank (PDB) at **http://www.pdb.org**

Analysis of such structures, have helped tremendously in our understanding of the macromolecular function at the molecular level. Like for example, the structure surrounding a drug binding site or an enzyme active site are critical in order to design potent drugs or modify enzyme activity/substrate specificity or design potent enzyme inhibitors, respectively.

In this laboratory session you shall obtain a few important structural parameters of the protein assigned to you employing the SWISS-PDB Viewer DEEP VIEW software (http://**www.expasy.org/spdbv/**).

Objective:

A) Open pdb file, write the name of the protein, PDB code, number of amino acids, number of chains and source of protein.

B) To determine the distance between the C_α atoms in the N and C terminus in Å

C) i) To calculate the volume of the given protein in $Å^3$ ii) To calculate in cm^3, the volume occupied by 1 g of protein (also called the partial specific volume).

D) Select Trp residues. Determine the number of Trp residues (N) and their sequence number (like W23 & W45). If N > 1, the distance between each pair of Indole N atoms (in case N > 2, write the distances as a matrix table). In case no Trp exists, repeat the same with either His or Cys or Met.

E) Identify the C_α atoms that lie within a distance of 5 Å from the N terminal C_α atom.