Course: BT 305

Lab Session 3: De novo Peptide/Protein Design

Date:

Aim: Design peptides and proteins from scratch using simple downloadable tools.

The objectives of current session are as follows:

1. Download and Install Ribosome and PROSS. You may use VADAR instead of PROSS

(Both the tools will be shared by TAs)

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2. Download 1PGB.pdb from Protein Data Bank

      A) Run PROSS to get the Phi, Psi, Chi1, Chi2 dihedral angles.

      Note down the dihedral angles of helix, Beta Strand, Anti parallel Beta Sheet

3. Design peptides with the following structure:

Reconstruct the protein structure using Ribosome

A) Alpha helix (right handed)
B) Beta strand
C) Beta sheet

Extract the helix and antiparallel beta sheet from 1PGB.pdb and compare the designed molecule by visualizing it side by side using any protein visualization software.

Material and methods

Operating System: linux
Computational tools: Ribosome, PROSS, Pymol/Swiss Pdb viewer