

## **BT 305 Lab Session 4: De novo Protein Design**

**Date:**

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

The objective of the current session are as follows:

1. Use Ribosome and PROSS already installed
2. Design peptides with the following structure:

Step 1: Download the structure TRP CAGE motif from pdb (1L2Y.pdb)

Step 2: Deduce phi psi chi1 chi2 etc angles using PROSS/VADAR

Step 3: Reconstruct the protein structure using Ribosome and name it as yournametpcage.pdb (if your name is ajay, then “ajaytrpcage.pdb” should be the file name)

Step 4: Super impose the structures using SPDB Viewer and calculate RMSD of your designed protein with original 1L2Y.pdb

Step 5: Take snap shots of both proteins by saving it as picture file, and present as side by side images in your record book.

(RMSD: Root mean square deviation)

Step 5: Use ‘diff’ program in shell and print out the two (original 1L2Y.pdb) and re-designed protein molecule.

### **Material and methods**

Operating System: linux

Computational tools: Ribosome, PROSS, Swiss Pdb viewer

Swiss pdb viewer can be downloaded from

[https://spdbv.vital-it.ch/download\\_prerelease.html](https://spdbv.vital-it.ch/download_prerelease.html)