Lab Session 9: Prediction of protein structure

Date: April 2023

Download the tool open babel and install it in your system.

https://openbabel.org/docs/dev/Installation/install.html

http://www.cheminfo.org/Chemistry/Cheminformatics/FormatConverter/index.html

Exercise 1

Convert all the structures that you have designed and downloaded small protein molecules 1L2Y.pdb and 1PGB from PDB to internal coordinate format.

Convert it back, means internal coordinate to PDB file.

Calculate the RMSD between the original pdb and newly generated pdb from internal coordinate.

Comment on the efficacy of file conversion tools.

Exercise 2

Browse through the open babel tool. Design a question yourself and find answer with open babel, and present it in your record book as a regular exercise.