Lab Session 1: Installation of LINUX and dual booting

By Chandan Nath, TS, BSBE, IITG

Assignments:

No assignments in this lab session

Lab Session 2: LINUX Assignment

1. Download Dihydrofolate reductase 4DFR.pdb from Protein data bank
2. Use vi editor to print 4DFR.pdb file without header, save it as file1
3. Write C-alpha (CA), N and CB atoms in separate files (file2, file3, file4).
4. Replace 'ATOM' string with your 'first name' and save it as a separate file (file 5).
   3A) Replace 'ATOM' with first name of three of your friends; and save them as separate files.
   3B) append all those into a single file (file6).
5. Print CG atoms in a separate file (file 7).
   4A) How many amino acids have large side chains, sidechains with CG, CD etc atoms; which all are those amino acids (file 8)
   4B) How many of them are acidic side chains (file 9)
   4C) How many have basic side chains (file 10)
   4D) What could be the net charge of this particular protein, write answer in your record book.

6. Open 4DFR.pdb using vi editor, remove the header files, and write your own header file with the following details (file 11):
   A) Total number of amino acids
   B) No. of alanines in the proteins
   C) No. of tryptophans in the proteins
   D) Total number of aminoacids with polar side chains

7. Using awk, Sum the X coordinates, Y coordinates and Z coordinates, and write it in the above file (file 11)

   Optional assignment for additional weightage

8. Find out the central atom of this protein, means atom with minimal distance among all atoms. Write a code in any language, save it as file 12. Send the code and executable

   (Note: If I get two identical codes, both will be disqualified)

(Each action 1-8 carries one mark each, total marks is 8)

Timeline: 1 week from the date of announcement (always)

Submit your assignments, properly arranged in soft copy on or before Sep 19, 2020. Because this is the first assignment, I am extending the date to Sep 25, 2020

Email: bclab2012@gmail.com