BT2042: Fundamentals of Biophysical Chemistry
Assignment I
February 23, 2022

Deadline for Submission: 4 pm on March 6, 2022

<u>Instructions</u> The code employed to do the calculations, details of the calculations and a write-up in a document should be sent to my email athi@iitm.ac.in (**as one zipped file with the title Name1_Name2.zip or Name1.zip**). This will account for 20% of the total points. Late submissions or incomplete submissions (without the code used or the write-up explaining the results) will NOT be entertained.

The submission will not be evaluated without the code employed – each group should write their own code. ***Any kind of plagiarism or copying will not be accepted and will be reported to the Disciplinary Committee followed by a U grade.***

Questions

Every group is provided a PDB id in the table below. Use only one chain in the PDB file (corresponding to the protein; typically chain A or the first model if it is an NMR structure) and disregard any heteroatoms, ligands, waters and nucleic acids in the PDB. Download the PDB structure and answer the following questions:

1. Calculate the pairwise interaction energy between all pairs of charged residues assuming a dielectric constant of 78 and using the Coulomb's law at pH 7. Construct a square matrix whose cells will contain information on the magnitude of the charge-charge interactions. This could be visualized using the command 'pcolor' in MATLAB.

2. How does the magnitude of the charge-charge interaction vary as the pH is raised from 7 to 14 or lowered from 7 to pH 5 or pH 2. Will the protein be stabilized or destabilized in each of the three conditions (pH 2, pH 5, pH 14) compared to pH 7? For this question, assume that all other interactions are identical and do not change on modulating pH.

3. What is the pI of the protein?

4. Construct pH titration curves for every residue in the protein assuming known pKa values for the side-chains.

Group	Name	Roll No.	Name	Roll No.	PDB ID
1	Arvinth S	BS20B008	Boneshwar V K	BS20B012	2ABD
2	Pankaj Bhardwaj	BS20B024	Ghanshyam	BS20B016	2ACY
3	Sapna R	BS20B032	Mohanapriya	BS20B023	1APS
4	Ahire Ganesh Ravindra	BS20B004	Aniket Sonje	BS20B007	1O6X
5	Darpan Balar	BS20B013	Sachin Choudhary	BS20B030	1E65

6	Deven Arya	BS20B014	Amrith K	BS20B005	1K0S
7	Livingston	BS20B011	Sujith	BS20B017	1YZA
8	Fathima Bensha	BS20B015	Sarath S	BS20B033	1FKB
9	Seema Rani	Bs20B034	Prasheela	BS20B026	1AYI
10	Mayank Anand	BS20B021	YATHARATH	BS20B039	1IMQ
11	Yashraj Singh	BS20B038	Abhishek Sharma	BS20B003	1N88
12	Vatsal Arya	BS20B037	Sanket Patil	BS20B025	1PNJ
13	Prince Kumar Gupta	BS20B027	Rajeev Ranjan	BS20B028	1DIV
14	Aarohee Vora	BS20B002	Malavika Venkatesh	BS20B020	1RIS
15	Ananya Sangeetha	BS20B006	Aakash B	BS20B001	1SPR
16	Arjun S	BE19B001	Ramshid N K	BE19B028	1TEN
17	Mohammed Nazeem	BS20B022	Rethik vishweshar	BS20B029	3AIT
18	Rashmi Athota	BE18B035	-	-	1URN
19	Tanush Kalantri	BS20B036	Jithin L	NA19B006	2QJL