

Indraprastha Institute of Information Technology Delhi (IIITD)

Department of Computational Biotechnology

BIO213 – Introduction to Quantitative Biology

ASSIGNMENT-2

Instructions:

1. You are required to submit the assignments by next Sunday, 11 April 2021.
2. Use Python to write your program.
3. Submit all your work as a single jupyter notebook (.ipynb). Use your roll number as the file name.
4. The code should be well commented.
5. Requests for extension of submission deadline will not be entertained.

Question 1. Write a program to implement Chou and Fasman method of secondary structure prediction for the following protein sequence:

SGFRKMAFSPGKVEGCMVQVTCGTTTLNGLWDDTVYCPRHVICTAEDMLNPNYEDL
LIRKSNHSFLVQAGNVQLRVIGHSMQNCLRLKVDTSNPKTPKYKFVRIQPGQTFSVLA
CYNGSPSGVYQCAMRPNHTIKGSFLNGSCGSVGF

- a) Provide a well commented code for the same. (20 marks)
- b) Display the output using the notation – H: Helix, S: Beta strand, and T: turn. (10 marks)

Question 2. Use the given protein.pdb file (structural coordinates for the protein from question 1) to predict the secondary structural elements using the STRIDE webserver (<http://webclu.bio.wzw.tum.de/cgi-bin/stride/stridecgi.py>). When prompted to choose from the PDB entries, do not use the same and proceed with the secondary structure prediction with the server.

- a) Display the output and compare with the result obtained in question 1. Mention the regions differing in both in terms of assigned secondary structure. (10 marks)
- b) Comment on the differences observed with proper reasoning. (10 marks)

Chou and Fasman parameters to be used for the prediction are as following:

Residue	P α	Residue	P β	Residue	Pt
Glu	1.53	Met	1.67	Asn	1.68
Ala	1.45	Val	1.65	Gly	1.68
Leu	1.34	Ile	1.60	Ser	1.56
His	1.24	Cys	1.30	Pro	1.54
Met	1.20	Tyr	1.29	Asp	1.26
Gln	1.17	Phe	1.28	Tyr	1.25
Trp	1.14	Gln	1.23	Cys	1.17
Val	1.14	Leu	1.22	Trp	1.11
Phe	1.12	Thr	1.20	Lys	1.01
Lys	1.07	Trp	1.19	Arg	1.00
Ile	1.00	Ala	0.97	Thr	1.00
Asp	0.98	Arg	0.90	Phe	0.71
Thr	0.82	Gly	0.81	His	0.69
Ser	0.79	Asp	0.80	Met	0.67
Arg	0.79	Lys	0.74	Ile	0.58
Cys	0.77	Ser	0.72	Ala	0.57
Asn	0.73	His	0.71	Gln	0.56
Tyr	0.61	Asn	0.65	Leu	0.53
Pro	0.59	Pro	0.62	Glu	0.44
Gly	0.53	Glu	0.26	Val	0.30