

# Indraprastha Institute of Information Technology Delhi (IIITD)

## Department of Computational Biotechnology

### BIO213 – Introduction to Quantitative Biology

#### ASSIGNMENT-2 (April 13, 2022)

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##### **Instructions:**

1. You are required to submit the assignments by next Wednesday, 20 April 2022.
2. Use Python to write your program.
3. Use your Roll no. and name to save the file.
4. You have to submit well commented scripts, and a PDF file with all the properly labelled answers.
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 (Helix and Beta strand) for the following protein sequence:

SGFRKMAFSPGKVEGCMVQVTCGTTTLNGLWLDDTVYCPRHVICTAEDMLNPNYEDL  
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. (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 $\alpha$ | Residue | P $\beta$ |
|---------|------------|---------|-----------|
| Glu     | 1.53       | Met     | 1.67      |
| Ala     | 1.45       | Val     | 1.65      |
| Leu     | 1.34       | Ile     | 1.60      |
| His     | 1.24       | Cys     | 1.30      |
| Met     | 1.20       | Tyr     | 1.29      |
| Gln     | 1.17       | Phe     | 1.28      |
| Trp     | 1.14       | Gln     | 1.23      |
| Val     | 1.14       | Leu     | 1.22      |
| Phe     | 1.12       | Thr     | 1.20      |
| Lys     | 1.07       | Trp     | 1.19      |
| Ile     | 1.00       | Ala     | 0.97      |
| Asp     | 0.98       | Arg     | 0.90      |
| Thr     | 0.82       | Gly     | 0.81      |
| Ser     | 0.79       | Asp     | 0.80      |
| Arg     | 0.79       | Lys     | 0.74      |
| Cys     | 0.77       | Ser     | 0.72      |
| Asn     | 0.73       | His     | 0.71      |
| Tyr     | 0.61       | Asn     | 0.65      |
| Pro     | 0.59       | Pro     | 0.62      |
| Gly     | 0.53       | Glu     | 0.26      |