

Indraprastha Institute of Information Technology Delhi (IIITD)
Department of Computational Biotechnology

BIO213 – Introduction to Quantitative Biology

ASSIGNMENT-2 (April 14, 2024)

Instructions:

1. You are required to submit the assignments by next **Sunday, 21 April 2024**.
2. Use Python and submit a well commented working code.
3. 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.

Use the following notation – H for Helix, S for Beta strand.

```
MNASSEGESFAGSVQIPGGTTVLVELTPDIHICGICKQQFNNLDAFVAHKQSGCQLTGTSAAAP
STVQFVSEETVTPATQTQTTRTITSETQTITVSAPEFVFEHGYQTYLPTESNENQTATVISLPA
KSRTKKPTTPPAQKRLNCCYPGCQFKTAYGMKDMERHLKIHTGDKPHKCEVCGKCFSRKDKLKT
HMRCHTGVPKYKCKTCDYAAADSSSLNKHLLRIHSDEPFKQCICPYASRNSSQLTVHLRSHTAS
ELDDDVPKANCLSTESTDTPKAPVITLPSEAREQMATLGERTFNCCYPGCHFCTVHGMKDLDHRH
LRIHTGDKPHKCEFCDKCFSRKDNLTMHMRCHTSVKPHKCHLCDYAAVDSSSLKKHLRIHSDE
PYKCQLCPYASRNSSQLTVHLRSHTGDTPFQCWLCSAKFKISSDLKRHMIVHSGEKPFKCEFC
VRCTMKANLKSHIRIKHTFKCLHCAFQGRDRADLLEHSRLHQADHPEKCPECSYSCSSAAALRV
HSRVHCKDRPFKCFDFCSFDTKRPSSLAKHVDKVRDEAKTENRAPLGKEGLREGSSQHVAKIVT
QRAFRCETCGASFVRDDSLRCHKKQHSDQSENKNSDLVTFPPESGASGQLSTLVSVGQLEAPLE
PSQDL
```

- a) Display the sequence regions that are helical in nature. **(20 marks)**
- b) Display the sequence regions that have the tendency to form beta strands. **(20 marks)**
- c) Display the conflicting regions. Also solve these conflicts to reach to the final assignment of secondary structural elements. Display the output for the complete sequence. **(10 marks)**

Use the Chou and Fasman parameters provided on the next page for all the calculations in your program.

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

Residue	P_{α}	Residue	P_{β}
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