

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2025

B.Tech-V Semester (BI)

COURSE CODE (CREDITS): 18B1WBI531 (3)

MAX. MARKS: 35

COURSE NAME: Structural Bioinformatics

COURSE INSTRUCTORS: Dr. Raj Kumar

MAX. TIME: 2 Hours

**Note:** (a) All questions are compulsory.

(b) The candidate is allowed to make Suitable numeric assumptions wherever required for solving problems

Q.No	Question	CO	Marks
Q1	Explain protein structure classification by CATH database.	2	3
Q2	Comparative modeling is a computational method used to predict the 3D structure of a protein from its amino acid sequence. What are the major sources of error in comparative modeling, and how do they arise during model construction?	2	5
Q3	Consider two proteins with PDB IDs 1ABC and 2XYZ. How would you compare these proteins, and what approaches or criteria would you use to interpret the results of the comparison?	3	3
Q4	A protein has 100 amino acids. Its actual secondary structure is H = 40, E = 40, and C = 30. The predicted structure is H = 35, E = 25, and C = 40. What is the Q3 score for this secondary structure prediction?	4	3
Q5	Calculate the statistical propensities of Leucine and Alanine residues in helix conformation of the given sequence. SS- HHHHHCCCCCCCCCHHHHHCCCCCCC Seq: AVLLTSAPLPTPLESR YRARIYRGNAITV	5	6
Q6	What is energy minimization process? Why it is essential to minimize a biomolecular system before production run?	6	4
Q7	To compute the intermolecular potential between two like atoms is calculates using Lennard-Jones (LJ) potential. Give explanation and mathematical expression for calculating LJ potential.	6	5

Q8

Evaluate the first seed window for the given sequence using the given Chou-Fasman parameters.

Seq - LDVRDSKSVAAARERVTEGRVDVLVCNAGLGLLGP

5

6

TABLE B.2 Chou-Fasman parameters

Residue	P <sub>e</sub>
Glu	H <sub>e</sub> 1.53
Ala	1.45
Leu	1.34
His	h <sub>e</sub> 1.24
Met	1.20
Gln	1.17
Tro	1.14
Val	1.14
Phe	1.12
Lys	l <sub>e</sub> 1.07
Ile	1.00
Asp	l <sub>e</sub> 0.98
Thr	0.82
Ser	0.79
Arg	0.79
Cys	0.77
Asn	b <sub>e</sub> 0.73
Tyr	0.61
Pro	B <sub>e</sub> 0.59
Gly	0.53