## JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT TEST -2 EXAMINATION- 2025

## B.Tech-V Semester (BI)

COURSE CODE (CREDITS): 18B1WBI531 (3)

MAX. MARKS: 25

**COURSE NAME: Structural Bioinformatics** 

COURSE INSTRUCTORS: Dr. Raj Kumar

MAX. TIME: 1 Hour 30 Min

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	A bond has an equilibrium bond length of $r_0$ =1.50 Å, $k_b$ =200 kcal/mol/Å <sup>2</sup> . If potential energy $E$ =0.5 kcal/mol, find the actual bond length $r$ .	CO-5	3
Q2	Consider two atoms <i>i</i> and <i>j</i> , respectively. The minimum distance between the two atoms upon superimposition is 2Å in 1D. What is the RMSD of the two atoms?	CO-5	3
Q3	For an actual sequence (10 residues), the secondary structures (SS) is: HHEECCHECH  For a predicted sequence SS is: HEEECHHECC.	CO-4	3
	Compute Q3 score for above prediction.	<u></u>	
Q4	Describe the secondary structure assignments by the STRIDE program.	CO-4	3
Q5	Define a typical potential energy function.	CO-4	3
Q6	Describe the simplest criteria for the hydrogen bond assignment? How can you improve this assignment to suite more sophisticated H-bond assignment by compute programs such as DSSP?	CO-4	5
Q7	Structural alignment attempts to establish homology between two or more polymer structures based on their shape and three-dimensional conformation. Describe working of a method which utilizes distance matrix for structural alignment.	CO-5	5