JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2024

B.Tech-V Semester (BI)

COURSE CODE (CREDITS): 18B1WBI531 (3) MAX. MARKS: 35

COURSE NAME: Structural Bioinformatics

COURSE INSTRUCTORS: 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	(i)	At the end of energy minimization in a biomolecular modelling process, the forces acting on the atoms in the system become close to_____.	3-6	**(5X1=5)**
	(ii)	The _____structure of a protein describes the local folding simultaneously in the protein translation process.		
	(iii)	True or False: Like quantum mechanical methods, molecular mechanics force fields are equally suitable for accurately predicting chemical reactions or properties that involve significant changes in molecular electronic structure, such as bond breaking and formation or charge transfer processes.		
	(iv)	Determine whether the provided reason for the given assertion is accurate? *Assertion*: Potential energy surfaces are useful tools for studying chemical reactions and molecular dynamics. *Reason*: Potential energy surfaces provide insights into the energetics and stability of different molecular configurations, facilitating the prediction of reaction pathways and the analysis of molecular motion, but only in certain cases and not universally applicable.		
	(v)	In molecular modeling, what technique is often used to prevent the optimization algorithm from getting stuck in local energy minima during energy minimization? A) Time step adjustment B) Metropolis criterion C) Line search D) Restart from multiple initial configurations		
Q2		Write the mathematical formulation used to model the potential energy of two charged atoms in a typical potential energy function.	5-6	**3**

Q3	Calculate the intermolecular potential between two like atoms separated by a distance of 5.0 Angstroms. Given, ε =0.997 kJ/mol and σ =2.50 Angstroms.	4-5	3
Q4	Calculate the number of steps required to achieve a simulation run of 10ns for a given time step of 2fs.	4-5	3
Q5	Write a brief note on thermodynamic ensembles used in molecular dynamics simulations?	6	3
Q6	There are different zones of sequence alignment identity that indicate the likelihood of adopting similar structures. How do zones of homology influence the process of homology modeling and template selection?	4	3
Q7	There are several model building steps in homology modelling. Discuss backbone generation and loop modeling steps.	4	5
Q8	Describe the various metrics you would use to measure and assess the results of a protein structure comparison. Explain how these measures are interpreted in terms of structural similarity and functional relevance.	4,5	3
Q9	Describe the key steps involved in the system preparation for molecular dynamics (MD) simulations. Discuss the processes required to prepare the molecular system, including initial setup, solvation, ionization, and energy minimization. How do these steps contribute to ensuring the accuracy and stability of the simulation results?	4-6	7