JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2023

B.Tech-V Semester (BIBT)

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)Marks are indicated against each question in square brackets.

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

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Q1. Explain the following in context to molecular mechanics: (CO-4) [3×3]

1) Geometry optimization
2) Energy gradient
3) Steepest descent

Q2. Biomolecular simulations are increasingly important for understanding and designing biological molecules and their interactions. Discuss the timescales involved in biomolecular dynamics and how experimental techniques capture these dynamics. (CO-5) [3]

Q3. Discuss the importance of equilibration. Which ensembles can be used to equilibrate a system of 'protein in water'? (CO-4) [3]

Q4. Identification of structural domains in proteins by a graph heuristic is a promising approach. Describe the automatic procedure for identifying domains from protein atomic coordinates employed in STRUDL. (CO-3) [5]

Q5. Give a brief account on bonded-terms used by a typical potential energy function with graphical representations of energy terms. (CO-6) [5]

Q6. Interactions between single atoms obey the Lennard-Jones (LJ) potential. How does the LJ potential vary with changes in the distance between particles? Illustrate with a simple explanation. (CO-5) [5]

Q7. Molecular dynamics (MD) is a computer simulation method for analyzing the physical movements of atoms and molecules. Discuss the working of a global MD algorithm. (CO-6) [5]