

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATIONS-2022

B.Tech-IV Semester (BI)

COURSE CODE (CREDITS): 18B1WBI531 (3)

MAX. MARKS: 25

COURSE NAME: Structural Bioinformatics

COURSE INSTRUCTORS: Dr. Raj Kumar

MAX. TIME: 1 Hour and 30 Minutes

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*Note: All questions are compulsory. Marks are indicated against each question in square brackets.*

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Q1. Protein structure comparison aims to measure the structural similarity between two different proteins. What are important outputs of protein structure comparison? [2] (CO-3)

Q2. Cite some examples of methods for protein structure prediction employing '1D to 3D' alignment. [2] (CO-3)

Q3. Secondary structure assignments are used in 3D structure visualizations to simplify the presentation of a protein in order to highlight functional aspects. Which is the simplest representation for hydrogen bond assignment? [2] (CO-2)

Q4. Consider a system of 1000 atoms. What level of representation will you apply to study the simulations upto nanoseconds time scale? [2] (CO-2)

Q5. Bottoms-up and Top-down approaches have been implemented in identifying protein domains. Cite some suitable examples of each approach. [2] (CO-3)

Q6. Tertiary structure prediction includes several model building and model selection criteria. Describe the energy function used in *ab initio* modeling of protein structure? [3] (CO-4)

Q7. Protein structure is more conserved than the protein sequences. Justify your answer by citing a suitable example. [3] (CO-4)

Q8. Consider two rigid bodies with atoms 'i' and 'j', respectively. The minimum distance between the two atoms upon superimposition is 4Å. What is the RMSD between two atoms? [3] (CO-4)

Q9. Discuss the calculations of Coulomb hydrogen bond energy in DSSP algorithm. [3] (CO-4)

Q10. STRUDL program implements graph heuristic procedure for identifying protein domains. How does the residue exchange procedure in STRUDL works? [3] (CO-3)