

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATION- 2023

B.Tech-V Semester (BIBT)

COURSE CODE (CREDITS): 18B1WBI531 (3)

MAX. MARKS: 25

COURSE NAME: Structural Bioinformatics

COURSE INSTRUCTORS: Dr. Raj Kumar

MAX. TIME: 1 Hour 30 Minutes

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

Q1. Describe the following in context to tertiary structure prediction: (CO-5) [2 × 3]

- a) Principles of fold recognition
- b) Physics-based energy function
- c) Conformational search

Q2. Consider two rigid bodies with atoms i and j , respectively. The minimum distance between the two atoms upon superimposition is 4\AA . What is the RMSD of the two atoms? (CO-5) [3]

Q3. Describe the conventions and challenges for defining structural domains in proteins. (CO-2) [2]

Q4. Describe the necessary motions required to compare protein structures? (CO-3) [2]

Q5. Describe the working principle and applications of DALI program. (CO-3) [3]

Q6. Hydrogen bonds are a very special class of intermolecular attractive forces that arise only in compounds featuring hydrogen atoms bonded to a highly electronegative atom. Describe the simplest criteria for the hydrogen bond assignment? (CO-4) [2]

Q7. The secondary structure of proteins is defined by patterns of hydrogen bonds between backbone amide and carboxyl groups. Discuss the helix assignments by the DSSP program. (CO-4) [3]

Q8. An empirical hydrogen bond energy calculation can be derived from the hydrogen bond geometry in crystal structures. Discuss the hydrogen bond assignment by STRIDE program. (CO-4) [3]