Or Y.M

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT
TEST-3 EXAMINATION DECEMBER 2018
B.Tech. (Bioinformatics) Vth Semester

COURSE CODE: 15B11BI511 **MAX. MARKS: 35**
COURSE NAME: Structural Bioinformatics
COURSE CREDITS: 4 **MAX. TIME: 2HR**

Note: All questions are compulsory. Carrying mobile phone during examinations will be treated as a case of unfair means.

Q1. State the problem of Energy Minimization in mathematical terms. Explain the methods of steepest descent, conjugate gradient, and Newton-Rhapson with appropriate mathematical terms.

5 Marks (CO IV and V)

Q2. What are internal and external coordinates? How will you convert external coordinates to internal coordinates? Are the coordinates in a .pdb format belong to internal or external coordinate system? **5 Marks (CO I)**

Q3. Define a structural domain of a protein? What do you understand by top-down, bottom-up, first-generation, and second generation methods of structural domain identification algorithms. Give examples. **5 Marks (CO II)**

Q4. "In SCOP database, only 100 folds account for about half of all protein superfamilies." What are the possible explanations for this phenomenon? How is this information used in fold recognition methods? **5 Marks (CO II and III)**

Q5. Why is the time-step of molecular dynamics (MD) simulation in femto-seconds? Explain what convergence means in MD simulations. Why should a molecule not see its own image in a simulation box? What is the minimum distance between two molecules to prevent seeing its own image? **5 Marks (CO IV and V)**

Q6. What is the pipeline for automating and using computational approaches for structure determination of proteins? Explain the steps where the pipeline still lacks automation and what are the limiting steps for automation? **5 Marks (CO III and IV)**

Q7. Draw schematically the format of PDB and mmCIF format for a biomolecule, labeling the different parts of the file. What are the advantages and disadvantages of both the formats?

5 Marks (CO I)