

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT
TEST-3 EXAMINATION-2021

B.Tech V Semester

COURSE CODE: 18B1WBI531

MAX. MARKS: 35

COURSE NAME: Structural Bioinformatics

COURSE CREDITS: 04

MAX. TIME: 2 Hours

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

- Q1. A systematic modification of the atomic coordinates to achieve the most stable conformer of a molecule is called ___. (1 Mark)
- Q2. To avoid edge effects in molecular dynamics simulations ___ conditions are used. (1 Mark)
- Q3. Forcefields are also called as ___ functions. (1 Mark)
- Q4. In what situations should we use a quantum mechanical calculation?(2 marks)
- Q5. How will you express the rotation along the bond motion mathematically? (2 marks)
- Q6. There are various biophysical methods to study molecular motions. What are advantages of computer simulations over these methods?(2 marks)
- Q7. Consider a system of 1000 atoms. What level of representation will you apply to study the simulations upto nanoseconds time scale? (3 marks)
- Q8. What will be the bond stretch energy if force constant is 10, optimal bond length 0.2nm, and observed bond length is 0.25nm? (3 marks)
- Q9. If you have charged atoms in your system, what type of potential will you use for calculating its potential energy? (3 marks)
- Q10. If your system has a single coordinate (x), how can the force acting on two atoms be expressed?(3 Marks)

Q11. How will the distance between two atoms affect the potential energy of the system if you are using 6-12 potential? Explain. **(3 Marks)**

Q12. Can we achieve global minima using energy minimization procedure? Justify your statement. **(3 Marks)**

Q13. Which algorithm uses a small displacement with every minimization step? How can these steps be manipulated to enhance algorithm's speed? **(4 Marks)**

Q14. What is a collection of points in phase space satisfying the conditions of a particular thermodynamic state called? Discuss its different characteristics. **(4 Marks)**