JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION-2022

B.Tech-V Semester (BI)

COURSE CODE (CREDITS): 18B1WBI531 (3) MAX. MARKS: 35

COURSE NAME: Structural Bioinformatics

COURSE INSTRUCTORS: Dr. Raj Kumar MAX. TIME: 2 Hour

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

Q1. Biomolecules are structurally dynamic in nature. What strategies will you utilize to understand their dynamic motions computationally? [3] (CO-3)

Q2. If you have two neutral atoms in your system, what type of function will you use for calculating its potential energy? Explain. [3] (CO-4)

Q3. If your system has a single coordinate (x), how can the force acting on two atoms be expressed? [3] (CO-4)

Q4. What will be the bond stretch energy if force constant is 5, optimal bond length 0.2nm, and observed bond length is 0.3nm? [3] (CO-5)

Q5. Find out the cumulative charge of the system containing two atoms located at 5nm apart and whose potential energy is -10 kJ/mol? [3] (CO-5)

Q6. Taylor series is implemented in potential energy function. Justify the statement by giving suitable example. [3] (CO-6)

Q7. Differentiate between out-of-plane bending and rotate-along-bond terms. [3] (CO-5)

Q8. Explain the characteristics if a potential energy surface in context to molecular modeling. [3] (CO-6)

Q9. Give a brief account on geometry optimization. [3] (CO-4)

Q10. Conjugate gradient find minima much quicker than the steepest descent algorithm. Justify this statement. [3] (CO-4)

Q11. What is a collection of points in phase space satisfying the conditions of a particular thermodynamic state called? Discuss its different characteristics. [3] (CO-6)

Q12. Can we achieve global minima using energy minimization procedure? Justify your statement. [2] (CO-5)