

END-Term Examinations, June-2023

Centre for Computational Biology and Bioinformatics

Course: M.Sc. Bioinformatics Subject: Fundamentals of Molecular Dynamics Simulations

Semester: 2nd Course Code: BIN469

Credit: 2 Time: 2:00 Hr Maximum Marks: 60

Date: 28-06-2023

Section -A (All Questions are COMPULSORY)

(10 X 1 = 10M)

Q1). Answer the ALL Following Questions

- i. Nucleotide is made up of _____
- ii. Define Docking?
- iii. What is canonical ensemble?
- iv. In isothermal isobaric- ensemble constant is _____
- v. What is steep length?
- vi. Find out the MD software
(a) Desmond (b) GROMACS (c) Both (d) None
- vii. An ensemble is a large group of microscopically described states of a system with all constant macroscopic properties. **True (or) False**
- viii. Verlet Algorithm introduced by
(a) Verlet (b) Stromer (c) Newton (d) None
- ix. Reversible binding of Protein Example
(a) Myoglobin (b) Hemoglobin (c) Both (d) None
- x. 1ps is equal to
(a) 10^{-12} seconds (b) 10^{-11} seconds (c) 10^{-14} seconds (d) 10^{-16} seconds

II. Section -B (Attempt any FOUR Questions)

(4 X 5 = 20 M)

Q2). Define Amino Acid and write down the types with examples?

Q3). What are bonded and Non-bonded interactions and explain?

Q4). Explain the First Order Reaction briefly.

Q5). Discuss about the Ramachandran Plot with diagram.

Q6). Write about the Newton's Equation of Motion

Q7). Write about the Monte Carlo Simulations.

III. Section - C (Attempt any FOUR Questions)

(4 X 7.5 = 30 M)

Q8). What is Homology Modeling and explain the brief Procedure?

Q9). Discuss the Biomolecular Dynamics Methodology?

Q10). Discuss the Protein-Ligand Interaction analysis after Molecular Dynamics Simulation

Q11). What is mean by Energy minimization and write the down the Steepest Descent Algorithm

Q12). Write briefly about the Verlet algorithm (or) Velocity Verlet algorithm

Q13). What are Nucleotides and Draw the Chemical Structures based on Types