Centre for Computational Biology and Bioinformatics

CENTRAL UNIVERSITY OF HIMACHAL PRADESH

(Established under Central Universities Act 2009, Accredited with NAAC A+)

Shahpur, District: Kangra, Himachal Pradesh-176206

MID-TERM EXAMINATIONS, APRIL-2024 (SPRING SESSION)

M.SC. BIOINFORMATICS

Semester: II

Name of the Course: Fundamentals of Molecular Dynamics Simulation

Course Code: BIN463 Credit: 2 Time Duration: 1 Hour Maximum Marks: 20

Date of Exam: 15-4-2024 **Roll No:**

Q3). Discuss the advantages and disadvantages of the steepest descent and conjugate gradient algorithms for energy minimization in molecular mechanics.

Q4). Describe the key features of the Leapfrog algorithm and its significance in molecular dynamics simulations.

Q5). Explain the importance of equilibration time and adaptive time steps in molecular dynamics simulations.

SECTION-C

ANSWER ANY TWO OF THE FOLLOWING QUESTIONS 2 X 5= 10 M

Q6). Discuss the concept of non-bonded interactions in molecular mechanics force fields. How do Van der Waals interactions and electrostatic interactions contribute to the overall potential energy of a system?

Q7). Explain the significance of the Ramachandran diagram in protein structure analysis. How do point charges in force fields affect the conformational behavior of proteins?

Q8). Compare and contrast the Verlet algorithm with the Leapfrog algorithm in the context of molecular dynamics simulations. What are their respective advantages and limitations?

Q9). Describe the role of Boltzmann velocity distribution in molecular dynamics simulations. How are initial atomic velocities assigned based on this distribution?