BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: BTECH. **SEMESTER : V**
BRANCH: BIOTECHNOLOGY **SESSION : MO/2025**

SUBJECT: BE328 MOLECULAR SIMULATION OF BIOMOLECULES

TIME: 3 Hours **FULL MARKS: 50**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 10 marks and total 50 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
***4*. Before attempting the question paper, be sure that you have got the correct question paper.**
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

			CO	BL
Q.1(a)	Determine the equilibrium distance r_{min} at which the Lennard-Jones potential reaches its minimum for σ = 0.34nm.	[5]	1	3
Q.1(b)	Derive the general expression for the total potential energy of a molecule in molecular mechanics. Discuss the physical meaning of each term.	[5]	1	2
Q.2	Explain the terms PBC, MIC, Cut-off distance, Neighbour list, and Time step used in MD simulations. Describe their importance and, where applicable, discuss the criteria for selecting appropriate values for each.	[10]	2	2,4
Q.3(a)	Discuss the assumptions underlying classical force fields. Why is it necessary to assign different atom types even for the same element in a force field? Illustrate with examples from organic molecules.	[5]	3	1,2
Q.3(b)	Explain any one of the commonly used time integration algorithms. Derive its mathematical formulation and present the final position and velocity update equations. Discuss its advantages and limitations with respect to computational speed, memory efficiency, choice of time step, energy conservation, and time reversibility.	[5]	3	2.4
Q.4(a)	Explain the algorithm of either the Steepest Descent or Conjugate Gradient method used for energy minimization. Describe the step-by-step procedure and discuss the advantages and limitations of the chosen method.	[5]	4	1,2
Q.4(b)	Discuss three common convergence criteria and two practical considerations used in energy minimization during Molecular Dynamics simulations.	[5]	4	3
Q.5(a)	Define docking power, scoring power, ranking power, and screening power. Discuss how each reflects a different aspect of a docking program's accuracy and reliability.	[5]	5	2
Q.5(b)	briefly explain the following five terminologies used in Genetic Algorithms in the context of molecular docking: Population, Fitness Function, Selection, Crossover, and Mutation.	[5]	5	1

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