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

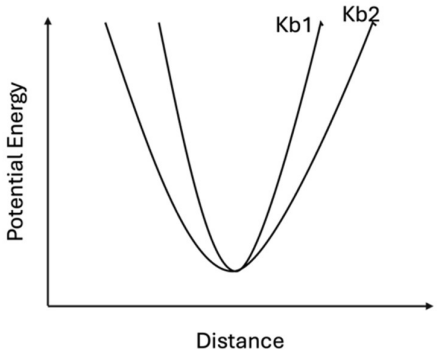
CLASS: B. TECH. **SEMESTER : V**
BRANCH: BIOTECHNOLOGY **SESSION : MO/2025**

SUBJECT: BE328 MOLECULAR SIMULATION OF BIOMOLECULES

TIME: 02 HOURS **FULL MARKS: 25**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 5 marks and total 25 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
***4*. Tables/Data handbook/Graph paper etc., if applicable, will be supplied to the candidates**

			CO	BL
Q.1(a)	Explain the following terms briefly in the context of molecular docking: **1.** Conformation **2.** Orientation	[2]	1	2
Q.1(b)	Define molecular docking and explain its significance. List any two applications where this technique is commonly used in biological research.	[3]	1	1
Q.2	Explain the role of the genetic algorithm in molecular docking. How does it help in identifying optimal binding poses?	[5]	1	2
Q.3	Explain the bonded energy terms in molecular mechanics. How do these terms contribute to the overall potential energy of a molecular system?	[5]	2	1
Q.4(a)	Calculate the intermolecular potential energy between two atoms separated by 0.4 nm using the Lennard-Jones potential. Given that ϵ = 0.997 kJ/mol and σ = 3.40 Å.	[2]	2,5	3
Q.4(b)	For the Lennard-Jones 6–12 potential, derive the relationship between r_m (the separation at which the potential energy is minimum) and σ (the distance parameter).	[3]	2,5	3
Q.5(a)	Which curve corresponds to the bond with a higher bond strength? Justify your choice.	[2]	2,5	4



Q.5(b)	What is a force field in molecular simulations? Why is it generally not advisable to mix parameters from two different force fields in a single calculation?	[3]	2,5	2

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