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

CLASS: B.TECH. **SEMESTER: V**
BRANCH: BIOTECH. **SESSION: MO/2022**

SUBJECT: BE328 MOLECULAR SIMULATION OF BIOMOLECULES

TIME: 2 HOURS **FULL MARKS: 25**

INSTRUCTIONS:
1. The total marks of the questions are 25.
2. Candidates may attempt for all 25 marks.
3. Before attempting the question paper, be sure that you have got the correct question paper.
4. The missing data, if any, may be assumed suitably.
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

			Marks	CO	BO
Q1	(a)	Why molecular docking considered as a power tools in drug design? Explain in detail.	[2]	CO1	Understanding
Q1	(b)	Discuss the conformation ensemble-based docking procedure. Why it is considered superior than other two docking procedure?	[3]	CO1	Understanding
Q2	(a)	Explain the term "pose" in molecular docking and how the information of pose is useful to improve the affinity of the ligand.	[3]	CO1	Application
Q2	(b)	What is dissociation constant and how to calculate it in molecular docking?	[2]	CO1	Knowledge
Q3	(a)	Which of the following statements is true? Justify your choice. 1) The most stable conformation of a drug is also the active conformation. 2) The active conformation is the most reactive conformation of a structure. 3) The active conformation can be determined by conformational analysis. 4) The active conformation is the conformation adopted by a drug when it binds to its target binding site.	[2]	CO1	Understanding
Q3	(b)	What is Molecular Mechanics? Enlist its applications and assumptions.	[3]	CO2	Knowledge
Q4	(a)	What is the main difference between the proper and improper dihedral angles? Why the improper dihedral angle is used in molecular mechanics? Give one example of how to model it.	[3]	CO2	Application
Q4	(b)	Drive the relationship between separation (r) and sigma (σ) at the equilibrium distance (r_m) for LJ 6-12 potential.	[2]	CO2	Analysis
Q5	(a)	What are the partial charges? How to calculate them? Explain with an example.	[3]	CO2	Understanding
Q5	(b)	Calculate the LJ 6-12 potential between two atoms using the following data. (Separation between atoms 4.0Å, ϵ=0.997 kJ/mol and σ=0.340 nm).	[2]	CO2	Application

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