Roll No_____

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BSc. Hons. Chemistry (FYUP), Chemistry/Semester-I
Paper Title: Molecular Modeling and Drug Design
Paper Code: BCH-MIC 401

Time: 2 ½ hours **Maximum Marks: 60**

Abbreviations Used: CLO- Course Outcome, PLO- Program Outcome, BTL- Bloom Taxonomy Level: BT level 1-Remember; BT level 2-Understand; BT level 3-Apply; BT level 4-Analyse; BT level 5-Evaluate, BT level 6-Create.

Q. No.		BTL	CLO	PLO
	SECTION A			
Very Short Type Questions (Attempt all):		**(1x15=15 marks)**		
A1	What is the fundamental difference between Newtonian mechanics and Schrodinger's equation?	2	2	2-3
A2	Define Molecular Mechanics.	2	2	2-3
A3	What are Van der Waals Interactions?	1	2	2
A4	Name one type of molecular surface representation used in molecular graphics.	2	2	3
A5	What does LCAO stand for in molecular orbital theory?	1	1-2	1-2
A6	Give an example of an extended basis set.	2	3	3
A7	State the Born-Oppenheimer Approximation.	1	2	2
A8	What is a potential energy surface?	1	2	3
A9	Define Energy Minimization in the context of molecular modeling.	1	1-2	1-2
A10	What is the Metropolis method used for?	2	2-3	2-3
A11	What does CADD stand for?	1	1-2	1-2
A12	Define Molecular Docking.	2	2-3	3
A13	What is Homology Modeling used for?	2	3	2-3
A14	Name one software used for molecular docking, briefly	2	1-2	1-2
A15	What is a scoring function in molecular docking?	1	1	2
	SECTION B			
Long Type Questions (Attempt any two out of four):		**(10x2=20 marks)**		
B1	Explain the components of a typical Molecular Mechanics force field, including (a) bonded and (b) non-bonded interaction terms.	3	1-3	1-3
B2	(a) Describe the Hartree-Fock method. What are its main approximations and limitations? (b) Discuss the role of basis sets in HF calculations.	4-6	2-6	4-6

B3	(a) Explain the principles of Molecular Dynamics (MD) simulation. (b) Discuss how temperature and pressure are controlled in MD simulations.	3-4	3-5	3-5
B4	(a) Describe the process of Homology Modeling for protein structure prediction. (b) What are the key steps involved, and how is the final model evaluated?	4-5	3-6	3-6
	SECTION C			
Short Type Questions (Attempt all Questions):				**(5x5=25 marks)**
C1	Discuss the different types of coordinate systems used in molecular Modeling and their relevance. Or Explain the concept of normal modes of vibration and how they are treated using Quantum Mechanics (QM).	3-4	3-4	3-4
C2	Define the following: (a) Bond length, (b) Bond Angle and (c) dihedral angle (d) Derive value of tetrahedron angle Or Discuss different types of basis sets used in QM calculations (e.g., STO/nG, polarization functions).	3-5	4-5	4-5
C3	Compare and contrast Molecular Dynamics (MD) and Monte Carlo (MC) simulation methods. Or Explain how long-range forces are typically handled in computer simulations like MD or MC.	3	4	3-4
C4	Describe different types of scoring functions used in molecular docking (e.g., Forcefield-based, Empirical, Knowledge-based). Or Describe the process of protein structure comparison and classification. Why is it important?	4-6	4	4-5
C5	What is Virtual Screening? Explain its importance in drug discovery. Or Explain the difference between structure-based drug design and ligand-based drug design.	5-6	3-6	4-6

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