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MSc Chemistry
Semester-IV Examination-2025
Paper Title: Molecular Modelling and Drug Design
Paper Code: MCH-DCE406

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 a Potential Energy Surface (PES)?	2	2	1-2
A2	Name one type of coordinate system used in molecular modelling.	2	2	01-Feb
A3	What are ab initio methods in quantum chemistry?	1	2	2
A4	Define Hartree-Fock equations.	2	2	3
A5	What is a Gaussian basis set?	1	1-2	1-2
A6	Give an example of a bonded term in a molecular force field.	2	3	3
A7	What are van der Waals forces?	1	2	2
A8	Define parameterisation in the context of force fields.	1	2	3
A9	What is energy minimisation?	1	1-2	1-2
A10	What does MD stand for in simulation methods?	2	2-3	2-3
A11	What is Homology Modelling?	1	1-2	1-2
A12	Define Molecular Docking.	2	2-3	3
A13	What is Chemo-informatics?	2	3	2-3
A14	What is meant by free energy of solvation?	2	1-2	1-2
A15	Name one application of simulations in modern drug design.	1	1-2	2
SECTION B				
Long Type Questions (Attempt **any two** out of four):		(10x2=20 marks)		
B1	(a) Discuss the fundamental concepts of quantum chemistry relevant to molecular modelling, including single/multiple electron systems, *Density Functional* methods, and the Hartree-Fock equations.	3	1-3	1-3
B2	(a)Explain the different types of interactions included in molecular force fields (bonds, angles, torsions, electrostatics, van der Waals). (b) Discuss the limitations of force fields.	4-6	2-6	4-6
B3	(a) Explain Born-Oppenheimer Approximation theory	3-4	3-5	3-5

	(b)How Neutral Entities, Ionic entities and radical entities are classified based on Hartree-Fock theory			
B4	Discuss advanced applications of molecular simulations in drug design, (a) free energy calculations, (b) chemical reactions, and (c) molecular docking.	4-5	3-6	3-6
SECTION C				
Short Type Questions (Attempt all Questions):		(5x5=25 marks)		
C1	Explain the role and importance of different types of basis sets (e.g., Gaussian basis sets) in *ab initio* calculations. Or Describe the Hartree-Fock method in quantum chemistry. What are its main approximations?	3-5	4-5	4-5
C2	Discuss the concept of Weak Forces and how they are considered and evaluated using Hartree-Fock matrix. Or Explain the concept of effective pair potentials and their role in simplifying force field calculations, especially for phenomena like hydrogen bonding.	3	4	3-4
C3	Compare and contrast energy minimization algorithms and Molecular Dynamics simulations in exploring conformational space. Or Discuss the Statistical importance of Ramachandran Plot and its importance in Homology modelling.	4-6	4	4-5
C4	Describe the process and importance of homology modeling in predicting protein 3D structures. Or Describe the Monte Carlo method and its application in conformational analysis.	3-4	2-3	3-5
C5	Outline the principles of molecular docking and its application in identifying potential drug candidates. Or Explain the various steps of performing QSAR analysis.	5-6	3-6	4-6
