Enrollment No./Seat No.:

GUJARAT TECHNOLOGICAL UNIVERSITY

POST GRADUATE DIPLOMA IN BIOINFORMATICS - SEMESTER - I EXAMINATION - WINTER 2025

Subject Code: 1310206 **Date: 26-12-2025**

Subject Name: Computer Aided Drug Designing

Time: 10:30 AM TO 01:00 PM **Total Marks: 70**

Instructions

1. Attempt all questions.

2. Make suitable assumptions wherever necessary.

3. Figures to the right indicate full marks.

4. Draw neat and clean diagrams as required.

		Marks
Q.1	Write a note on following	**20**
(1)	Write a short note Z-matrix representation of a molecule.	
(2)	Differentiate between global minimum conformation and bioactive conformation.	
(3)	Explain the role of hydrophobic interactions in the protein folding process.	
(4)	What is the full form of ADMET? Give the reason why predicting ADMET properties is important in drug design.	
(5)	How does flexible docking differ from rigid docking?	
(6)	Write a short note on GPCR receptors as the most widely found drug targets.	
(7)	Write a short note on internal 2D structure representations of a small molecule.	
(8)	What is the Zinc Database? Discuss its significance in drug discovery.	
(9)	What is Free Wilson analysis, and how does it differ from Hansch analysis?	
(10)	Give the advantages of structure-based virtual screening.	
Q.2	Answer the following (Any 2 out of 3)	**20**
(1)	Define the Empirical force field and give its role in the calculation of the energy of a molecule.	
(2)	Compare and contrast quantitative structure-activity relationship (QSAR) modeling with molecular dynamics simulations in drug design.	
(3)	Describe the integration of structure-based and ligand-based approaches in the context of Computer-Aided Drug Design.	
Q.3	Answer the following (Any 6 out of 8)	**30**
(1)	What is fragment-based drug design (FBDD)? How does it differ from traditional drug design?	
(2)	Based on the information stored in a SMILE notation, explain how it is better than any other line notation, like Wiswesser line notation.	

(3) Describe the conjugate gradient method for energy minimization. What makes it more advantageous than the steepest descent method when dealing with large molecules?

(4) How does pharmacophore-based screening differ from similarity-based methods?

(5) Describe the difference between internal and external 2D structure representation of a molecule with the help of an example.

(6) What parameters are typically evaluated in docking studies? Explain.

(7) How can genomic and proteomic information be used in discovery of a novel target? explain in detail.

(8) A given protein has been identified as a potential drug target. The required protein 3D structure has been created, comprising of 500 amino acids. All the hydrogen atoms have been added and the structure has been optimized, now the structure requires to be energy minimized. Which energy minimization algorithm are you going to use to minimize the energy of the same. Give reasons for your answer

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