GUJARAT TECHNOLOGICAL UNIVERSITY
Integrated Master of Science (Biotechnology)
Semester: 6
Subject Name: Computer Aided Drug Designing
Subject Code: 1360405

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks				Total Marks
				Theory Marks		Practical Marks		
L	T	P	C	ESE (E)	PA (M)	PA (I)	ESE (V)	
4	0	0	4	70	30	0	0	100

Prerequisite:
Students should have the basic knowledge of Computer and Bioinformatics.

Rationale:
The subject of Computer Aided Drug Designing (CADD) is crucial in modern drug discovery, providing efficient computational tools to expedite the identification and optimization of lead compounds. Understanding the principles and techniques in CADD is essential for drug design researchers and pharmaceutical professionals.

Course Content:

Unit No.	Content	No. of Hours	Weightage (%)
1	**Introduction to Computer Aided Drug Design (CADD)** History, different techniques and applications Quantitative Structure Activity Relationships: Basics History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters, lipophilicity effects and parameters, steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physicochemical parameters.	6	10
2	**Quantitative Structure Activity Relationships** Applications Hansch analysis, Free Wilson analysis and relationship between them, Advantages and disadvantages; Deriving 2D-QSAR equations. 3D- QSAR approaches and contour map analysis. Statistical methods used in QSAR analysis and importance of statistical parameters.	15	25
3	**Molecular Modelling and Docking** Molecular and Quantum Mechanics in drug design, Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation, Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra-precision docking.	15	25
4	**Molecular Properties and Drug Design** Prediction and analysis of ADMET properties of new molecules and its importance in drug design. De novo drug design: Receptor/enzyme- interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design. Homology modeling and	12	20

	generation of 3D- structure of protein.		
5	**Pharmacophore Mapping and Virtual Screening** Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modelling; Conformational search used in pharmacophore mapping In Silico Drug Design and Virtual Screening Techniques Similarity based methods and Pharmacophore based Screening, structure based In-silico virtual screening protocols.	12	20
	Total Hours:	60	100

Textbook:

1. Robert M troud and Janet.F Moore Computational and structural approaches to drug discovery, RCS Publishers. Latest edition
2. Y.C. Martin, Introduction to Quantitative Drug Design, Taylor & Francis. Latest edition

Reference Books:

1. Ariens, Drug Design, Elsevier Publishers, Latest Edition
2. Smith and Williams, Principles of Drug Design. Taylor & Francis. Latest Edition
3. Richard B. Silverman, The Organic Chemistry of the Drug Design and Drug action. Elsevier Publishers. Latest Edition

Course Outcomes:

No.	Course Outcomes	RBT Level*
1	Understand the basic concepts, terminology of molecular modelling, molecular docking and 3D QSAR	UN,RM
2	Gain knowledge of different molecular modelling, molecular docking and 3D QSAR tools	UN,RM
3	Develop skills to study and analyze biological macro-molecules in drug design framework.	UN,RM, AN

*RM: Remember, UN: Understand, AP: Apply, AN: Analyze, EL: Evaluate, CR: Create

Suggested Course Practical List:

NA

List of Laboratory/Learning Resources Required

- https://nptel.ac.in/courses/102106070
- https://www.springer.com/journal/10822
- https://github.com/volkamerlab/TeachOpenCADD.