GUJARAT TECHNOLOGICAL UNIVERSITY

Bachelor of Pharmacy
Subject Code: BP807TT
SEMESTER: VIII
Subject Name: Computer Aided Drug Design

Scope: This subject is designed to provide detailed knowledge of rational drug design process and various techniques used in rational drug design process.

Objectives: Upon completion of the course, the student shall be able to understand
- Design and discovery of lead molecules
- The role of drug design in drug discovery process
- The concept of QSAR and docking
- Various strategies to develop new drug like molecules.
- The design of new drug molecules using molecular modeling software

Teaching scheme and examination scheme:

Teaching Scheme				Evaluation Scheme			
Theory	Tutorial	Practical	Total	Theory		Practical	
				External	Internal	External	Internal
3	1	0	4	70	30	0	0

Sr No	Topics	% weightage
1.	**Introduction to Drug Discovery and Development** Stages of drug discovery and development **Lead discovery and Analog Based Drug Design** Rational approaches to lead discovery based on traditional medicine, Random screening, Non-random screening, serendipitous drug discovery, lead discovery based on drug metabolism, lead discovery based on clinical observation. **Analog Based Drug Design:**Bioisosterism, Classification, Bioisosteric replacement. Any three case studies	10
2.	**Quantitative Structure Activity Relationship (QSAR)** SAR versus QSAR, History and development of QSAR, Types of physicochemical parameters, experimental and theoretical approaches for the determination of physicochemical parameters such as Partition coefficient, Hammet's substituent constant and Tafts steric constant. Hansch analysis, Free Wilson analysis, 3D-QSAR approaches like COMFA and COMSIA.	10
3.	**Molecular Modeling and virtual screening techniques** **Virtual Screening techniques:** Drug likeness screening, Concept of pharmacophore mapping and pharmacophore based Screening, **Molecular docking**: Rigid docking, flexible docking, manual docking, Docking based screening. *De novo* drug design.	10
4.	**Informatics & Methods in drug design** Introduction to Bioinformatics, chemoinformatics. ADME databases, chemical, biochemical and pharmaceutical databases.	8
5.	**Molecular Modeling:** Introduction to molecular mechanics and quantum mechanics. Energy Minimization methods and Conformational Analysis, global conformational minima determination.	7

Recommended Books (Latest Editions)

1. Robert GCK, ed., "Drug Action at the Molecular Level" University Prak Press Baltimore.
2. Martin YC. "Quantitative Drug Design" Dekker, New York.

3. Delgado JN, Remers WA eds "Wilson & Gisvolds's Text Book of Organic Medicinal & Pharmaceutical Chemistry" Lippincott, New York.
4. Foye WO "Principles of Medicinal chemistry 'Lea & Febiger.
5. Koro lkovas A, Burckhalter JH. "Essentials of Medicinal Chemistry" Wiley Interscience.
6. Wolf ME, ed "The Basis of Medicinal Chemistry, Burger's Medicinal Chemistry" JohnWiley& Sons, New York.
7. Patrick Graham, L., An Introduction to Medicinal Chemistry, Oxford University Press.
8. Smith HJ, Williams H, eds, "Introduction to the principles of Drug Design" Wright Boston.
9. Silverman R.B. "The organic Chemistry of Drug Design and Drug Action" Academic Press New York.