FACULTY OF PHARMACY

Marwadi University

B. PHARMACY

Syllabus ◆ Semester-8

Elective subject-**5** name with code: **13PH0807 Computer-Aided Drug Design**

Course Objective

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

Course Outcomes

Upon completion of the course, the student shall be able to

1. Design and discovery of lead molecules.
2. The role of drug design in the drug discovery process.
3. The concept of QSAR and docking.
4. Various strategies to develop a new drug-like molecule.
5. The design of new drug molecules using molecular modelling software.

Teaching and assessment scheme

Teaching Scheme (Hours)			Credits	Theory/ Tutorial Marks			Practical Marks		Total Marks
Theory	Tutorial	Practical		CSE	IA (I)	ESE (E)	TW	Viva (V)	
3	1	0	4	10	15	75	0	0	100

Theory syllabus **Teaching hours: 45 Hours**

Unit-1 10 Hours

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, Bio isosteric replacement. Any three case studies

Unit-2 10 Hours

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, Hammett's substituent constant and Tafts steric constant. Hansch analysis, Free Wilson analysis, 3D-QSAR approaches like COMFA and COMSIA.

Unit-3 10 Hours

Molecular modelling and 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.

Unit-4 8 Hours

Informatics & methods in drug design: Introduction to Bioinformatics, chemoinformatic. ADME databases, chemical, biochemical and pharmaceutical databases.

Unit-5 7 Hours

Molecular modelling: Introduction to molecular mechanics and quantum mechanics. Energy Minimization methods and Conformational Analysis, global conformational minima determination.

Tutorials will be based on the above syllabus. **Teaching hours: 15 Hours**

Recommended references (Latest edition)

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 & Fibiger.
5. Koro Ikovas A, Burckhalter JH. "Essentials of Medicinal Chemistry" Wiley Interscience.
6. Wolf ME, ed "The Basis of Medicinal Chemistry, Burger's Medicinal Chemistry" John Wiley& Sons.
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.