

INSTITUTE	FACULTY OF PHARMACY
PROGRAM	BACHELOR OF PHARMACY
SEMESTER	8
COURSE TITLE	COMPUTER AIDED DRUG DESIGN
COURSE CODE	13PH0807
COURSE CREDITS	4

Objective:

- 1 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: After completion of this course, student will 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.

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

Teaching and Examination Scheme

Theory Hours	Tutorial Hours	Practical Hours	ESE	IA	CSE	Viva	Term Work
3	1	0	75	15	10	0	0

Contents : Unit	Topics	Contact Hours
1	Introduction to drug discovery and development 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	10

Contents : Unit	Topics	Contact Hours
2	Quantitative Structure-Activity Relationship (QSAR) 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.	10
3	Molecular modelling and virtual screening techniques 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.	10
4	Informatics & methods in drug design Informatics & methods in drug design: Introduction to Bioinformatics, chemoinformatic. ADME databases, chemical, biochemical and pharmaceutical databases.	8
5	Molecular modelling Molecular modelling: Introduction to molecular mechanics and quantum mechanics. Energy Minimization methods and Conformational Analysis, global conformational minima determination.	7
Total Hours		45

Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
1	Tutorials Tutorial 1, Tutorial 2, Tutorial 3, Tutorial 4, Tutorial 5, Tutorial 6, Tutorial 7, Tutorial 8, Tutorial 9, Tutorial 10, Tutorial 11, Tutorial 12, Tutorial 13, Tutorial 14, Tutorial 15	15
Total Hours		15

Textbook :

- 1 Martin YC. "Quantitative Drug Design", Dekker,, New York., 1978

References:

- 1 Robert GCK, ed., "Drug Action at the Molecular Level" University Prak Press Baltimore.
- 2 Delgado JN, Remers WA eds "Wilson & Gisvolds's Text Book of Organic Medicinal & Pharmaceutical Chemistry" Lippincott, New York.
- 3 Foye WO "Principles of Medicinal chemistry 'Lea & Fibiger.
- 4 Koro lkovas A, Burckhalter JH. "Essentials of Medicinal Chemistry" Wiley Interscience.
- 5 Wolf ME, ed "The Basis of Medicinal Chemistry, Burger's Medicinal Chemistry" John Wiley& Sons.

References:

- 6 Patrick Graham, L., An Introduction to Medicinal Chemistry, Oxford University Press.
- 7 Smith HJ, Williams H, eds, "Introduction to the Principles of Drug Design" Wright Boston.
- 8 Silverman R.B. "The Organic Chemistry of Drug Design and Drug Action" Academic Press New York.

Suggested Theory Distribution:

The suggested theory distribution as per Bloom's taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery					
Remember / Knowledge	Understand	Apply	Analyze	Evaluate	Higher order Thinking / Creative
20.00	30.00	25.00	15.00	10.00	0.00

Instructional Method:

- 1 The course delivery method will depend upon the requirement of content and the need of students. The teacher in addition to the conventional teaching method by the blackboard may also use any tools such as demonstration, role play, quiz, brainstorming, MOOCs etc.
- 2 The internal evaluation will be done based on continuous evaluation of students in the laboratory and classroom.
- 3 Students will use supplementary resources such as online videos, NPTEL videos, MOOCs/ e-courses, virtual laboratories.