INSTITUTE	**FACULTY OF PHARMACY**
PROGRAM	**BACHELOR OF PHARMACY**
SEMESTER	**6**
COURSE TITLE	**COMPUTER-AIDED DRUG DESIGN**
COURSE CODE	**13OE0002**
COURSE CREDITS	**3**

Objective:

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

Course Outcomes: After completion of this course, student will be able to:

1 Design and discovery of lead molecules The role of drug design in the drug discovery process

2 The concept of QSAR and docking Various strategies to develop new drug-like molecules

3 The design of new drug molecules using molecular modelling software.

Pre-requisite of course: Nil

Teaching and Examination Scheme

Theory Hours	Tutorial Hours	Practical Hours	ESE	IA	CSE	Viva	Term Work
3	0	0	50	30	20	0	0

Contents : Unit	Topics	Contact Hours
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. Analogue-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 the Tafts steric constant. Hansch analysis, Free Wilson analysis, 3D-QSAR approaches like COMFA and CoMSIA.	10

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Contents : Unit	Topics	Contact Hours
3	**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
Total Hours		**30**

Textbook :

1 Drug Action at the Molecular Level, Robert GCK, ed., University Prak Press Baltimore , 1977

References:

1 Quantitative Drug Design, Quantitative Drug Design, Martin YC, Dekker, New York, 2010

2 Wilson & Gisvolds's Text Book of Organic Medicinal & Pharmaceutical Chemistry, Wilson & Gisvolds's Text Book of Organic Medicinal & Pharmaceutical Chemistry, Delgado JN, Remers WA eds , Lippincott, New York, 2010

3 Principles of Medicinal chemistry , Principles of Medicinal chemistry , Foye WO , Lea & Febiger, 2008

4 Essentials of Medicinal Chemistry, Essentials of Medicinal Chemistry, Koro lkovas A, Burckhalter JH. , Wiley Interscience, 2008

5 The Basis of Medicinal Chemistry, Burger's Medicinal Chemistry, The Basis of Medicinal Chemistry, Burger's Medicinal Chemistry, Wolf ME, ed , John Wiley & Sons, New York, 2012

6 An Introduction to Medicinal Chemistry, An Introduction to Medicinal Chemistry, Patrick Graham, L., Oxford University Press, 2013

7 Introduction to the Principles of drug design, Introduction to the Principles of drug design, Smith HJ, Williams H, eds, Wright Boston, 2005

8 The Organic Chemistry of Drug Design and Drug Action, The Organic Chemistry of Drug Design and Drug Action, Silverman R.B. , Academic Press New York, 2014

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**
10.00	20.00	25.00	25.00	10.00	10.00

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