18BP092 COMPUTER AIDED DRUG DESIGN

Hours Per Week :

L	T	P	CP	CL
3	1	-	-	4

Total Hours :

L	T	P
45	1	-

WA/RA	SSH/HSH	CS	SA	S	BS

SCOPE:

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

COURSE OUTCOMES:

Upon completion of the course, the student will be able to achieve the following outcomes:

COs	Course Outcomes	POs	PSOs
1	Design and discovery of lead molecules	3	1,2
2	The role of drug design in drug discovery process	3	1,2
3	The concept of QSAR and docking	3	1,2
4	Various strategies to develop new drug like molecules	3	1,2
5	The design of new drug molecules using molecular modeling software	3	1,2

UNIT - I **10HOURS**

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: Bio isosterism, Classification, Bio isosteric replacement. Any three case studies

UNIT - II **10HOURS**

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.

UNIT - III **10HOURS**

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. *Denovo* drug design.

UNIT - IV **08HOURS**

INFORMATICS & METHODS IN DRUG DESIGN: Introduction to Bioinformatics, chemo informatics. ADME databases, chemical, biochemical and pharmaceutical databases.

UNIT - V **07HOURS**

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

RECOMMENDED BOOKS (LATEST EDITIONS)

1. Robert GCK, ed., "Drug Action at the Molecular Level" University Park 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 Inter science.
6. Wolf ME, eds "The Basis of Medicinal Chemistry, Burger's Medicinal Chemistry" John Wiley & 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.