

DISCIPLINE SPECIFIC CORE COURSE -8 (DSC-8) MEDICINAL CHEMISTRY

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
MEDICINAL CHEMISTRY	4	3	-	1		Basic knowledge of Enzymes and proteins

Learning objectives

The introduction of Medicinal Chemistry course at undergraduate level to Biomedical Science students has been conceived to make them understand:

- Concealed chemical science interlinked to other science disciplines such as biophysics, chemistry, biology, biochemistry, pharmacology etc.
- Application of the area in revealing new drug design and targets through studying the drug-receptor interactions and signaling mechanism in cell for lead discovery.
- Various drug targets in the body and drug development strategies with mechanism of action and concept of drug resistance.

Learning Outcomes

- After completing the course, students shall be able to understand the various stages involved in drug development. Further, they will be able to explore various kinds of drug targets including protein, enzymes, nucleic acids etc.
- They will also appreciate the process of drug-receptor interactions; identify association between chemical structure and its physicochemical properties. After the completion of the course, the learners will demonstrate a strong foundation via problem solving, critical thinking and analytical reasoning in the fundamentals of medicinal chemistry, physicochemical principles of drug action and measurement of drug effects, comprehend the physicochemical basis for the rational drug design, analogue synthesis, and mechanism of action of drugs.
- Additionally, this course will involve extensive laboratory work. The students will be able to design and carry out small molecule (low molecular drug-relevant compounds) synthesis. They will do the natural product isolation along with their purification and characterization through chromatography and spectroscopic methods and analyze the results of such experiments.
- They will also actively participate group exercises; communicate the results of experiments conducted in oral as well as written formats. Further, they will appreciate the central role of chemistry in our daily life and will also learn safe handling of hazardous chemicals and follow the SOP for chemical waste disposal.

SYLLABUS OF DSC-8

Unit-1: General introduction

(02 Hours)

Definition and scope of Medicinal Chemistry

Unit-2: Principles of Drug Design

(10 Hours)

Introduction to Structure Activity Relationship (SAR) of morphine/salicylic acid, strategies in the search for new lead compounds, analogue synthesis versus rational drug design, concept of prodrugs. Affinity, efficacy and potency of drugs. Concepts of agonist, antagonist and inverse agonist, competitive, non-competitive, suicide inhibitors.

Unit-3: Physicochemical principles of drug action and measurement of drug effects (10 Hours)

Partition coefficient, drug dissolution, acid-base properties, surface activity, bioavailability, stereochemical aspects of drug action, electronic structure (Hammett correlations) and determining relationship between chemical and biological data (Hansch approach). Kinetic analysis of ligand receptor interactions using Scatchard plot, Double reciprocal plot, Hill plot, forces involved, relationship between dose and effect (graded and quantal response).

Unit-4: Drug target classification

(15 Hours)

- a. Proteins as drug targets.
 - i. Receptors: the receptor role, ion channels, membrane bound enzyme activation, desensitization and sensitization of receptors, agonist (e.g. endorphins) and antagonists(e.g. caffeine)
 - ii. Enzymes: Enzyme inhibitors, medicinal use of enzyme inhibitors (e.g. clavulanic acid)
- b. Nucleic acids as drug targets. Classes of drugs that interact with DNA: DNA intercalators (amsacrine), Groove binders (netropsin), DNA alkylators (amines: mechlorethamine; nitrosoureas: carmustine), concept of antisense therapy.

Unit-5: How drugs trigger the signals-molecular aspects

(08 Hours)

Structure and functions of cell surface receptors, signal transduction mechanism (GPCRs, tyrosine kinase, guanylate-cyclase linked receptors and intracellular receptors that regulate DNA transcription).

Practical Component

(30 hours)

(Wherever wet lab experiments are not possible, the principles and concepts can be demonstrated through any other material or medium including videos/virtual labs etc.)

1. Preparation, recrystallization and purity of following drugs/compounds by melting point and TLC
 - i. Hippuric acid.
 - ii. Benzocaine,
 - iii. Benzoquinone
 - iv. Phenacetin
 - v. s-benzyl thiuronium salt.
2. Determination of partition coefficient of aspirin in octanol-water system.
3. Extraction of caffeine from tea leaves.
4. Study absorption properties of caffeine.
5. Extraction of piperine from black pepper.
6. Phytochemical screening of *Curcuma longa* by solvent extraction: Terpenes and polyphenols

Essential Readings:

- Patrick G.I. (2017). 6th Edition. Introduction to medicinal chemistry. Oxford, UK: OxfordUniversityPress.ISBN-13: 978-0198749691.
- Silverman, R.B. and Holladay, M.W. (2015). 3rd Edition. The organic chemistry of drug design and drug action. San Diego, USA:Elsevier,AcademicPress.ISBN-13:9780123820303.
- Ashutosh Kar (2020) Advanced Practical Medicinal Chemistry 3rd Edition New Age International Private Limited, ISBN-10 : 9388818458

Suggestive Reading for Basics:

- Gringauz, A. (1996). 1st Edition. Introduction to medicinal chemistry: How drugs act and why. Brooklyn, New York, USA: WileyVCH.ISBN-13:978-0471185451.
- King F.D. (2003). 2nd Edition. Principles and practice of medicinal chemistry. London, UK: The Royal Society of Chemistry. ISBN-13: 978-0854046317.
- Nogrady, T. and Weaver, D.F. (2005). 3rd Edition. Medicinal chemistry: A molecular and biochemical approach. New York, USA: Oxford University Press. ISBN-13:978-0195104561.
- Wermuth, C.G., Aldous, D., Raboisson, P. and Rognan, D. (2015). 4thEdition. The practice of medicinal chemistry. San Diego, USA: Elsevier, Academic Press. ISBN-13:978-0124172050.