

## DISCIPLINE SPECIFIC ELECTIVE COURSE – 20 (DSE-20)

### Fundamentals of 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		
Fundamentals of Medicinal Chemistry (DSE-20)	04	02	--	02	Class 12 <sup>th</sup> with Physics, Chemistry	--

#### **Course Objectives**

**The objectives of this course are as follows:**

This course aims to introduce students to the foundational concepts of medicinal chemistry, highlighting its historical development and the significance of natural products as drug sources. Additionally, the course examines the structure, synthesis, therapeutic use, and basic SAR of key drugs like Ibuprofen, Paracetamol, Aspirin, and Penicillin.

#### **Learning outcomes**

**By studying this course, the students will be able to:**

- Understand the development and role of medicinal chemistry, understand the stages of drug discovery, and evaluate drug screening and clinical processes.
- Interpret how stereochemical and physicochemical properties influence drug behavior and efficacy.

#### **Unit 1: Introduction to Medicinal Chemistry and Drug discovery: (15 Hours)**

History and development of medicinal Chemistry. Sources of drugs, including natural products with examples, Stages of drug discovery, Stereochemical aspects, Physicochemical properties: solubility, acid-base, partition coefficient.

Target identification and validation, Screening of drugs, High throughput screening (HTS), Random and Systematic screening. Structure activity relationship (SAR), Hit identification, and Lead optimization

#### **Unit 2: Pharmacokinetics (ADME): (5 Hours)**

Drug administration/absorption, drug distribution, drug metabolism - Phase 1 and Phase 2, drug excretion, Half-Life of drugs, and Clinical trials.

#### **Unit 3: Representative Synthetic Drugs: (7 Hours)**

Structure, Synthesis, and Therapeutic Value of Representative Drugs: Fluconazole (antifungal), Penicillin (antibiotic), Isoniazid (antibiotic), and Azidothymidine (AZT; anti-HIV).

**Unit 4: Bioin-formatics:** Use of computational tools for drug design.

**(3 Hours)**

**Practicals:**

**Credits: 02**

**(Laboratory periods:15 classes of 4 hours each)**

1. Isolation and estimation of aspirin from commercial tablets
2. Synthesis of paracetamol from *p*-aminophenol
3. Synthesis of benzotriazole/benzimidazole.
4. Synthesis of 5,5'-Diphenylhydantoin.
5. Synthesis of dihydropyridine (DHP)/dihydropyrimidine (DHPM).
6. Study of physicochemical properties of pharmaceutically active compounds using computational methods.
7. Synthesis of Benzocaine, a topical pain reliever.
8. Isolation of Caffeine from tea leaves using solvent extraction techniques.
9. Estimation of Vitamin C.

**Essential/recommended readings**

**Theory:**

1. Patrick, G. L. *Introduction to Medicinal Chemistry*, Oxford University Press (2001)
2. Lemke, T. L. & William, D. A., *Foye's Principles of Medicinal Chemistry*, 5th Ed., USA (2002)
3. Dunlap, N. K. & Huryn, D. M., *Medicinal Chemistry*, Garland Science, New York (2018)
4. Mark W. Holladay, Richard B. Silverman. *The Organic Chemistry of Drug Design and Drug Action*, 3<sup>rd</sup> Ed. Academic Press (2014)

**Practical:**

1. Vogel, A. I. (2012), Quantitative Organic Analysis, Part 3, Pearson Education.
2. Mann, F. G., Saunders, B.C. (2009), Practical Organic Chemistry, Pearson Education.
3. Furniss, B. S., Hannaford, A. J., Smith, P.W.G., Tatchell, A.R. (2012), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
4. Ahluwalia, V.K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
5. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
6. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume-I, I K International Publishing house Pvt. Ltd, New Delhi
7. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume-II, I K International Publishing house Pvt. Ltd, New Delhi

**Assessment Methods:** All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.