SEMESTER –VI

MEDICINAL CHEMISTRY AND CATALYSIS

THEORY

Program: B.Sc.   **Max. Hours: 45**
Course Code: U20/CHE/DSE/604   **Hours per week: 3**
Course Type: DSE 4   **Max. Marks: 100**
 No. of Credits: 3

COURSE OBJECTIVES:

- To introduce students to the action of drugs on biological systems.
- To explain about the drug formulation and discovery process.
- To discuss the synthetic routes for some commonly used drugs.
- To gain the knowledge of characteristics of catalysts, mechanism and design of catalytic reactions.
- To learn to calculate and assess the effect of catalysts.

COURSE OUTCOMES:

CO1:   Learn and understand the action of drugs on biological systems.

CO2:   Differentiate between Pharmacodynamic and Chemotherapeutic agents.

CO3:   Comprehend about the drug formulation and discovery process.

CO4:   Discuss the synthetic routes and therapeutic activity for some commonly used drugs.

CO5:   Understand the mechanism of catalytic reactions and characterize a catalyst.

CO 6: Assess the effect of catalysts and design different types of catalytic reactions.

MODULE 1: MEDICINAL CHEMISTRY   (12 Hrs)

TERMINOLOGY IN MEDICINAL CHEMISTRY   (2 Hrs)
Disease, Drug, Pharmacology, Pharmacophore, Pharmacodynamics, Pharmacokinetics, metabolites, antimetabolites, agonist, antagonist and therapeutic index.

Nomenclature   (1 Hr)
Chemical name, Generic name and Trade names. Trade names for the given generic names – (i) Aspirin (ii) Amoxycillin(iii) Ciprofloxacin (iv) Paracetamol (v) Mebendazole.

ADME   (3 Hrs)
a) Absorption: Definition, absorption of drugs across the membrane – active and passive absorption, routes of administration of drugs. b) Distribution: definition and effect of plasma protein binding. c) Metabolism: definition, phase I and phase II reactions. d) Elimination: definition and renal elimination.

CLASSIFICATION OF DRUGS
Classification of Drugs based on therapeutic action–Chemotherapeutic agents, and Pharmacodynamic agents (brief explanation for the following)
(i) Chemotherapeutic agents   (1Hr)
Antimalarials – Chloroquine; Antibiotic – Amoxicillin; Antitubercular drugs – isoniazid; Antiprotozoals – metronidazole: Antibacterial – Sulphanilamide; Anthelmentics –Albendazole.
(ii) Pharmacodynamic agents   (5 Hrs)
(a) Drugs acting on CNS: General (thiopental sodium)and local anaesthetics (Benzocaine),Analgesics (Ibuprofen),Antipyretics (Aspirin, Paracetamol), Sedatives &Hypnotics (Phenobarbital), Anticonvulsants (Diazepam), Anti-psychotics (Chlorpromazine) and Antidepressants (Fluoxetine).
(b) Drugs acting on PNS: Adrenergic (Salbutamol, Propranolol) &Cholinergic (Carbachol, Diphenhydramine) Drugs.
(c) Drugs acting on Cardiovascular System-Antihypertensive Drugs (Captopril, Nifedipine)
(d) Drugs acting on renal system- Diuretic drugs (Furosemide, Acetazolamide)

MODULE 2: MEDICINAL CHEMISTRY II   (11Hrs)

SAR STUDIES   (1Hr)
Introduction to Structure Activity Relationship Studies, Lead modification strategies.SAR of benzodiazepines.
ANTIBIOTICS   (1Hr)
Discovery- Isolation of Penicillin, Striucture of Penicillin G, Penicillin-V, Penicillin-O &Amoxycillin.
SYNTHETIC ROUTE AND BRIEF THERAPEUTIC ACTION OF THE FOLLOWING DRUGS: (4 Hrs)
Chemotherapeutics: Chloroquin, Ciprofloxacin, Sulphanilamide, Metronidazole.

Drugs to treat metabolic disorders: Paracetamol, Salbutamol, Omeprazole, Mephensin, Aspirin, Thiobarbituric acid, L-Dopa, Phenobarbital, Oil of wintergreen, Nifedipine

FORMULATIONS   **(2 Hrs)**
(a) Introduction: Need of conversion of drugs into medicine. Additives & their role (Brief accountonly). (b) Classification of Drug formulations: Oral, parenterals and topical dosage forms – advantages and disadvantages.

BRIEF OVERVIEW OF DRUG DEVELOPMENT PROCESS: **(3 Hrs)**
   (a) Lead drug-Definition & example (b) Drug design-i) Based on Lead compound ii) Based on Target Structure(De novo drug design) iii) Computer aided Drug Design (Molecular modelling) (c) Drug Testing-Clinical trials.

MODULE 3: CATALYSIS I   (11 Hrs)

Homogeneous and heterogeneous catalysis - Definition of a catalyst and catalysis.Comparison of homogeneous and heterogeneous catalysis with specific examples.General characteristics of catalytic reactions.

Acid-base catalysis- Examples of acid and base catalysed reactions, hydrolysis of esters. Kinetics of acid catalysed reactions. Specific acid and general acid catalysis, Kinetics of base catalysed reactions. Specific base and general base catalysis.Examples-Aldol condensation and decomposition of nitramide, base catalysed conversion of acetone to di acetone alcohol. Effect of P H on reaction rate of acid and base catalysed reactions.
Phase transfer catalysis: Principle of phase transfer catalysis, classification of phase transfer catalysts. Factors influencing the rate of PTC reactions.

MODULE 4: CATALYSIS II   (11Hrs)

Enzyme catalysis- Characteristics of enzyme catalysis, Examples: (i) Invertase in inversion of cane sugar (ii) Maltase in conversion of maltose to glucose (iii) Urease in decomposition of urea and (iv) Zymase in conversion of glucose to ethanol. Factors affecting enzyme catalysis. Effect of temperature, pH, concentration and inhibitor on enzyme catalysed reactions.

Kinetics of enzyme catalysed reactions: Michaelis-Menton Equation. Mechanism of enzyme catalysed reactions. Significance of Michaelis constant (Km) and maximum velocity (Vmax), Lineweaver-Burk plot.

Text Books:

1. G.L. David Krupadanam, D.Vijaya Prasad, K.Varaprasad Rao, K.L.N. Reddy,   C. Sudhakar, Drugs, Universities Press (India) Limited 2007.
2. Graham L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, New York. 1995
3. Chemistry text book for B.Sc., Vol. IV published by Telugu Academy, Govt. of Telangana.
4. Principles of Physical Chemistry by Puri, Sharma and Pathania, 2017.
5. Text Book of Physical Chemistry P.L Soni, O.P Dharmaha, U.N Dash.
6. Physical Chemistry by Atkins and De Paula, 8 th Edn.
7. Chatwal. R.G., (2006) Chemistry And Industry, New Delhi, Himalaya Publishing House.

Reference Books

1. Thomas Nogrady, Medicinal Chemistry, Oxford Univ. Press, New York.2005.
2. David William and Thomas Lemke, Foye's Principles of Medicinal Chemistry, Lippincott Williams & Wilkins, 2008.
3. AshutoshKar Medicinal Chemistry, New Age International, 2005.
4. O.D. Tyagi & M.Yadav Synthetic Drugs by, Anmol Publications, 1998.
5. Medicinal Chemistry by Alka L. Gupta, Pragati Prakashan.
6. Kinetics and mechanism of chemical transformations by Rajarajm and Kuraiacose, Published by Macmillan India Ltd.
7. Text book of Physical Chemistry by K.L. Kapoor Macmillan, 1999.
8. Catalysis by J.C. Kuriacose, Macmillan Macmillan Publishers India Limited, 1980.

MEDICINAL CHEMISTRY AND CATALYSIS
MODEL QUESTION PAPER
THEORY

Course Code: U20/CHE/DSE/604   **Max. Marks: 60**
Credits: 3   **Max Time: 2 Hrs**

SECTION - A

I.   Answer the following   **4 x 10 = 40 M**

1. a) Explain briefly about agonist and antagonist. (CO 1)   5 M
    b) Write about anaesthetic and antipyretic drugs. (CO 2)   5 M
                                OR
2. Explain about ADME.   (CO 1)   10 M
3. a) Describe the isolation of Penicillin and give the structure of Penicillin G.   (CO 1)   5 M

    b) What are additives? Explain briefly about diluents and stabilizing agents with
       examples.   (CO 3)   5 M
                                OR
4. The synthetic route and brief therapeutic action of   Write   10 M
    i) Ciprofloxacin   ii) Aspirin iii) Salbutamol   iv) Omeprazole (CO 4)
5. Discuss the Kinetics of Acid-base catalyzed reaction.   (CO 5)   10 M
                                OR
6. a) Define catalysis. Give the characteristics of catalysis. (CO 5)   5 M
    b)Explain types of catalysis with examples.   5M

7. Derive Michaelis - Menten Equation   (CO 6)   10 M
                                OR
8. Explain with mechanisms   (CO 6)   10M
    (i)   Invertase in inversion of cane sugar
    (ii)   Urease in decomposition of urea

SECTION - B

II. Answer any FOUR.   **4 x 5 = 20 M**

I.
9. Write a note on drugs acting on renal system. (CO 2)
10. Write a short note on clinical trials. (CO 3)
11. What are chemotherapeutic agents? Discuss about antimalarial and antitubercular drugs. (CO 2)
12. What are the factors effecting Enzyme catalysis. (CO 5)
13. Explain the principle involved in PTC. (CO 5)
14. Explain Lineweaver-Burk plot. (CO 6)