

Punyashlok Ahilyadevi Holkar
Solapur University, Solapur

SCHOOL OF CHEMICAL
SCIENCES

M. Sc. II, Sem.-III & IV
MEDICINL CHEMISTRY SYLLABUS
(Choice Based Credit System-CBCS)

(w.e.f. June, 2020)

**PUNYASHLOK AHILYADEVI HOLKAR
SOLAPUR UNIVERSITY, SOLAPUR
M. Sc. II, MEDICINAL CHEMISTRY COURSE SYLLABUS
CHOICE BASED CREDIT SYSTEM (CBCS) (w.e.f. June 2020)**

A two-year duration M. Sc. Medicinal Chemistry course syllabus has been prepared as per the CBCS semester system. M. Sc. II, SEM-III & SEM-IV Organic Chemistry syllabus will be implemented from June 2020. The syllabus has been prepared taking into consideration the syllabi of other Universities, SET, NET, UGC guidelines, and the specific inputs of the Expert Committee Members from Pune University, Pune and Dr. BAMU, Aurangabad.

General Structure of the Course:

The course will be of four semesters spread over two academic years. Each semester will have four theory papers of 70 marks for university external examination and 30 marks for internal examination of each semester and two practical's of 70 marks, 30 marks for internal practical of each semester. The distribution of marks is mentioned below

Theory Paper (Semester exam), 16 X 70+30 marks	1600 marks
Practicals (semester end exam.), 8 X 70+30 marks	800 marks
Tutorials for each semester, 4 X 25	<u>100 marks</u>
	Total: 2500 marks

Ratio of marks (Theory: Practical): (73:27)

Semester	Paper Code	Title of the Paper	Semester exam			L	T	P	Credits
			Theory	IA	Total				
I		Hard core							
	HCT-1.1	Inorganic Chemistry -I	70	30	100	4		-	4
	HCT-1.2	Organic Chemistry -I	70	30	100	4		-	4
	HCT-1.3	Physical Chemistry -I	70	30	100	4		-	4
		Soft Core (Any one)							
	SCT-1.1	Analytical Chemistry -I	70	30	100	4		0	4
	SCT-1.2	Chemistry in Life Sciences	70	30	100	4		0	
		Practicals							
	HCP-1.1	Inorganic Chemistry	35	15	50	-	-	2	6
	HCP-1.2	Organic Chemistry	35	15	50	-	-	2	
	HCP-1.3	Physical Chemistry	35	15	50	-	-	2	
		Soft core (Any one)							
	SCP-1.1	Analytical Chemistry	35	15	50	-	-	2	2
SCP-1.2	Analytical Chemistry	35	15	50	-	-	2		
T-1	Tutorial/Seminar					25		1	
	Total for 1st semester	420	180	600		25		25	

II		Hard core							
	HCT-2.1	Inorganic Chemistry -II	70	30	100	4	--	-	4
	HCT-2.1	Organic Chemistry -II	70	30	100	4		-	4
		Soft core (Any one)							
	SCT-2.1	Physical Chemistry -II	70	30	100	4		=	4
	SCT-2.2	Green Chemistry	70	30	100	4		-	
		Open elective (Any one)							
	OET-2.1	Instrumental Methods of Analysis	70	30	100	4		-	4
	OET-2.2	Medicinal Chemistry -I	70	30	100	4		-	
		Practicals							
	HCP 1.1	Inorganic Chemistry	35	15	50	-		-	2
	HCP 1.2	Organic Chemistry	35	15	50	-	-	2	
		Soft core (Any one)							
	SCP 1.1	Physical Chemistry	35	15	50	-	-	2	2
	SCP 1.2	Physical Chemistry	35	15	50	-	-	2	
		Open elective (Any one)							
	OEP 1.1	Analytical Chemistry	35	15	50	-	-	2	2
	OEP 1.2	Medicinal Chemistry	35	15	50	-	-	2	
	T-2	Tutorial/Seminar					25		1
		Total for 2nd semester	420	180	600		25		25

III		Hard core							
4	HCT-3.1	Biochemistry and Bioinorganic Chemistry	70	30	100		--	-	4
	HCT-3.2	Advanced Spectroscopic Methods	70	30	100	4		-	4
		Soft core (Any one)							
	SCT-3.1	Drugs Synthestic Methods	70	30	100	4		-	4
	SCT- 3.2	Fundamentals of Medicinal Chemistry	70	30	100	4		-	
		Open elective (Any one)							
	OET- 3.1	Bioactive Heterocyclic Chemistry	70	30	100	4		-	4
	OET- 3.2	Unit operations of chemical Engineering	70	30	100	4		-	
		Practicals							
		HCP -3.1	Organic Mixture (Ternary)	70	30	100		-	-
	SCP -3.1	Preparation (2 stages)/Drug assay	35	15	50	-	-	2	2
		Open elective (Any one)							
	OEP -3.1	Spectral Problems	35	15	50	-	-	2	2
	OEP- 3.2	Colum chromatography	35	15	50	-	-	2	
	T-3	Tutorial/Seminar					25		1
		Total for 3rd semester	420	180	600		25		25

IV		Hard core							
	HCT-4.1	Medicinal Chemistry	70	30	100	4	--	-	4
	HCT-4.2	Stereo Chemistry	70	30	100	4		-	4
	HCT-4.3	Chemistry of Natural Products	70	30	100	4		-	4
		Soft Core (Any one)						-	4
	SCT-4.1	Drug Discovery	70	30	100	4		-	4
	SCT-4.2	Chemical Industries	70	30	100	4		-	4
		Practicals							
	HCP -4.1	Preparations (3 Stages)	70	30	100	-	-	4	4
	HCMP-4.2	Major Project/In plant training & Chemdraw assignment	70	30	100	-	-	4	4
	T-4	Tutorial/Seminar					25		1
		Total for 4th semester	420	180	600		25		25
		Total			2500				100

L = Lecture T = Tutorials P = Practical
4 Credits of Theory = 4 Hours of teaching per week
2 Credit of Practical = 4 hours per week
HCT = Hard core theory,
SCT = Soft core theory,
HCP = Hard core practical
SCP = Soft core practical,
OET = Open elective theory,
OEP = Open elective practical,
HCMP = Hard core main project

Nature of Examination:

Each semester will have theory external examination of four papers of 70 marks each (2.5 hrs. duration). The practical examination of Semesters I to IV will be conducted at the end of the each Semester. Duly certified copy of laboratory record must be produced at the time of examination.

Practical Examination of M. Sc. II

The practical examination will be of 3 days for each semester.

Practical experiments: 60 marks

Oral: 05 marks

Journal: 05 marks

Project work / In-plant training Report:

60**+10 marks for presentation

** The valuation of project/ In plant training report to be done by both external and internal examiners at the time of examination. Valuation of Tutorials is to be done in each semester by the teaching faculty involved in organic chemistry course.

Nature of question paper (M. Sc. II):

Time: 2.5 hours Max. Marks 70

Instructions

1. Attempt 05 questions.
2. All questions carry equal marks.
3. Figures to the right indicate full marks.
4. Use of log tables and calculators is allowed.

Question Paper Pattern

Q 1. Answer the following (14 sub-questions) Marks 14 (1 x 14) Multiple choice questions, predict the product, provide the reagent and conditions etc.

Sub-questions (i) to (xiv)

Q 2. a) - - - - -Marks 08

b) - - - - -Marks 06

Q 3. a) - - - - -Marks 08

b) - - - - -Marks 06

Q 4. a) - - - - -Marks 10

b) - - - - -Marks 04

Q 5. - - - - -Marks 14

At least 40 % questions should be problem oriented, where-ever possible, in view to train students for the SET/NET/GATE and other competitive examinations. These questions should test the understanding of candidate rather than the memory. The question paper should cover all the Units included in the syllabus of the respective paper and the weightage of the questions should correspond to the number of lectures allotted to the respective Units / Topics.

HCT 3.1: BASIC BIOCHEMISTRY, BIOMOLECULES, BIOINORGANIC CHEMISTRY

Credits: 04

60 L

UNIT I: (15 L)

Introduction of Biochemistry: Introduction: The molecular logic of life; Structural hierarchy in the molecular organization of Cells. Chemical unity of diverse living organisms, prokaryotic and Eukaryotic, Scope of the subject in pharmaceutical Sciences

Carbohydrates Biomolecules: Classification, basic chemical structure, monosaccharides, aldoses, and ketoses, cyclic structure of monosaccharides, stereoisomerisms, anomers and epimers. Reducing properties of monosaccharides, disaccharides, oligosaccharides, polysaccharides, structural studies methylation and periodate oxidation. Polysaccharides structure and function of complex carbohydrates, proteoglycans, glycoproteins, glycolipids, mucopolysaccharides.

UNIT II: (15 L)

Lipids Biomolecules: Classification, structure and function of major lipid subclasses- acylglycerols, circulating lipids: lipoproteins, chylomicrons, LDL, HDL, and VLDL. Pathological changes in lipid levels. Formation of micelles, monolayers, bilayer, liposomes.

Vitamins and Co-enzymes: Classification, water-soluble and fat-soluble vitamins. Structure, dietary requirements, deficiency conditions, coenzyme forms.

UNIT III: (15 L)

Amino acids: Classification, Properties, reactions of amino acids

Proteins: Peptide bond, properties, functions

- (a) Protein structure: Primary structure, Secondary structure; alpha-helix and beta pleated sheets, beta-turns, super secondary structure, and Tertiary structure: forces stabilizing and prediction of tertiary structure, fibrous and globular proteins, and Quaternary structure – hemoglobin.
- (b) Working with proteins: Fractionation and purification by gel filtration and chromatographic techniques. Characterization by gel electrophoresis and isoelectric focusing
- (c) Protein sequencing: end group analysis, Sangers method and Edman degradation method
- (d) Solid phase peptide synthesis

Nucleic acids

- (a) Molecules of Heredity: Structure of deoxyribonucleic acid (DNA) and ribonucleic acid (RNA), DNA double helix, major groove and minor groove, A, B, and Z forms of DNA.
- (b) DNA as genetic material, genetic code, flow of genetic information, DNA replication, transcription and translation
- (c) Drugs acting on DNA: nucleoside analogues, Intercalating agents, Alkylating agents, UV radiations and thymine dimers, Drugs acting by chain cutting

Reference Books:

1. *Principle of Biochemistry, Lehinger D.L. Nelson and M.M. Cox. Macmillan worth Publishers.*
2. *Biochemistry, L. Stryer, W.H. Freeman, San Francisco.*
3. *Schaum's Outline Series of Theory and Problems of Biochemistry, Philip W. Kuchel and G.B. Ralston. Int. Ed., McGraw-Hill Book Co.*
4. *Problem Approaches in Biochemistry. Wood and Hood*

UNIT IV: Bioinorganic Chemistry (15 L)

1. Principles of coordination Chemistry related to Bioinorganic–Proteins, nucleic acids and other metal binding biomolecules.
2. Choice, uptake and assembly of metal containing units in Biology
3. Control and utilization of metal ion concentration in cells.
4. Metal ion folding and cross –linking of biomolecules.
5. Binding of metal ions and complexes to biomolecular active center

Text Books:

1. *Ligand field theory & its application: B.N.Figgis & M.A. Hitchman (2000) Wiley-VCH publ. Chapters 5, 6, 8, 9, 11.*
2. *Principles of Bioinorganic Chemistry: S.J. Lippard & J.M Berg (1994), University science books, Mill Valley, California Chapters- 1,2,3,5,6,7,8.*
3. *Inorganic Chemistry: Shriver & Atkins (1999) Oxford.*
4. *Inorganic Electronic spectroscopy: A.B.P.Lever, 2nd edn (1984), Elsevier Science Publishers, New York.*
5. *Biological Chemistry of the Elements: R.J.P. Williams & F.R.deSalvia, Oxford University, Press-(1991)*
6. *Bioinorganic Chemistry: Inorganic elements in the Chemistry of life: An introduction & guide: W.Kaim, B.Schwederski, VCH, (1991)*

Reference Books:

1. *Principle of Biochemistry, Lehinger D.L. Nelson and M.M. Cox. Macmillan Worth Publishers.*
2. *Biochemistry, L. Stryer, W.H. Freeman, San Francisco.*
3. *Schaum's Outline Series of Theory and Problems of Biochemistry, Philip W.Kuchel and G.B. Ralston. Int. Ed., McGraw-Hill Book Co.*
4. *Problem Approaches in Biochemistry. Wood and Hood*

HCT 3.2: ADVANCED SPECTROSCOPIC METHODS

Credits: 04 (60 L)

UNIT I: ¹H NMR (16 L)

Recapitulation of basic principle, Fourier Transform technique, Pulse sequence, and relaxation processes. Use of Integration in the quantitative determination of isomers, Chemical Shift, Factors affecting on chemical shifts (inductive, resonance and anisotropic effect and solvent effect with examples), Chemical shift of different types of protons (alkane, alkene, alkyne and allene, aromatic protons)

Spin-Spin coupling: Coupling constant and its mechanism, factors affecting coupling constants (dihedral angle, Karplus equation-graph, electronegativity, bond order, hybridization, bond angle with examples), Chemical equivalence and non-equivalence, rate processes. Different types of spin coupling, first order analysis of spectra, Ramsay mechanism of spin coupling, roofing effect with example, different spin systems with examples (AB, AM, AX, ABX/AMX etc.), calculations of line intensities and chemical shifts in AB spin system, Effect of high field NMR for simplification of spectra, Shift reagents.

Resonance of other nuclei- ^{19}F & ^{31}P . Spin decoupling and Nuclear Overhauser effect with examples. NMR of Intra & intermolecular hydrogen bond, C...H---N, C—H...O, Ar-H...O=C etc., explanation of NMR with x-ray, determination of stereoisomer using NMR.

UNIT II:

A] ^{13}C NMR (10 L)

Elementary ideas, instrumental difficulties, FT technique advantages and disadvantages, Proton noise decoupling technique advantages and disadvantages, off-resonance technique, Chemical shifts of solvents, factors affecting on chemical shifts, analogy with ^1H NMR, calculations of chemical shift of hydrocarbons, effect of substituents on chemical shifts, different types of carbons (alkene, alkyne, allene, carbonyl, nitrile, oxime and aromatic carbons and effect of substituent on chemical shifts of carbons. Chemical shifts of solvents

B] Two-dimensional (2D) NMR techniques (08 L)

principle and pulse technique, DEPT, ^1H - ^1H COSY, ^1H - ^{13}C COSY (HETCOR, HMQC, HMBC, HSQC), interpretation of 2D spectra and examples, Spin decoupling and Nuclear Over Hauser effect (NOE) with examples.

UNIT-III: Mass spectrometry (15 L)

Theory, instrumentation various methods of ionization (field ionization, FAB, MALDI, californium plasma), different detectors [magnetic analyser, ion cyclotron analyser, quadruple mass filter, time of flight (TOF)]. Importance of HRMS, Rules of fragmentation of different functional groups, factors controlling fragmentation. Fragmentation of alkanes alkenes, nitriles, aromatic and carbonyl compounds etc.

UNIT-IV: Problems -based on joint application of UV, IR, ^1H and ^{13}C NMR, 2D and Mass (Including reaction sequence) (11 L)

References:

1. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).
2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed. John Wiley
3. Spectroscopic methods in organic chemistry – D. H. Williams and I. Fleming Mc Graw Hill.
4. Absorption spectroscopy of organic molecules – V. M. Parikh
5. Nuclear Magnetic Resonance – Basic Principles- Atta-Ur-Rehman, Springer- Verlag (1986).
6. One and Two dimensional NMR Spectroscopy- - Atta-Ur-Rehman, Elsevier (1989).
7. Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998).
8. Organic structural spectroscopy- Joseph B. Lambert, Shurvell, Lightner, Cooks, Prentice-Hall (1998).
9. Organic structures from spectra- Field L. D., Kalman J.R. and Sternhell S. 4th Ed. John Wiley and sons
10. NMR spectroscopy of Organic compounds. Jackmann and Sternhell S

SCT-3.1: DRUGS SYNTHETIC METHODS

Credits: 04

(60 L)

Unit- 1:

[15L]

Introduction, Classification, Mechanism of action and Synthesis of the following drug molecules (at least one convenient synthetic route with possible mechanism) from following classes:

Anaesthetics: Lidocaine, Thiopental, mechanism of action.

Analgesic and antipyretics: Paracetamol, Meperidine, Methadone, Aminopyrine

Anti-neoplastic agent

Introduction, cancer chemotherapy, special problems; Role of alkylating agent, and anti-metabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors, synthesis of some antineoplastic agent-e.g. Taxol

(a)**Antagonist:** Fluorouracil (b) **Alkylating agents:** i) Chlorambucil (ii) Cis-Platin

UNIT- II:

[15 L]

Antibiotics

Preparation of semi synthetic penicillin, conversion of penicillin into cephalosporin, general account of tetracycline and macaracyclic antibiotics (no synthesis)

Introduction, Classification, Mechanism of action and Synthesis of the following drug molecules (at least one convenient synthetic route with Possible mechanism) from following classes:

Antibiotics: (a) Chloramphenicol (b) Ampicillin (c) Amoxycillin (d) Cefepime (e) Cefpirome

Antimycobacterial: Ethambutol, **Antiviral:** Acyclovir, **Antimicrobial:** Sulfamethoxazole, Trimethopim.

Antitubercular and anti-leprotic:Ethanbutol, Isoniazide, Dasone, mechanism,Pathways, inhibition of cyclooxygen.

Anti-inflammatory: Ibuprofen, Oxyphenbutazone, Dichlorophenac, Indomethacin,Arachidonic acid.

Unit-III: Antidiabetics, Antihistamines and Anti-hypertensive drugs

[15L]

Introduction, Classification, Mechanism of action and Synthesis of the following drug molecules (at least one convenient synthetic route with possible mechanism) from following classes:

Anti-hypertensive Drugs: (a) Verapamil (b) Captopril (c) d-sotalol (d) Atenolol (e) Diltiazem (f) Semotiadilfumarate.

Antidiuretics: (a) Troglitazone (b) Chlorpropamide (c) Tolbutamide

Antihistamines; Phenobarbiton, Fenediazole, Diphenylhydramine, mechanism of action

Unit-IV: Tranquilizers, Anti AIDS and Cardiovascular Drugs:

[15L]

Introduction, Classification, Mechanism of action and Synthesis of the following drug molecules (at least one convenient synthetic route with Possible mechanism) from following classes:

Tranquilizers: Diazepam, Trimeprazin

Anti AIDS drugs: Cause, Antimetabodies and Anti-AIDS drugs

Cardiovascular Drugs: Dilliazem, Quindine, Methyldopa, Atenolol, Oxyprenol

Antacids / Antiulcer: Omeprazole, Ranitidine

Reference Books:

- 1.Synthesis of Essential Drugs- R. S. Vardanyan and V. J. Hruby, Elsevier
- 2.Contemporary Drug Synthesis- J. J. Li, D. S. Johnson, D. R. Sliskovic, B. D. Roth, John Wiley
- 3.Medicinal chemistry (Vol. I and II)-Burger
- 4.The organic chemistry of drug design and drug action-R. B. Silverman (Academic Press)
- 5.Strategies for organic drug synthesis and designing - D. Lednicer Wiley
- 6.Medicinal Chemistry- Ashutosh Kar
- 7.Medicinal Chemistry- Balkishen Razdan
- 8.W. O. Foye: Principals of medicinal chemistry
- 9.Wilson, Gisvold and Dirque: Text book of Organic medical and pharmaceutical Chemistry
- 10.Pharmaceutical manufacturing encyclopedia
- 11.Introduction to Medicinal Chemistry, Alex Gringuaz

SCT-3.2: Fundamentals of Medicinal Biochemistry

4 Credits: 04 **(60 L)**

UNIT 1:

Medicinal Biochemistry **(14 L)**

Introduction to development of antimicrobial agents, historical development of antimicrobials, chemotherapy, use of synthetic compounds and antibiotic revolution. Mechanism of action at molecular level of selected antibiotics: inhibitors of cell wall :introduction to bacterial cell wall, peptidoglycan structure synthesis , mechanism of antibiotics inhibiting cell wall synthesis. Plasma membrane antiseptics, mechanism of antiseptics, disinfectants, cationic antibiotics, polypeptide antibiotics ionophoric and polyene antibiotics. Mechanism of inhibition of Nucleic acids synthesis: inhibitors of nucleotide synthesis, inhibitor of polymerization of nucleic acids, inhibitors of polymerases. Mechanism of inhibition of protein synthesis: inhibitors of amnoacetyl tRNA formation, t RNA ribosome interaction inhibitors, and inhibitors of peptide bond formation.

UNIT II: **(10 L)**

A] Antiviral, antifungal, antiprotozoal, analgesic drugs: mechanism of action at molecular level of some antiprotozoal: antimalarial, antiviral antiflu, anti HIV etc, analgesic drugs. Mechanism of resistance to antibiotics and other drugs: mechanism of resistance at biochemical level of some antibiotics: conversion of active drug to inactive, modification of drug sensitive site, loss of cell permeability to drug.

B] Immunology **(08 L)**

UNIT III

Chemistry of amino acids **(10 L)**

Chiral Synthesis of alpha and Beta amino-acid, Difficulties involved in synthesis of peptides, Importance of peptides in drug discovery, Protection and Deprotection of amino acids General aspects, need for protection, minimal versus global protection, protection of amino group by acid and base labile groups, protection of carboxyl group, concept of orthogonal protection in peptide synthesis, importance of side-chain functional group protection and details of protective groups used for masking individual amino acids, methods used for deprotection. Coupling reactions in peptide synthesis Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, over-activation and side reactions of individual amino acids

UNIT IV:

A] Peptides, nucleotides, nucleosides (12 L)

Principle of solid phase peptide synthesis, t-BOC and Fmoc protocols, various solid supports and linkers: Activation procedures, peptide bond formation, deprotection and cleavage from resin, low and high HF cleavage protocols, formation of free peptides and peptide amides, purification and case studies, site-specific chemical modifications of peptides
Chemistry of nucleosides and nucleotides

B] Synthesis of Antibiotics-penicillins, cephalosporins, macrolides, aminoglycosides, cyclins, ofloxacin (Nicolae) (04 L)

References:

1. Biochemistry of antimicrobial action (4th ed) t J Franklin, Chapman Hall (1989)
2. Mechanism of microbial diseases, M Schaechter et. al. Williams and Wilkins Int. Ed (1989)
3. Medicinal Chemistry,- Molecular and Biochemical approach – Thomas Mogarty and Donald Weaver (3rd ed) Oxford press.
4. Biochemistry- L, Stryer (3rd ed) Freeman and Co.
5. Text book Biochemistry with clinical correlations Thomas Devlin (2nd ed) John Wiley and sons.
6. General microbiology, Pelczar, Rardhan (1987).
7. Asymmetric Reactions and Processes in Chemistry: Ernest L. Eliel
8. Catalytic Asymmetric Synthesis: 2nd Ed., Iwao Ojima
9. Asymmetric Organocatalysis: From Biomimetic Concept to Applications in Asymmetric Synthesis: David MacMillan
10. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press.)
11. Asymmetric synthesis Vol.1-5 by J. D. Morrison
12. Chirotechnology: Industrial synthesis of optically active compounds, R. A. Sheldon
13. Organic Chemistry - R. P. Morrison and R. N. Boyd
14. Organic Chemistry – I. L. Finar, volume II
15. Chiron approach in organic synthesis – S. Hanessian
16. An introduction to medicinal chemistry-Graham L. Patric Oxford press
17. The organic chemistry of drug design and drug action- R.B. Silverman
18. Exploring OSAR fundamentals and applications in chemistry and biology-Corwin Hansch and Albert Leo

OET 3.1 Bioactive Heterocyclic Chemistry

Credits: 04

60 L

Heterocyclic compounds - Synthesis, reactivity, aromatic character and medicinal importance of following heterocycles:

UNIT I [15L]

3-membered rings: Aziridines, Oxiranes, Thiiranes,

4-membered rings: Azetidines, Oxitanes and Thietanes

UNIT II: 5-membered rings [15L]

Five-membered rings with *one* heteroatom: Pyrrolidine, Furan, Pyrrole and Thiophene

Five-membered rings with *two* heteroatoms: Imidazole, Pyrazole, Oxazole, Isoxazole, Thiazole, Isothiazole.

Five-membered rings with *three* heteroatoms: Triazoles, Oxadiazole, Thiadiazole, Tetrazole.

UNIT III: 6-membered rings [15L]

Six-membered rings with *one* heteroatom: Pyran, Pyridine

Six-membered rings with *two* heteroatoms: Piperazine, Morphine, Thiomorphine, Pyridazines, pyrimidines, pyrazines,

Six-membered rings with *three* heteroatoms: Hexahydro-1,3,5-triazine

Six-membered rings with *three* heteroatoms: Tetrazine

UNIT- IV: [15L]

Benzofused heterocycles

Benzopyrroles, Benzofuran, Indole, Benzothiophene, Benzoxazole, benzthiazole, Benzimidazole, Quinolines, Isoquinoline, Quinazolines, Coumarins and Chromones, Purines and Pteridines

Reference Books and Text Books

- 1.R. M. Acheson: An introduction to chemistry of heterocyclic compounds (Interscience)
- 2.Joule and Smith: Heterocyclic chemistry (Van Nossstrand)
- 3.R.K. BANSAL: Heterocyclic chemistry (Wiley E)
- 4.L.A. Paquette: Principals of modern heterocyclic chemistry
- 5.M.H. Palamer: The structure and reactions of heterocyclic compounds.
- 6.A.R. Katritzky and A.V. Bootton: Advances in Heterocyclic chemistry (A.P.)
- 7.Finar: Organic chemistry (Vol. 1 and 2)
- 8.Conn and Stumpf: Outline of Biochemistry
- 9.Williams, Introduction to the chemistry of enzyme action.
- 10.The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman AcademicPress.
- 11.Strategies for Organic Drug Synthesis and Design. D. Lednicer, John Wiley.
- 12.Heterocyclic Chemistry Vol. 1-3, R. R. Gupta, M. Kumar, and V. Gupta, SpringerVerlag.
- 13.The Chemistry of Heterocycles, T Eicher and S. Hauptmann, Thieme.
- 14.Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman ans Hall.
- 15.Heterocyclic Chemistry, T. L. Gilchrist, Longman ScietificTechinal
- 16.Contemporary Heterocyclic Chemistry, G. R. Newkome and W. W. Poudler, Wiley.
- 17.An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.
- 18.Comprehensive Heterocyclic Chemistry, A. R. Katrizky and C. W. Rees, eds, Pergamon Press.

OET 3.2 UNIT OPERATIONS OF CHEMICAL ENGINEERING

Credits: 04

60 L

Unit I: Nitration

[15L]

Introduction; Nitrating agents, Aromatic nitration, Thermodynamics of Nitrations; Heat of Nitration; Process equipment for technical nitration; Mixed acid for nitration-Acid processing, Mixed acid composition, D.V.S. Calculation, Relation between D.V.S. and Stability of Nitrator Charge; Typical industrial Nitration process (Nitrobenzene, and α -Nitronaphthalene)

Unit II: Sulphonation

[15L]

Introduction; Sulphonating agents and their applications; Thermodynamics of sulfonation; The Desulphlonation Reaction – General consideration, Sepaeration of isomers, Raw

material and waste Recovery; working-up procedures; Industrial equipments and Techniques, Material of construction, Commercial Sulfonation Methods; Technical preparation of Sulfonates -Aromatic Sulfonates (The mono sulfonation of Benzene, Anthraquinone -1-Sulfonates).

Unit III: A) Halogenation [15L]

Introduction; Chlorination of cycloparaffins; Preparation of Ethylene dichloride; Design and construction of Equipment for Halogenation; Technical Halogenations – Manufacturing processes for monochloroacetic acid, Chloral, Monochlorobenzene, and Vinyl chloride (Ethylene and Acetylene).

Unit III: B) Esterification

Introduction; Esterification by organic acid; Esterification of carboxylic acid Derivative; Ester by addition to unsaturated system; Manufacture of ethyl acetate, Vinyl acetate, Cellulose acetate.

Unit IV: A) Polymerization [15L]

Introduction; Chemistry of polymerization reactions; Methods of polymerization, polymerization kinetics; Industrially important polymerization and polymers: Phenolic, urea and melamine and alkyl resins, Polyamides, Polyesters, Epoxy resins, Polyethylene, Polypropylene, Vinyl polymers, Polystyrene, Acrylonitrile polymers.

Unit IV: B) Oxidation

Introduction; Types of oxidative reactions; Liquid phase oxidation with oxygen, Acetaldehyde to Acetic acid, Vapour phase oxidation aliphatic compound- oxidation of Methanol.

HCT 4.1: MEDICINAL CHEMISTRY

Credits: 4

60 L

UNIT –I (15 L)

Introduction to Medicinal Chemistry: History and development of medicinal chemistry, Physicochemical properties in relation to biological action, Ionization, Solubility, Partition Coefficient, Hydrogen bonding, Protein binding, Chelation, Bioisosterism, Optical and Geometrical isomerism. **Drugs:** Essential Drugs, Nomenclature of Drugs, Routes of Drug Administration, Adverse effects of Drugs, IUPAC Naming of Drugs.

UNIT –II (15 L)

Drug discovery process: Brief introduction to bioinformatics and chemoinformatics, Molecular modeling: Energy minimization, geometry optimization, conformational analysis. Drug discovery process: Computer Aided Drug Design (CADD), Development of New Drugs, Factors Affecting development of New Drugs. Concept of prodrugs and soft drugs, Drug Receptors. Molecular docking: Rigid docking, flexible docking, manual docking. Autodock and Dock softwares with examples.

UNIT-III (15 L)

Pharmacokinetics: Introductions, Drug Absorption, Distribution, Metabolism (Phase I and Phase II), Excretion and Toxicity (ADMET). **Pharmacodynamics:** Introduction, Drug-receptor interaction, Types of Interactions, Enzyme Stimulation, Enzyme Inhibition, Membrane Active Drugs, QSAR- 2D QSAR and 3D-QSAR.

UNIT-IV (15 L)

Drug Action: Theories of Drug Action, Molecular Recognition in Drug-Receptor Binding, Enzyme Inhibitors (Modes of inhibition). **Antibacterial, Antifungal, Antiviral and Anticancer drugs** (Major drug classes, mechanism of drug action, Drug resistance). Analgesic Drugs, anesthetics (general, local), Neurotransmitters (adrenergic, cholinergic effects; psychopharmacology), CNS depressants (sedative/hypnotic, major/minor tranquilizers), CNS stimulants, Steroids.

Medicinal Chemistry Textbooks

1. *The Organic Chemistry of Drug Design and Drug Action*, by Richard B. Silverman, 2nd Edition. Elsevier Academic Press, 2004, ISBN 0-12-643732-7.
2. *Foye's Principles of Medicinal Chemistry*, 5th Edition, by David A. Williams and Thomas L. Lemke, Lippincott Williams & Wilkins, 2002.
3. *Medicinal Chemistry: A Molecular and Biochemical Approach*, 3rd Edition, by Thomas Nogrady and Donald F. Weaver, 2005.
4. *Medicinal Chemistry, An Introduction*, by Gareth Thomas, John Wiley & Sons, 2000.
5. *The Practice of Medicinal Chemistry*, ed. Camille Wemuth, Academic Press, 1996.

Selected Medicinal Chemistry Journals

1. *Journal of Medicinal Chemistry*
2. *Journal of Medicinal Chemistry Letters* (starting with 2010, Volume 1)
3. *Bioorganic & Medicinal Chemistry*
4. *Bioorganic & Medicinal Chemistry Letters*
5. *European Journal of Medicinal Chemistry*
6. *ChemMedChem*

HCT-4.2: STEREOCHEMISTRY

Credits: 04

60 L

UNIT-I Conformation and reactivity in acyclic compounds and of cyclohexanes [15L]

Stability and reactivity of diastereoisomers. Curtin- Hammett principle.

The shapes of the rings including six membered: Shapes of five, and seven eight membered rings, Reactivity of six-member ring system

Conformational effects in medium sized rings, Concept of I strain.

UNIT-II Fused and Bridged rings [15L]

Fused bicyclic ring systems: Cis- and trans- decalins and nine methyl decalines and perhydrophenanthrene, perhydroanthracene. Bridged rings, Nomenclature stereo chemical restrictions. The Bredts rule, Reactivities. Stereochemistry of Allenes, spiranes and biphenyls

UNIT-III Newer methods of Stereo selective synthesis [15L]

Introduction and Stereoselective and stereospecific reactions. Enantioselective synthesis (Chiral approach) reactions with hydride donors, catalytic hydrogenation via chiral hydrazones and oxazolines, enantiotopic and diastereotopic atoms, groups and faces. Use of calculations of optical purity and enantiomeric excess.

UNIT-IV Asymmetric Synthesis [15L]

Chiral pool, Chiral auxiliary, Enantio- & Diastereoselective synthesis, Chiral reagent and chiral catalyst including CBS reagent, NADH, Asymmetric hydrogenation including BINAP,

Hydroboration-Ipc₂BH, IpcBH₂, Asymmetric epoxidation- (+) DET & (-) DET, Sharpless, Jacobson, Asymmetric dihydroxylation-(DHQD)₂PHAL & (DHQ)₂PHAL, Felkin-Anh model, Zimmermann-Traxler transition state model.

Reference Books:

1. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
2. Stereochemistry: Conformation and Mechanism: P. S. Kalsi
3. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
4. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
5. Organic Chemistry: Clayden, Greeves, Warren and Wothers
6. Organic Synthesis: M. B. Smith

HCT-4.3: CHEMISTRY OF NATURAL PRODUCT

Credits: 04

60 L

UNIT-I Steroids

(15 L)

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, structure determination and synthesis of Bile acids, Androsterone, Testosterone, Estrone, Progesterone.

UNIT-II

(15 L)

- (a) Structure, stereochemistry, synthesis and biogenesis of Hardwickiiic acid, Camptothecin and Podophyllotoxin. (Ref. 1 to 4 and 11)
- (b) Structure determination and Synthesis of i) Reserpine (Woodward synthesis) Ref. 5, 6 ii) Taxol – Ref. 6 iii) Estrone and Mifepristone – Ref. 6, 7 iv) Strychnine (Overman's synthesis) – Ref. 6 v) Fredericamycin A – Ref. 5.

UNIT-III Biogenesis

(15 L)

The building blocks and construction mechanism of

- (i) Terpenoids – Mono, Sesqui, Di and Triterpenoids and cholesterol
- (ii) Alkaloids derived from ornithine, lysine, nicotinic acid, tyrosine and tryptophan.
- (iii) The Shikimate pathway – cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbers, isoflavanoids and terpenoid quinones. Ref. 8, 9, 10.
- (iv) Arachidonic acid – Prostaglandins & thromboxanes.

UNIT-IV

(15 L)

Synthesis and biological Functions involving vit. B₁, B₂, B₆, Biotin, NAD/NADP – NADH/NADPH, Folic acid, Riboflavin and Prostaglandins

References

1. J. Am Chem. Soc. 88, 3888 (1966).
2. M. C. Wani and M.E. Wall J. Org. Chem. 34, 1364 (1969)
3. (i) Tetrahedron Letters, 3751 (1964)
(ii) Tetrahedron Letters, 2861 and 2865 (1968)

4. Chemistry of Natural products-Kalsi
5. Principles of organic synthesis by R.O.C. Norman and J. M. Coxon; Chapman and Hall
6. Classics in organic synthesis – K.C. Nicolaou and E.J. Sorensen
7. J. Indian Inst. Sci. 81, 287 (2001).
8. Medial Natural Products – A Biosynthetic approach by Paul M. Dewick 2nd edition (Wiley)
9. Secondary metabolism – J. Mann, 2nd edition.
10. Chemical aspects of Biosynthesis – J. Mann (1994)
11. i) J.C.S. Perkin Transactions II, 288-292, (1973)
ii) J. Am. Chem. Soc. Vol. 77, 432-437, (1955).
12. Apsimon: The Total synthesis of natural products.
13. Manskey and Holmes: Alkaloids
14. A.A. Newmen: Chemistry of Terpenes.
15. P. D B.Mayo: The Chemistry of natural products.
16. Simonson: Terpenes.
17. T.W. Goddwin: Aspects of terpenoid chemistry and biochemistry
18. Woguer: Vitamins and Co- enzymes.
19. Bently: Chemistry of natural products,
20. Fieser and Fieser: Steroids
21. Finar: Organic chemistry Vol. II and I
22. J.B. Hendrickson: The molecules of nature.
23. Peter Bernfield: The biogenesis of natural products,
24. R.T. Slickenstaff A.C. Ghosh and G.C. Wole: Total synthesis of steroids.
25. The Chemistry of natural products: by Nakanishi

SCT-4.1: FUNDAMENTALS OF DRUG DISCOVERY

Credits: 04

60 L

Unit-1: Introduction to drug discovery and dosage forms

[15L]

Introduction, drug discovery and design: a historical outline, sources of drugs and lead compounds, classification of drugs, brief discussion on methods of drug administration, introduction of drug action and bioavailability

Dosage forms: oral solids, oral liquids, solution properties, suspensions, emulsions, parenteral, aerosols, inhalation products, topical semisolids, typical lipids and powders, ophthalmic products, rectal and vaginal products. Oral solids: tablets, types of tablets, methods of tablet production- wet granulation, coating of tablets. Quality control methods and measurement of tablet properties, Oral liquids: introduction, type, oral suspensions and oral emulsions.

Unit-2: Drug screening methods

[15L]

General principles of screening of drugs, general screening methods, clinical trial, experimental animals used in pharmacological assays, invitro, invivo studies, tissue experiments and whole animal experiments. Bioassay, scope, principals involved and general methods. Bioassay of acetylcholine, insulin and atropine. Screening method for evaluation of

analgesic, anti-inflammatory, antiulcer, anticonvulsants, hepatoprotective, antidiabetic and antifertility activities. Methodology for microbial assay of penicillin and miconazole. Enzyme inhibition studies: inhibition of acetylcholine esterase activity in rat striatum, Cox inhibition studies.

Unit-3: GMP and Drug Regulations [15L]

Introduction, requirements of good manufacturing practice and quality management, guidelines to manufacturing practice for medicinal products, premises and equipments, documentation, production and quality control.

GCP-guidelines and related management, Principles of ICH and GCP, ethical principles related to GCP. Regulations for obtaining permission for clinical trial, application for permission, report: clinical trial report, trial management, data monitoring committee (DMC).

Unit-4: Drug delivery systems [15L]

Fundamental of novel drug delivery: Rationale of sustained release, controlled release dosage forms. Physicochemical and biological factors influencing design, performance of CR products, Pharmacokinetics and pharmacodynamic basis of NDDS. Bioavailability assessment of CR systems, Regulatory requirements, Theory of mass transfer, Fick's law and its application in NDDS, Polymers in CR- classification, properties biocompatible and biodegradable polymers. Modeling of drug release from porous polymer, drug release from nonporous and hydrophobic polymers, Oral controlled drug delivery systems, mucosal drug delivery system, ocular drug delivery systems, parenteral drug delivery systems, transdermal drug delivery systems

References:

1. Pharmacology and Pharmacotherapeutics – Satoshkaret. Al
2. Basic pharmacology- N M Ghosh
3. Drug discovery and Evaluation. pharmacological assay, III Ed. Vol-2, H G Vogel
4. Biopharmaceutics and clinical pharmacokinetics IV Ed.- Gibaldi
5. Pharmaceutics and Pharmacokinetics – G R chatwal
6. Biopharmaceutics – S N Jogdand
7. Pharmcaeutical codex Principles and practice of pharmaceutics 11 Ed. Waterland.

SCT 4.2 CHEMICAL INDUSTRIES

Credits: 04

60 L

Unit I:

(15 L)

A) Metallurgy Industry

Extraction and applications of metal alloys

- a) Iron and steel: Iron, steel alloy, tool steel, stainless steel.
- b) Aluminum

B) Cement Industry

Introduction; Classification and Manufacturing processes of Cement and Lime; Setting and Hardening process

C) Glass Industry

Introduction; Physical and Chemical properties; Characteristics of glass; Raw material Manufacturing process of glass; Ceramic- Raw material, Manufacturing process of White ware, Glazing.

Unit II: (15 L)

A) Paints and Pigments Industries

Paints- Introduction; Classification of paints; Constituents of paints; Formulation of paints; Mixing of paints; Manufacturing processes of paints ; Failure of paints; Varnishes, Enamals, Emulsion paints- Constituents.

Pigment- Manufacturing processes of zinc oxide and titanium dioxide, properties and application

Special paints- Luminescent paints, Heat resistant paints, cellulose paints.

B) Dyes

Classification of dyes according to the mode of applications and according to the chemical constitution; Methods of preparation of commercial dyes of different classes with suitable examples; Typical manufacturing processes of dyes; Fluorescent brightening agents

Unit III: (15 L)

Agrochemicals:

- a) Organo chlorine pesticides: BHC, Aldrin, Dieldrin, Endosulphan,
- b) Organo phosphorus pesticides: Malathion, monocrotophos, Dimethoate, chloropyrifos.
- c) Carbamates: Carbaryl, Bygon, Ziram, Zineb, Maneb.
- d) Insect pheromones and Repellants: Pheromone, general introduction and application in integrated pest management (no synthesis), Repellent: Survey and synthesis of following repellants: N,N Diethyl-3-methyl benzamide, N,N, Diethylenebenzamide, 2-ethyl-1,3, hexanediol, Butopytranexyl, Dimethylcarbamate, Dimethylphthalate

Unit IV: (15 L)

Petrochemicals

Crude oil, Natural gas, Petroleum hydrocarbons- Types and source of crude oil; Refining various petroleum fractions- Thermal cracking, Recycle cracking, Thermal cracking of fuel ; outline of chemicals derived from natural gases/ paraffin hydrocarbon-Ethylene, Propylene Butylenes, Benzene, Toluene.

References

1. F.A. Henglein: Chemical Technology (Pergamon)
2. R.W. Thomas & P.Farago: Industrial Chemistry (HEB)
3. R.N. Shreve: Chemicals Process Industrial (MGH)
4. Riegel's: Industrial Chemistry (Reinhold)
5. D.S.T: Perspectives in science and technology Vol I & II (Vilas)
6. W.H. Dennis: Foundation of iron and steel metallurgy (Elsevier)

7. Prakash G. More, Comprehensive Industrial Chemistry, Pragati Prakashan, Meerut (Uttar Pradesh)
8. Kirk R Smith: Biofuels: Air pollution and Health: A Global Review (Kluwer Academic/Plenum publisher)
9. Plant oil as fuels- Present state of science and future developments Edited by N. Martini and J.S. Sebeli Springer Verlag 1998.

M. Sc. II Medicinal Chemistry Practicals

HCP 3.1 Qualitative Analysis

Separation, purification and identification of compounds of THREE components mixtures, chemical tests. derivatives etc. by micro scale technique. IR spectra to be used for functional group identification. TLC and Column Chromatography.

HCP 3.2 and HCP 4.1:

Two stage and Three stage Organic preparations starting with 5g or less.

(TLC Analysis is recommended)

1. Preparation of Benzanilide by Beckmann rearrangement.
2. Preparation of Anthranilic acid.
3. Preparation of Phthalimide.
4. Preparation of N- Bromosuccinamide.
5. Preparation of p- Aminobenzoic acid.
6. Preparation of p- chloronitrobenzene by Sandmeyer reaction.
7. Preparation of p- Iodonitrobenzene by Sandmeyer reaction.
8. Pinacol- Pinacolone rearrangement.
9. Preparation of Acetophenones by Fries rearrangement
10. Preparation of aromatic aldehydes by Vilsmer Hack reaction or R. T.
11. Wittig reaction.
12. Preparation of Benzopyrazole

(Other suitable experiments may be added)

OEP 3.1 Spectral Problems

OEP 3.2 Drug Assay/ Analysis

HCMP 4.4: Major Project/In Plant training: Literature survey. Studies of reactions, synthesis, mechanism, isolation of natural products, standardization of reaction conditions, new methods etc. and Spectral Analysis

References

1. A Textbook of Practical Organic Chemistry - A. I. Vogel.
2. Practical Organic Chemistry - Mann & Saunders.
3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke. 4. Organic Synthesis Collective Volumes by Blat.
5. Reagents in Organic Synthesis by Fieser and Fieser.
6. Organic Practicals by Ahluwalia.
7. Systematic Lab Experiments in Organic Chemistry by Arun Sethi. (New Age).