DEPARTMENT OF CHEMISTRY
SATAVAHANA UNIVERSITY - KARIMNAGAR

REVISED SYLLABUS

From 2023-24 onwards

M.Sc. Chemistry

IV Semester

2024

DEPARTMENT OF CHEMISTRY

SATAVAHANA UNIVERSITY - KARIMNAGAR

M.Sc., Chemistry

Under Choice Based Credit System (CBCS)

(From the academic year 2023-24)

M.Sc. (Organic Chemistry) IV Semester

Paper Code	Title	Workload Per Week		Marks			Credits	Duration of the Exams.
		Theory	Practical	Internal	External	Total		
MCHE (ATG) 401T (Common Paper)	Analytical Techniques and Green Chemistry	**4**	**--**	**20**	**80**	**100**	**4**	**3 Hrs**
MCHE (OC) 402T	Drug design and Drug Discovery	**4**	**--**	**20**	**80**	**100**	**4**	**3 Hrs**
MCHE (OC) 403T (E-I) (OR) MCHE (OC) 403T (E-II)	Drug synthesis and mechanism of action (or) Biopharmaceutics and Pharmacodynamics	**4**	**--**	**20**	**80**	**100**	**4**	**3 Hrs**
MCHE (OC) 404T (E-I) (OR) MCHE (OC) 404T (E-II)	Advanced Natural Products (or) Bioorganic Chemistry	**4**	**--**	**20**	**80**	**100**	**4**	**3 Hrs**
MCHE (OC) 451P	Spectroscopic identification of organic compounds and Green syntheses	**--**	**6**	**-**	**100**	**100**	**4**	**4 Hrs**
MCHE (OC) 452P	Synthesis and analysis of drugs	**--**	**6**	**-**	**100**	**100**	**4**	**4 Hrs**
TOTAL		**16**	**12**	**80**	**520**	**600**	**24**	

COURSE NAME	M.Sc.	SUBJECT NAME	CHEMISTRY	Max. Marks	80+20
Semester	IV	TITLE	ANALYTICAL TECHNIQUES AND GREEN CHEMISTRY	No. of Credits	4

Paper-I MCHE (ATG) 401T: Analytical Techniques and Green Chemistry **4 Hrs/ Week**

ATG-25: Thermal methods
ATG-26: Separation methods
ATG-27: Nanotechnology
ATG-28: Green chemistry

ATG-25: Thermal methods (15Hrs)

Thermogravimetry, Differential Thermal Analysis and Differential Scanning Calorimetry, Instrumentation. Methodology of TGA, DTA and DSC.

Thermomechanical analysis, Dynamic mechanical analysis. Application of TGA, study of oxalates and chromates. Determination of Glass transition, Heat capacity determination, Characterization of polymer blends. Problems based on decomposition path way and % composition. Thermometric titrimetry – Theory, Instrumentation, applications.

ATG-26: Separation methods (15Hrs)

Solvent extractions: The Distribution coefficient, Distribution ratio, Relation between KD& D, the percent extracted. Solvent extraction of metals-metal chelates, Extraction process, Analytical separations, Solid phase extraction.

Column Chromatography: Retention Parameters, Separation Efficiency, Resolution, Asymmetric factor, Column efficiency, Column performance, HETP, Effective plate number, Van Deemter Equation,

Gel Exclusion Chromatography: Principle, Stationary phases, Instrumentation, Retention behaviour, Applications.

Super Critical Fluid Chromatography: Principle, Super Critical Fluids, Instrumentation, Stationary Phases and Mobile Phases, Detectors, Comparison of SFC with HPCL and GC Applications.

ATG-27: Nanotechnology (15Hrs)

Introduction to nanoparticles, Preparation of nanoparticles by co-precipitation and wet-impregnation method. Properties of the nanoparticles: Magnetic and electronic properties of the nanoparticles, Scanning electron microscopy (SEM), TEM and EDAX analysis and X-ray diffraction, A brief historical overview of atomic force microscopy (AFM) and an introduction to its basic principles & applications. Optical microscope and their description, operational principle and application for analysis of nanomaterials, UV-Vis-IR spectrophotometers, Principle of operation and application for band gap measurement.

ATG-28: Green chemistry (15Hrs)

Basic principles of Green Chemistry, Prevention of waste, hazardous/toxic products, designing safer chemicals, atom economy, green solvents efficiency and industrial applicability, Ionic liquids properties and applications in organic synthesis, Supercritical fluids, Supercritical carbon dioxide, solvent free liquid phase and solid phase reactions, green catalysts, Use of zeolites, silica and alumina. Phase transfer

catalysts applications, microwave and ultrasound assisted reactions, Green analytical techniques, micelle mediated extraction etc.

References:

1. Instrumental Techniques for Analytical Chemistry, Frank Settle.
2. Principles of Analytical Chemistry, M. Valcarcel.
3. Separation Methods - M. N. Sastri, 1st ed., Himalaya Publishers, 1991.
4. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
5. Analytical Chemistry - Gary Christian, 6th ed, John Wiley and sons. Inc., New York, sixth edition, 1994.
6. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill, New Delhi, 2007.
7. G.Cao, Nanostructures and Nanomaterials – Synthesis, Properties and Applications, Imperial College Press, London, 2004, chapters 3, 4 and 5.
8. C. N. R. Rao, A. Muller and A. K. Cheetham, The Chemistry of Nanomaterials, Volume Wiley –VCH Verlag GmbH & Co. KgaA, Weinheim, 2004, Chapter 4.
9. Nanoparticles- Theory and Applications by Schmid
10. Carbon Nanomaterials by Challa
11. Nanomaterials- Synthesis, properties and applications by Rao CNR, Miller A, Cheetham AK.
12. New trends in green chemistry, V. K. Ahluwalia, M. Kidwai, Springer, 2012, 1st Edition.
13. Green Chemistry: Environment Friendly Alternatives, Rashmi Sanghi, M.M Srivastava, Alpha Science International, 2009, 4th Edition.
14. Green Chemistry: Theory and Practice. P.T. Anastas and J.C. Warner. Oxford University Press, 2000, 1st Edition.
15. Introduction to green chemistry, Albert S. Matlack, CRC Press, 2001, 2nd Edition

COURSE NAME		M.Sc.	SUBJECT NAME	CHEMISTRY	Max. Marks	80+20
Semester	IV	TITLE	DRUG DESIGN AND DRUG DISCOVERY		No. of Credits	4

Paper-II MCHE (OC) 402T: Drug design and Drug Discovery **4 Hrs/ Week**

OC-29: Principles of drug design and drug discovery
OC-30: Lead modification and SAR studies
OC-31: Quantitive structure – activity relationship (QSAR) Studies
OC-32: Combinatorial chemistry

OC-29: Principles of drug design and drug discovery (15Hrs)

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery – disease, drug targets, bioassay. Discovery of a lead – screening of natural products and synthetic compound libraries, Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), Pharmacodynamics. Nature of drug – receptor interactions and their theories – occupancy theory, induced – fit theory, Macromolecular perturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – pharmacophore – structure pruning technique e.g., morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g., Salbutamol), Antagonists (e.g., cimetidine) and enzyme inhibitors (e.g., Captopril). Drug discovery without lead – serendipity – penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and clinical trials.

OC-30: Lead modification and SAR studies (15Hrs)

Lead modification strategies, Bioisosterism, variation of alkyl substituents, chain homologation and branching, Variation of aromatic substituents, Extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxamniquine, salbutamol, cimetidine and captopril structure – activity relationship studies in Sulfa drugs, Benzodiazepines and Taxol analogues.

OC-31: Quantitative structure – activity relationship (QSAR) Studies (15Hrs)

Introduction, physicochemical properties – p^{Ka}, electronic effects and Hammett constants(σ), Lipophilicity constant(π), Steric effects and Taft's constant, Linear and nonlinear relationship between biological activity and Hammett / Lipophilicity substituent constants. Lipinski rule of five. Hansch analysis, Craig's plot, Topliss scheme, Free Wilson approach, Cluster significant analysis. Three case studies.

OC-32: Combinatorial chemistry (15Hrs)

***Introduction*:** Combinatorial approach, Combinatorial libraries, technologies. Solid phase synthesis, types of Resins, Linkers. Reactants for solid phased synthesis.

Methods of parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis.

Methods in mixed combinatorial synthesis: general principles. Furka's mix and split combinatorial synthesis, structure determination of active compounds – deconvolution, Methods in deconvolution recursive deconvolution, tagging and use of decoded sheets. Examples of combinatorial chemistry. Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules. Automation in combinatorial chemistry. High throughput screening.

References:

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to medicinal chemistry by Graham L. Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical chemistry and drug synthesis by Roth and kleeman
8. Drug design by E. J. Arienes
9. Principles of medicinal chemistry Vol I & II by kadam et al
10. Medicinal chemistry an introduction by Gareth Thomas
11. Organic and pharmaceutical chemistry by Delgado
12. Organic pharmaceutical chemistry b Harikishan singh
13. Medicinal chemistry by Ashutosh kar
14. Medicinal chemistry by Chatwal
15. Organic drug synthesis by ledneiser vol 1-6
16. Strategies for organic drug synthesis and design by danie ledneiser.
17. Top Drugs: top synthetic routes by John saunders
18. Chirotechnology by roger A. Sheldon
19. Burger's medicinal chemistry and drug discovery: Principles and practice, vol 1.
20. Text book of drug design and discovery, edited by povl krogsgaard- Larsen, Tommy Liljefors.

COURSE NAME	M.Sc.	SUBJECT NAME	CHEMISTRY	Max. Marks	80+20
Semester	IV	TITLE	DRUG SYNTHESIS AND MECHANISM OF ACTION	No. of Credits	4

Paper-III MCHE (OC) 403T (E-I): Drug synthesis and mechanism of action **4 Hrs/ Week**

OC-33: Drugs acting on metabolic process, cell wall and specific enzymes
OC-34: Drugs acting on genetic material and immune system
OC-35: Drugs acting on receptors and ion channels
OC-36: Chiral drugs

OC-33: Drugs acting on metabolic process, cell wall and specific enzymes (15Hrs)

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a) Drugs acting on metabolic process: Antifolates -Discovery and mechanism of action of sulfonamides. Synthesis of Sulfamethoxazole, Sulfadoxine, Sulfaguanidine and Dapsone. Diaminopyrimidines - Trimethoprim, bacterial resistance to sulfonamides and drug synergism.

b) Drugs acting on cell wall: Structure of bacterial cell wall, ***ß-lactam antibiotics-*** mechanism of action of Penicillins and Cephalosporins. Synthesis of Penicillin-G and Cephalosporin-C, Cefalexin and Cycloserine. Resistance to Pencillins.
Broad spectrum penicillins- Cloxacillin, Methicillin, Ampicillin, Amoxicillin and Carbenicillin. ***ß-Lactamase inhibitors-*** Structural formulae and mode of action of Clavulanic acid and Sulbactum.

c)Drugs acting on specific enzymes: ***H^+/ K^+ -ATPase inhibitors-*** synthesis of Omeprazole and Carbonic anhydrase inhibitors- synthesis of Acetazolamide.

OC-34: Drugs acting on genetic material and immune system (15Hrs)

i. Drugs acting on genetic material: Introduction, classification and mechanism of action.

a) DNA-intercalating agents: Anticancer and antimalarial agents. Structural formulae of Daunomycin. Adriamycin and Amsacrine. Synthesis of Amsacrine, Nitracrine, Quinacrine and Chloroquine.

b) DNA-Binding and nicking agents: Antiprotozoal drugs, Synthesis of Metronidazole, Dimetridazole and Tinidazole.

c) DNA-Alkylators: Synthesis of Cyclophosphamide and Busulphan.

d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.

e) DNA-Topoisomerase inhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae of Ofloxacin and Lomefloxacin.

f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents. structural formulae of Rifamycins and partial synthesis of Rifampicin.

g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin.

ii. Drugs acting on immune system: Introduction to immune system. immunosuppressing agent-structural formula of Cyclosporin. Immunoenhancers-use of vaccines and structural formula of Levamisol.

OC-35: Drugs acting on receptors and ion channels (15Hrs)

Introduction to nervous system: structure of neuron. Definition and examples of agonist, antagonist, neurotransmitters and receptors.

Drugs acting on receptors:

a) Adrenergic receptors: Introduction and classification. α-Adrenergic-receptor agonists and antagonists-Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Terazosin.
β-Adrenergic-receptor - agonists and antagonists - Synthesis and pharmacological activity of Salbutamol, Terbutaline, Propranolol and Atenolol.

b) Cholinergic-receptors: Introduction and classification. Cholinergic-receptor agonists and antagonists-Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline

c) Dopamine receptors: Introduction and classification. Dopamine- receptor agonists and antagonists-Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.

d) Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists-synthesis and pharmacological activity of Serotonin and Metaclopramide.

e) Histamine receptors: Introduction and classification. Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chloropheneramine, and Ranitidine.

f) Hormone receptors: Introduction to estrogen receptors, Structural formula of Tamoxifen.

Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca^{2+}, Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis of Nifedipine, Diltiazem, Tetracaine and 4-Aminopyridine.

OC-36: Chiral drugs (15Hrs)

Introduction to chiral drugs Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule.
Role of chirality on biological activity: Distomers — a) with no side effects b) with undesirable side effects c) both isomers having independent therapeutic value d) combination products having therapeutic advantages e) metabolic chirality inversion.
Synthesis and pharmacological activity of S-Ibuprofen, S- Metaprolol, Indinavir sulfate, Levocetirizine, 2S-Verapamil, S,S-Ethambutol, (+)Lomefloxacin, Fluvastatin, Dextropropoxyphen, (+)Ephedrine, (+)Griseofulvin, Dexormaplatin, R-Indacrinone, Nateglinide, Oxybutynin hydrochloride, S,S.- Captopril and S,S,S- Enalaprilate.

References:

1. Introduction to Medicinal chemistry by Graham L. Patrick
2. Burger's medicinal chemistry and drug discovery by Manfred B. Wolf
3. Introduction to drug design by R. B. Silverman
4. Comprehensive medicinal chemistry Vol 1-5 by Hanzsch
5. Principles of medicinal chemistry by William O. Foye et. al.
6. Biochemical approach to medicinal chemistry by Thomas Nogrady
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Klecman
8. Drug design by El Arienes
9. Principles of Medicinal Chemistry Vols.1 & 2 by Kadam et. al
10. Medicinal chemistry an introduction by Gareth Thomas
11. Wilson and Gisvold's Textbook of organic medicinal and pharmaceutical chemistry by John M. Beale, Jr., John H. Block
12. Organic Pharmaceutical chemistry by Harikishan singh
13. Medicinal Chemistry by Ashutosh kar
14. Medicinal Chemistry by G. Chatwal
15. Organic Drug synthesis by Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design by Daniel Ledneiser
17. Top Drugs: Top synthetic routes by John Saunders
18. Chirotechnology by Roger A. Sheldon

COURSE NAME	M.Sc.	SUBJECT NAME	CHEMISTRY	Max. Marks	80+20
Semester	IV	TITLE	BIOPHARMACEUTICS AND PHARMACODYNAMICS	No. of Credits	4

Paper-III MCHE (OC) 403T (E-II): Biopharmaceutics and Pharmacodynamics **4 Hrs/ Week**

OC-33: Pharmacokinetics
OC-34: Pharmacodynamics
OC-35: Principles of Therapeutics
OC-36: Drug Interactions

OC-33: Pharmacokinetics (15Hrs)

Introduction and importance of ADME studies of drugs. Routes of administration.
i) Absorption: Definition, absorption of drugs across the membranes. Physico chemical factors affecting the drug absorption (emphasis on pH partition hypothesis and Drug Dissolution). Methods of determination of drug absorption. Bioavailability.
ii) Distribution: Apparent volume of drug distribution. Factors affecting distribution, plasma protein binding.
iii) Metabolism: Sites of drug metabolism, metabolic rate constant, bioactivation and biotransformation of drugs (phase I and phase II reactions)
iv) Elimination: Types of elimination and overall apparent elimination rate constant and half-life, concept of clearance.

OC-34: Pharmacodynamics (15Hrs)

Introduction, targets for drug action, receptor concept. Pharmacological binding terms. Two state receptor model, receptor families- structure and signal transduction mechanisms- channel linked proteins, gating mechanism, G-protein coupled receptors, G-protein and their role, Targets for G-proteins, Kinase linked receptors, receptors that regulate gene transcription. Theories of concentration -response relationship, dose-response curves.

OC-35: Principles of Therapeutics (15Hrs)

Plasma Drug concentration vs Time profile, Definition and explanation of various terms: MEC, MSC, MTC, AUC (graph). Peak plasma concentration, time of peak concentration. Therapeutic range. Steady state concentration, onset of action, onset of time, duration of action, intensity of action. LD50, ED50. Therapeutic objective. Dosage regimen, Design of dosage regimes: Dose size, dosing frequency, drug accumulation during multiple dosing, time to reach steady-state during multiple dosing, average concentration and body content on multiple dosing to steady state, loading dose, maintenance dose, maintenance of drug within the therapeutic range, design of dosage regimen from plasma concentration. Kinetics of fixed dose, fixed time interval regimes. Modification to dosage regime: Dosing of drugs in obese patients, dosing of drugs in Neonates, infants & children, dosing of drugs in geriatrics (elderly), dosing of drugs in Hepatic disease, dosing of drugs in renal disease.

OC-36: Drug Interactions (15Hrs)

Introduction, classification, Mechanisms of drug interactions. – pharmacokinetic Interactions (alteration of gastrointestinal absorption, complexation and adsorption, alteration of distribution, alteration of metabolism and alteration of excretion) & pharmacodynamic interactions (antagonistic effects, synergistic

effects, alteration of electrolyte levels, interactions involving adrenergic system, alteration of receptor site interaction and antibiotic combinations). Influence of alcohol (Anti biotics, Anti coagulants, Anti histamines, Anti psychotic drugs, sedatives and Hypnotics), smoking (Theophylline, Diazepam, a Tri cyclic antidepressants), food (Bronchodilators, Diuretics, ACE Inhibitors, Anti coagulants, Tetracyclines) on drug action.

References:

1. Pharmacokinetics. By Shobha Rani
2. Elements of Pharmacology. By Gandhi, Desani & Goyal.
3. Goodmann & Gilmann's "The pharmacological basis of therapeutics". By Gilman & Rali.
4. Pharmacology. By Rang.
5. Biopharmaceutics and pharmacokinetics By Brahmani kar
6. Pharmacology By Lippincott
7. Modern Pharmacology with Clinical Applications. By R. Craig.
8. Comprehensive pharmacy review by Leon Shargel
9. Hospital and clinical pharmacy.
10. Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
11. Introduction to Medicinal chemistry. By Patrick.
12. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
13. Principles of medicinal chemistry. By William Foye
14. Biochemical approach to medicinal chemistry. By Thomas Nogrady.

COURSE NAME	M.Sc.	SUBJECT NAME	CHEMISTRY	Max. Marks	80+20
Semester	IV	TITLE	ADVANCED NATURAL PRODUCTS	No. of Credits	4

Paper-IV MCHE (OC) 404T (E-I): Advanced Natural Products **4 Hrs/ Week**

OC-37: Biosynthesis of Natural products
OC-38: Study of the natural products by chemical methods
OC-39: Study of the natural products by spectral methods
OC-40: Total stereo selective synthesis of natural products

OC-37: Biosynthesis of Natural products (15Hrs)

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, feeding experiments — use of radioisotopes Measurement of incorporation — absolute incorporation, specific incorporation. Identification of the position of labels in labelled natural products by chemical degradation and spectral methods.

Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway; Biosynthesis of essential amino acids — phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway: Biosynthesis of terpenes — mono, sesqui, di, tri (β-amyrin) and carotenoids, steroids — cholesterol.

OC-38: Study of the natural products by chemical methods (15Hrs)

Determination of structure and stereochemistry of morphine, reserpine, abietic acid, quinine, atropine.

OC-39: Study of the natural products by spectral methods (15Hrs)

Spectroscopic techniques IR, UV, ^{1}H-NMR, ^{13}C-NMR, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines and isoquinolines.

Study of the following solved problems:

Mass, IR, ^{1}H, ^{13}C-NMR, HOMOCOSY, HETCOR, DEPT, 2D-INADEQUATE and NOE of **Geraniol**, INEPT of **Menthol**, APT of **Apparicine,** NOESY of **Buxaquamarine**, HETEROCOSY of **Strictanol**, 2D-INADEQUATE of **α-picoline** and **β-methyl tetrahydro furan.**

OC-40: Total stereo selective synthesis of natural products (15Hrs)

Woodward's synthesis of Reserpine, Corey's synthesis of Prostaglandins (E_2, $F_{2\alpha}$), Sharpless synthesis of L-Hexoses, Nicolaou's synthesis of Taxol, Danishefsky's synthesis of Indolizomycin, Takasago's synthesis of Menthol and Hoffmann-La Roche's synthesis of Biotin.

References:

1. Biosynthesis by Geismann
2. Textbook of organic chemistry, Vol II by I L Finar
3. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
4. An introduction to the chemistry of terpenoids and steroids, by William Templeton
5. Systematic identification of flavonoid compounds by Mabry & Markham
6. Steroids by Fieser arid Fieser
7. Alkaloids by Manske
8. Alkaloids by Bentley
9. Alkaloids by Pelletier
10. The chemistry of terpenes by A Pinder
11. The terpenes by Simenson
12. Terpenoids by Mayo
13. Principles of organic synthesis 3rd Ed. R O C Norman and J M Coxen
14. One- and two-dimensional NMR spectroscopy by Atta Ur Rahman
15. Spectrometric: identification of organic compounds by Silverstein and Webster
16. Classics in total synthesis K C Nicolaou and E J Sorenson
17. Total synthesis of Natural Products by Apsimon Vol 1-5

COURSE NAME	M.Sc.	SUBJECT NAME	CHEMISTRY	Max. Marks	80+20
Semester	IV	TITLE	BIOORGANIC CHEMISTRY	No. of Credits	4

Paper-IV MCHE (OC) 404T (E-II): Bioorganic Chemistry **4 Hrs/ Week**

OC-37: Carbohydrates
OC-38: Nucleic acids and Lipids
OC-39: Proteins and Enzymes
OC-40: Coenzymes and Vitamins

OC-37: Carbohydrates (15Hrs)

Introduction to the importance of Carbohydrates. Types of naturally occurring sugars. Deoxy sugars, amino sugars, branched chain sugars methyl ethers and acid derivatives of sugars. Determination of configuration and determination of ring size of D-glucose and D-Fructose. Conformational analysis of monosaccharides. 4C1 and 1C4 conformations of D-glucose.

Reactions of six carbon sugars: Ferrier, Hanesian reaction and Ferrier rearrangement. Synthesis of amino, halo and thio sugars. Structure, ring size determination of sucrose and maltose. Conformational structures of sucrose, lactose, maltose, cellobiose and gentobiose. Structure and biological functions of starch, cellulose, glycogen and chitin. Role of sugars in cell-to-cell recognition, blood groups.

OC-38: Nucleic acids and Lipids (15Hrs)

Nucleic acids: Retro synthetic analysis of nucleic acids - Nucleotides, Nucleosides, Nucleotide bases and Sugars. Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. DNA finger printing.

Lipids: Introduction and classification of lipids. Stereochemical notation in lipids. Chemical synthesis and biosynthesis of phospholipids and glycolipids. Properties of lipid aggregates, micelles, bilayers, liposomes and biological membranes.

OC-39: Proteins and Enzymes (15Hrs)

Proteins: Introduction. Peptide bond, classification and nomenclature of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods. Proteins – Biological importance and classification - Primary, secondary and tertiary structure of proteins.

Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis - Lock and Key, Induced- Fit and three point contact models. Enzyme selectivity –chemo, regio, diastereo and enantio selectivity – illustration with suitable examples. Factors affecting enzyme catalysis. Enzyme inhibition-reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes

OC-40: Coenzymes and Vitamins (15Hrs)

Coenzymes: Introduction. Co-factors - co-substrates -prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their Phosphates (NAD), NADH, NADP+ NADPH) ii) Flavin adenine nucleotide FAD, FADH2 and iii) Flavin mononucleotide (FMN, FMNH2) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine

(SAM) and uridine diphosphosugars (UDP-sugars) Mechanism of reactions catalysed by the above coenzymes.

Vitamins: Introduction, classification and biological importance of vitamins. Structure determination and synthesis of vitamins A, B1, and B2. Synthesis of vitamins - B6, C, E and K. Structure of vitamin B12.

References:

1. Organic Chemistry Vol. I and Vol. II by I. L. Finar
2. Carbohydrate Chemistry by Barton Volumes
3. Carbohydrate chemistry by G. J. Boons
4. The chemistry of natural products: vol. V - carbohydrates by S. F. Dyke
5. Organic Chemistry by McMurry
6. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
7. Lehninger Principles of Biochemistry by D L Nelson and M M Coxon
8. Outlines of Biochemistry by Conn and Stumpf
9. Enzyme structure and mechanism by Fersht and Freeman
10. Enzymes for green organic synthesis by V. K. Ahluwalia
11. Biotransformations in Organic Chemistry by K Faber.
12. Principles of biochemistry by Horton &others.
13. Bioorganic chemistry-A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
14. Concepts in Biotechnology by D. Balasubramanian & others
15. Chemistry and physiology of the vitamins by H. R. Rosenberg.

COURSE NAME	M.Sc.	SUBJECT NAME	CHEMISTRY	Max. Marks	100
Semester	IV	TITLE	Spectroscopic identification of organic compounds and Green syntheses	No. of Credits	4

Paper-V MCHE (OC) 451P: Spectroscopic identification of organic compounds and Green syntheses	**6 hrs/week**

A) Spectroscopic identification of organic compounds:
Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H NMR, ^{13}C NMR and mass spectral data. A minimum of 30 representative examples should be studied.

B) Green syntheses

i. Clay catalysed solid state synthesis of 7-hydroxy-4-methylcoumarin
ii. Nitration of phenol using calcium nitrate and acetic acid
iii. Bromination of acetanilide using ceric ammonium nitrate (CAN) and Potassium bromide
iv. Preparation of 1,1-bis-2-napthol
v. Synthesis of dihydropyrimidinone (Three component coupling)
vi. Synthesis of 2-cyano-3-(4-methoxyphenyl)-propionate (Microwave-assisted ammonium formate-mediated Knoevenagel reaction)
vii. **Solid state synthesis:** Ring opening reactions: Aniline react with anhydrides (Maleic, Succinic & Pthalic)

References:

1. Spectral identification of organic compounds Bassler, Silverstein 5th Edition
2. Monograph on Green Chemistry Laboratory Experiments

MODEL QUESTION PAPER

1) Determine the structure of compound by using the given spectral data of UV, IR, ^{1}H-NMR, ^{13}C-NMR and Mass spectral data.

2) Synthesize the given organic compound and calculate the yield of product.

SCHEME OF EVALUATION

Assessment	**Marks: 100**
Experiment 1	40
Experiment 2	40
Record submission	05
Samples & Viva-voce	15

COURSE NAME	M.Sc.	SUBJECT NAME	CHEMISTRY	Max. Marks	100
Semester	IV	TITLE	SYNTHESIS AND ANALYSIS OF DRUGS	No. of Credits	4

Paper- VI MCHE (OC) 452P: Synthesis and analysis of drugs	**6 hrs/week**

(A) Laboratory Synthesis of the following drugs:

Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone, 4-Aminobenzene, Sulfonamide, Fluorescein and Antipyrine.

(B) Estimation of the following drugs:

Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry), Chloride in Ringer's lactate (argentometry), Ascorbic acid {titrimetry (Iodometry and Cerimetry), colorimetry}, Isoniazid (Iodometry), Riboflavin (colorimetry).

References:

1. Text book of practical organic chemistry, Vogel.
2. Text book of practical organic chemistry, Mann and Saunders.

MODEL QUESTION PAPER

1) Synthesize the given drug compound, recrystallize and calculate the yield of product.

2) Estimate the amount of aspirin present in the given Aspirin tablets by using titrimetry.

SCHEME OF EVALUATION

Assessment	**Marks: 100**
Experiment 1	40
Experiment 2	40
Record submission	05
Samples & Viva-voce	15