VISVESVARAYA TECHNOLOGICAL UNIVERSITY
BELAGAVI

Syllabus

M.Sc. in Chemistry

(Specialisation: Analytical Chemistry / Organic Chemistry**)**

(Effective from the Academic year 2024-25)
IV Semester Syllabus

IV SEMESTER

ADVANCED ANALYTICAL CHEMISTRY			
Course Code	MSC401A	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- Understand the principles, instrumentation, and working mechanisms of thermal, electroanalytical, spectroscopic, and microscopic techniques.
- Analyze and interpret electrochemical and thermal data for qualitative and quantitative chemical analysis.
- Apply advanced voltammetric and coulometric methods to real-world analytical and research problems.
- Explain the structure–property relationships using advanced spectroscopic and microscopic techniques.
- Select appropriate instrumental techniques for material characterization, trace analysis, and research applications.
- Develop competency in modern analytical tools relevant to academia, industry, and R&D.

Module-1

Thermal Analysis: Introduction, principle and applications of TGA, DTG, DTA, DSC - combustion calorimetry- Thermal diffusivity by the laser flash technique- simultaneous techniques including analysis for gaseous products.

Module-2

Voltametry: Introduction, Principle, excitation signals in voltammetry, basic instrumentation based on operational amplifiers, voltammetric electrodes, modified electrodes. Hydrodynamic Voltammetry- Electrode profiles in stirred and unstirred solutions, Applications.

Cyclic Voltammetry: Instrumentation, Determination of analytes using cyclic voltammetry, Applications.

Pulse voltammetry: Introduction, Normal Pulse Voltammetry, Reverse pulse voltammetry, Differential pulse voltammetry, Square wave voltammetry.

Module-3

Stripping voltammetry: Cathodic and Anodic stripping voltammetry, Electrodeposition step, Voltametric completion of the analysis, adsorptive striping methods.

Voltammetry with microelectrodes. Practical applications in analytical chemistry and research.

Coulometry

Introduction: Theory and instrumentation, current-voltage relationship, controlled potential Coulometry, types of coulometric methods, coulometric titration, and applications. Practical applications in analytical chemistry and research.

Module-4

Advanced Spectroscopic Techniques

Principles, instrumentation, and applications of: Atomic Absorption Spectroscopy (AAS), Inductively Coupled Plasma – Atomic Emission & Mass Spectrometry (ICP-AES, ICP-MS), X-ray Fluorescence (XRF) and X-ray Photoelectron Spectroscopy (XPS), Mössbauer Spectroscopy.

Hyphenated Techniques: CE-MS, LC-MS, GC-MS

Module-5

Microscopic Techniques: Scanning Electron Microscope (SEM) - Introduction, principle, instrumentation, applications Transmission Electron Microscope (TEM) - Introduction, principle, instrumentation, applications Electron Dispersion Spectroscopy (EDS) - Introduction, principle, instrumentation,

applications Energy Dispersive X-ray Analysis (EDAX) - Introduction, principle, instrumentation, applications.

Scanning Tunneling Microscopy (STM) - Introduction, principle, instrumentation, applications Atomic Force Microscopy (AFM) - Introduction, principle, instrumentation, applications Practical applications and examples in analytical chemistry and research.

References

1. A. I. Vogel: A text book of Quantitative inorganic Analysis, Lonqmans
2. Instrumental methods of Chemical analysis-H. Kaur
3. Bhushan, Bharat 2004. Handbook of Nanotechnology. Springer.
4. Avouris, P, Klitzing, K. Von, Sakaki, H. & Wiesendanger,R .2003 NanoScience and Technology
5. Series. Scanning Probe Microscopy- Analytical Methods (R. Wiesendanger eds), Springer.
6. R.D. Braun, Introduction to Instrumental Analysis.
7. D.A.Skoog, F. J. Holler, Principles of Instrumental Analysis, 6th edition.
8. Willard, Deritt, Dean and Settle, Instrumental methods of Analysis.
9. F. J. Welcher, Standard Methods of chemical Analysis Vol.3,PartA & B.
10. G.W. Ewing, Instrumental Methods of Analysis 4th and 5th editions.
11. Chatawal and Anand, Instrumental Methods of Analysis.
12. Bassett, Denney-Jeffer and Mendham, Vogel's Textbook of Quantitative Inorganic Analysis, (5th edition).
13. Electro-analytical chemistry, edited by H.W. Nurnberg.
14. Stulic, Ion selective electrodes (John Wiley).

Course Outcomes: After completion of the course, students will be able to

CO1	Understand and explain the principles and instrumentation of modern analytical techniques.
CO2	Apply electroanalytical and thermal techniques for qualitative and quantitative chemical analysis.
CO3	Analyze and interpret complex instrumental data for research and industrial applications.
CO4	Select appropriate spectroscopic and microscopic techniques for material characterization.
CO5	Demonstrate problem-solving skills using advanced analytical tools in chemistry and allied research areas.

Mapping of Cos and Pos

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	**X**	**X**	**X**		**X**		
CO2	**X**	**X**	**X**	**X**	**X**		
CO3		**X**		**X**	**X**		
CO4			**X**	**X**	**X**		
CO5				**X**	**X**	**X**	

ENVIRONMENTAL AND PHARMACEUTICAL ANALYTICAL CHEMISTRY			
Course Code	MSC402A	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- Understand the chemical composition of soil, environmental pollutants, pesticides, drugs, and biological fluids**.**
- Explain the principles and methodologies used in environmental, pharmaceutical, forensic, and clinical analysis.
- Apply classical and instrumental analytical techniques for qualitative and quantitative determination of analytes.
- Interpret analytical data related to environmental contamination, drug purity, toxicological evaluation, and disease diagnosis**.**
- Develop analytical problem-solving skills relevant to regulatory, industrial, forensic, and research laboratories**.**

Module-1

Soil Chemistry: Physio-chemical composition of soil, humus, Inorganic and organic components of soil, nutrients (NPK) in soil, significance of C:N ratio, Cation exchange capacity (CEC), Environmental geochemistry: Concept of major, trace and REE. Classification of trace elements, Solubility and mobility of trace elements; Biochemical aspects of Arsenic, Cadmium, Lead, Mercury, Carbon monoxide, O3, PAN, MIC and other carcinogens.

Module-2

Pesticides Analysis

Introduction, classification of pesticides, sampling, sample pretreatment and processing, analysis of DDT, gammexane, endosulphan, zinab, ziram, malathion, thiram, thiometon, simazine and chloridane. Applications of colorimetric and chromatographic techniques (GC-MS, HPLC- MS) in analysis of pesticide residue. Introduction to EPA regulatory body. Practical applications and examples in analytical chemistry and research.

Module-3

Drug Analysis

Introduction to drugs, their classification, sources of impurities in pharmaceutical raw materials such as chemical, atmospheric and microbial contaminants etc. Limit tests: Limit test for impurities for Pb, As, Fe, Se, etc. Estimation of moisture (K-F method), halide (Schnoiger's oxygen flask method), sulfate, boron, etc. Analysis of commonly used drugs such as antihistamines, sulfa drugs, barbiturates, etc. using non-aqueous titrations, sodium nitrite titrations, differential UV methods, colorimetric and fluorimetric methods of analysis.

Module-4

Forensic Analysis

Special features of forensic analysis, sampling, sample storage, sample dissolution, classification of poisons, lethal dose, significance of LD-50 and LC-50. General discussion of poisons with special reference to mode of action of cyanide, organophosphate and snake venom. Estimation of poisonous materials such as lead, mercury and arsenic in biological samples. Practical applications and examples in analytical chemistry and research.

Module-5

Body fluid analysis

Composition and detection of abnormal level of certain constituents leading to diagnosis of diseases. Sample collection and preservation of physiological fluids, analytical methods to the constituents of physiological fluids (blood, urine and serum) Blood-Estimation of glucose, chlolesterol, urea, hemoglobin and bilirubin, Urine- urea, uric acid, creatinine, calcium, phosphate, sodium, potassium and chloride.

References

1. F. J. Welcher: Standard methods of Chemical analysis, 6th Ed. Vol. I and II (D. Van Nostard Comp.)
2. M. Kolthoff: Treatise on Analytical Chemistry Vol. I & II
3. F. D. Snell: Encyclopedia of industrial Chemical Analysis Vol. 1 to 20 (John Wiley)
4. Riech: Outline of Industrial Chemistry.
5. K. H. Buchel: Chemistry of Pesticides (John Wiley)
6. Indian, Pharmacopoeia, British Pharmacopoeia and U. S. Pharmacopoeia.
7. V. M. Parikh: Absorption spectroscopy of organic molecules (Addision Wesley)
8. Willard, Merrite, Dean and Settle: Instrumental methods of analysis (CBS)
9. D. H. Williams and J. Fleming: Specroscopic methods in organic chemistry (Mc Graw Hill) Silverstein: Spectroscopic Identification of organic compounds (John Wiley)
10. Jackmann and Sternhill: Applications of NMR spectroscopy of organic Chemistry (Pergamon Press)
11. J. D. Roberts : Nuclear Magnetic Resonance (Mc Graw Hill)
12. K. Benjamin : Mass Spectrometry
13. Nichollas: Aids to the Analysis of foods and Drugs.

Course Outcomes: After completion of the course, students will be able to

CO1	Analyze the physicochemical properties of soil and environmental matrices and evaluate the behavior, toxicity, and biochemical impact of major and trace environmental pollutants.
CO2	Apply appropriate sampling, pretreatment, and analytical techniques to detect and quantify pesticide residues in environmental samples in compliance with regulatory standards.
CO3	Evaluate the quality, purity, and composition of pharmaceutical substances using classical, instrumental, and pharmacopeial analytical methods.
CO4	Interpret forensic evidence through chemical analysis of poisons and toxic substances in biological samples for medico-legal and investigative applications.
CO5	Analyze physiological fluids to determine biochemical parameters essential for disease diagnosis and clinical interpretation.

Mapping of Cos and Pos

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	**X**	**X**					
CO2	**X**	**X**			**X**		
CO3	**X**		**X**		**X**	**X**	
CO4		**X**		**X**			**X**
CO5			**X**			**X**	**X**

INDUSTRIAL ANALYTICAL CHEMISTRY			
Course Code	MSC403A	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- Understand quality assurance systems, regulatory frameworks, and standardization practices relevant to industrial chemical analysis.
- Apply classical and instrumental analytical methods for quality control of food, pharmaceuticals, cosmetics, oils, detergents, paints, and petroleum products.
- Evaluate composition, purity, safety, and regulatory compliance of industrial products.
- Interpret analytical results for process control, product validation, and troubleshooting in industrial settings.

Module-1

Quality Assurance and Quality Control

Definition - Quality control and Quality assurance, concept and philosophy of TQM, GMP, ICH and ISO 9000. Standardization concept for products. Introduction to various pharmacopeia, Overview of ICH Guidelines: QSEM, with special emphasis on Q-series guidelines, Validation of Analytical Procedures, Good Manufacturing Practice (GMP) Guide for Active Pharmaceutical Ingredients, Good Laboratory Practice (GLP)

Module-2

Food Analysis

Estimation of moisture, ash, crude protein, fat, crude fibre, carbohydrate, calcium, potassium, sodium and phosphate in foods; Analysis of common adulterants in foods; milk and milk products alcohol test, fermentation test, dye reduction tests (methylene blue and resazurin), test to distinguish between butter and margarine, phosphatase test for pasteurization, estimation of added water; Beverages - caffeine and chicory in coffee, methanol in alcoholic drinks; Estimation of saccharin, coal tar dyes, aflatoxins in foods
Analysis of vitamins (thiamine, ascorbic acid, Vit. A, Vit. B6, Vit. K).

Module-3

Analysis of oils, fats and Soaps

Introduction to natural fats and oils; isolation of oils from natural resources and their purification. Analysis of oils and fats: Softening point, Congeal point, Titre point, Cloud point, Iodine, saponification, acid, hyroxyl, R-M and Polenske value, Elaiden test, etc.
Introduction to soaps, manufacture of soaps (in brief), analysis of soaps: total anhydrous soap and combined alkali, potassium, water, free fatty acids, saponifiable and non-saponifiable matter in soaps, estimation of phenol, copper and germicidal agents in soaps, determination of inorganic fillers and soap builders, and other additives, estimation of soap in detergents (THAM method)

Analysis of Detergents

Classification of detergents, analysis of raw materials, separation as alcohol soluble and alcohol insoluble matter, additives in detergent formulation (chlorides, sulfates, phosphates, silicates, borates, oxygen releasing substances, CMC, EDTA, etc.), their role and analysis; analysis of active ingredients in detergents (methylene blue and Hyamine-1622 method).

Module-4

Analysis of cosmetics products

Introduction to cosmetics, definition, types of cosmetics, background, development in cosmetic industry, issues in cosmetic industries (contamination and adulteration), future scope and role of analytical

chemistry.

Analysis of cream and lotions

Composition of creams and lotions, determination of water, propylene glycol, non-volatile matter and ash content; estimation of borates, carbonates, sulphates, phosphates, chlorides, ammonia, nitromethane, oxalic acid, 4- hydroxy benzoic acid, sodium iodate, free formaldehyde, H2O2, mercatoacetic acid, titanium and zinc oxides.

Analysis of face powder

Composition of face powder, estimation of boric acid, Mg, Ca, Zn, Fe, Al and Ba. Analysis of deodorants and antiperspirants-composition, analysis of fats and fatty acids, boric acid, magnesium, calcium, zinc, iron, titanium, aluminium, phenol, methanamine, hexachlorophenone, sulphonates, urea, etc.

Module-5

Analysis of Paints and pigments

Composition of paint, preliminary inspection of sample, test on the total coating, separation and estimation of pigments, binder and thinner of latex paints; modification of binder, flash point of paints. Practical applications and examples in analytical chemistry and research.

References

1. M. Sitting, Resources Recovery and Recycling, Handbook of industrial Waste.
2. B.K. Sharma, Industrial Chemistry.
3. S.P. Mahajan, Pollution Control in Process Industries.
4. R.A. Horne, Chemistry of our Environment
5. Gowenlock, B. G., et al. Vogel's Textbook of Qualitative Chemical Analysis (Longmans / Pearson)
6. Willard, Merritt, Dean & Settle *Instrumental Methods of Analysis* (CBS/Thomson)
7. Gunstone, F. D. (Ed.). *The Chemistry of Oils & Fats* (Blackwell)

Course Outcomes: After completion of the course, students will be able to

CO1	Explain and apply quality assurance systems, regulatory guidelines, and analytical validation principles for ensuring product quality and compliance in chemical industries.
CO2	Analyze food products, beverages, vitamins, and hormones for nutritional value, adulteration, and safety using standard chemical and instrumental methods.
CO3	Evaluate the physicochemical properties and quality parameters of oils, fats, soaps, and detergents to ensure performance, safety, and regulatory compliance.
CO4	Assess the composition, quality, and safety of cosmetic products using appropriate analytical techniques to detect contaminants, adulterants, and regulated substances.
CO5	Apply industrial analytical techniques to characterize paints, pigments, petroleum products, coal, and coke for quality control and performance evaluation.

Mapping of Cos and Pos

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	**X**	**X**			**X**	**X**	**X**
CO2		**X**			**X**		**X**
CO3		**X**	**X**				
CO4				**X**		**X**	**X**
CO5		**X**		**X**			**X**

ANALYTICAL CHEMISTRY PRACTICAL - III			
Course Code	MSC404A	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	1:6:0	SEE Marks	50
Total Hours of Pedagogy	72	Total Marks	100
Credits	4	Exam Hours	3

Course Learning Objectives are:

- Acquire hands-on skills in quantitative analysis of food and feed samples using classical and instrumental methods.
- Understand the principles and procedures involved in proximate analysis such as moisture, ash, fat, fiber, carbohydrate, and protein estimation.
- Apply wet digestion, spectroscopic, chromatographic, and electro-analytical techniques for food quality and safety assessment.
- Develop competence in instrument handling, calibration, data recording, and result interpretation.
- Follow good laboratory practices (GLP), safety protocols, and proper waste disposal methods during analytical work.

1. Estimation of moisture in foods and feeds.
2. Estimation of ash content in flour samples
3. Estimation of fat in oil seeds (peanut)
4. Estimation of crude fiber in Wheat bran or vegetable residue
5. Estimation of carbohydrate in Banana pulp or fruit samples
6. Estimation of protein Kjeldahl's method of protein estimation in foods and feeds.
7. Protein estimation by Biuret / Lowry / Bradford (colorimetric) as alternatives to Kjeldahl for quick assays. Egg white (albumin) solution or milk
8. Determination of saponification value and iodine value of oil
9. Estimation of lactose from milk sample using flame photometer.
10. Heavy metals in food (Pb, Cd, As, Hg) wet digestion and AAS
11. Gas chromatography for fatty acid methyl ester.

References

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Practical Clinical biochemistry methods and interpretations, R. Chawla, J.P. Bothers Medical Publishers (P) Ltd., 1995.
7. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.

8. Practical Clinical Biochemistry by Harold Varley and Arnold.Heinmann, 4th edition.
9. Watson, D. G. Pharmaceutical Analysis: A Textbook for Pharmacy Students and Pharmaceutical Chemists, Churchill Livingstone.

Course Outcomes:

CO1	Perform quantitative estimation of major nutritional components (moisture, ash, fat, fiber, carbohydrate, protein, and lactose) in food and feed samples using standard analytical procedures and interpret the results accurately.
CO2	Apply instrumental techniques such as flame photometry, atomic absorption spectroscopy (AAS), and gas chromatography (GC) to analyze trace metals and fatty acid profiles in food samples, demonstrating proficiency in modern analytical tools and laboratory practices.

Mapping of COs and POs

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	X	X	X				X
CO2	X	X	X				X

ADVANCED ORGANIC CHEMISTRY			
Course Code	MSC401B	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- To understand the functional group interconversions of organic compounds using various reagents.
- To understand the synthesis and retro-synthesis approaches in organic synthesis.

Module-1

Oxidation of Alkenes: (a) Peracids oxidation of alkenes and carbonyls.
(b) Alkenes to diols (manganese, osmium based), alkenes to carbonyls with bond cleavage (manganese, ruthenium, and lead based, ozonolysis), and alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, and selenium based allylic oxidation).
(c) Asymmetric epoxidations (Sharpless, Jacobsen, and Shi epoxidations) and Sharpless asymmetric dihydroxylation.
Oxidation of Alcohols: (a) Metal based and non-metal based oxidations of alcohols (chromium, manganese, silver, ruthenium, DMSO, and hypervalent iodine).

Module-2

Reduction: (a) Catalytic homogeneous and heterogeneous hydrogenation, Wilkinson catalyst. (b) Metal based reductions using Li/Na in liquid ammonia, sodium, magnesium, zinc, titanium, and samarium. (c) Hydride transfer reagents: $NaBH_4$, L- selectride, K-selectride, Luche reduction, $LiAlH_4$, DIBAL-H, Red-Al, Trialkylsilanes, and Trialkylstannane. (d) Enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata) and Noyori asymmetric hydrogenation.

Module-3

Modern Synthetic Methods: (a) Baylis-Hillman reaction, Henry reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Brook rearrangement, Tebbe olefination.
(b) Metal mediated C-C and C-N coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions, directed ortho metalation. (c) Stereoselective synthesis of tri- and tetra-substituted olefins. Synthetic applications of Claisen rearrangement, ene reaction (metallo-ene, Conia ene).

Module-4

Construction of Ring Systems: (a) Alternate approaches towards the synthesis of three, four, five, and six-membered rings. (b) Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization, inter-conversion of ring systems (contraction and expansion). (c) Construction of macrocyclic rings and ring closing metathesis.

Module-5

Retrosynthetic Analysis: Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions. Protecting groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

References

1. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996.
2. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier

Academic Press, 2005.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
4. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
5. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
6. S. Warren, Organic Synthesis, The disconnection Approach, John Wiley & Sons, 2004.
7. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley & Sons, 2003.
8. I. Ojima, Catalytic Asymmetric Synthesis, 2nd edition, Wiley−VCH, New York, 2000.
9. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.

Course Outcomes: After completion of the course, students will have

CO1	Students are familiar about chemistry of oxidants and various types of oxidants used for oxidation reactions
CO2	Better understanding of reducing agents and reduction reaction mechanisms
CO3	Familiar about various moderns synthetic methods and reactions
CO4	Able to construct various ring systems
CO5	Analyse the reactions by Retro-synthetic approach

Mapping of Cos and Pos

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	**X**		**X**			**X**	**X**
CO2	**X**						
CO3	**X**	**X**					
CO4	**X**	**X**	**X**			**X**	**X**
CO5	**X**	**X**	**X**			**X**	**X**

ADVANCED MEDICINAL AND BIOORGANIC CHEMISTRY			
Course Code	MSC402B	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- To gain a comprehensive understanding of advanced concepts in medicinal chemistry, including contemporary drug design methodologies.
- To investigate detailed mechanisms of action of various drug classes at the molecular and cellular levels.
- To analyze complex structure-activity relationships to predict drug efficacy and optimize lead compounds.
- To explore advanced synthetic methodologies for the development of novel therapeutic agents, including asymmetric synthesis and combinatorial chemistry.

Module-1

Fundamental aspects of drugs: Forms, application, biological action, placebo effect, metabolism, drug interactions, adverse effects, classification of drugs, nomenclature of drugs, drug combinations, selection of essential drugs. Physicochemical properties of drug molecules in relation to biological activity; solubility, partition coefficient, hydrogen bonding, protein binding, chelation, pka values, isomerism, Geometrical and optical isomers, steric effect, ionization.

SAR and QSAR: SARs, Changing size and shape, introduction of new substituents-the introduction of a group in an unsubstituted position, the introduction of a group by replacing the existing group. QSAR-Lipophilicity, partition coefficient (log P), lipophilic substitution constants(π). Electronic effect (Hammet constant σ), steric effect, Taft's steric parameter (Es), Hansch analysis and application, craigs plot, Free-Wilson analysis and application.

Lipinski's rule/Pfizer rule of 5 – if possible sir.

Module-2

Prodrugs: Enzyme activation of drugs, Utility of prodrugs, types of prodrugs, mechanism of drug activation- Carrier linked prodrugs, carrier linkages for various functional groups, carrier linked bipartite prodrugs. Bioprecurssor prodrugs(Proton activation, hydrolytic activation, elimination activation, oxidative activation, reductive activation, nucleotide activation, phosphorylation activation, sulfation activation, decorboxylation activation

Module-3

Combinatorial Chemistry: Introduction, the design of combinatorial synthesis, the general techniques used in combinatorial synthesis, the solid support method, parallel synthesis, Furka's mix and split techniques, Encoding methods-Sequential chemical tagging method, stills binary core tag system, computerized tagging, combinatorial synthesis in solution, screening and deconvolution.

Module-4

Carbohydrates: Carbohydrates: Introduction, Ring size determination of monosaccharides, configuration and conformations of monosaccharides, anomeric effect, Hudson's rules, epimerization and mutarotation. Synthesis, industrial and biological importance of glycosides, amino sugars, sucrose, maltose and lactose. Polysaccharides: General methods of structure elucidation. Industrial importance and biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar- agar. Photosynthesis and biosynthesis of carbohydrates.

Module-5

Amino Acids: General structure, physiological properties, protection of functional groups.

Protecting groups: Protection of hydroxyl, carboxyl, carbonyl, thiol and amino groups. Illustration of protection and deprotection in synthesis.

Peptides: Structure and conformation of peptide bond, peptide synthesis: Solution phase and Merrifield's solid phase synthesis, Racemization and use of HOBt, Synthesis of oxytocin and vasopressin, biological importance of insulin, selective cleavage of polypeptide bonds (chemical and enzymatic). Proteins: Structure determination: *C* and *N* terminal residue determination, primary, secondary, tertiary and quartenary structure determination, denaturing and renaturing of proteins.

Nucleic acids: Introduction, structure and synthesis of nucleosides and nucleotides, protecting groups for hydroxy group in sugar, amino group in the base and phosphate functions. Methods of formation of internucleotide bonds: DCC, phosphodiester approach and phosphoramide methods. Solid phase synthesis of oligonucleotides. Structure of RNA and DNA, Crick-Watson model, role of nucleic acids in the biosynthesis of proteins.

References

1. Introduction to quantitative Drug Design-Y.C.Martin.
2. Comprehensive Medicinal chemistry-Crowin and Hansch.
3. Medicinal Chemistry-Burger.
4. Principles of Drug Design-Smith.
5. Principles of Medicinal Chemistry- William Foye.
6. Drug design volumes-Ariens.
7. Strategy of drug design-Brucell.
8. The Organic Chemistry of drug design and drug action-Richard. B. Silverman.
9. Fundamentals of medicinal chemistry-Gareth Thomas. John Wiley and sons England.

Course Outcomes:

CO1	Demonstrate an in-depth understanding of advanced concepts in medicinal chemistry and their application in drug discovery.
CO2	Understand and articulate the regulatory processes involved in drug approval, including the significance of clinical trials.
CO3	Demonstrate proficiency in advanced synthetic methodologies, including combinatorial chemistry, for the development of novel therapeutic agents.
CO4	Synthesis, industrial and biological importance of carbohydrates.
CO5	General synthesis of amino acids, peptides, nucleic acids and their biological significance.

Mapping of COs and POs

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	**X**	**X**					
CO2	**X**	**X**	**X**				
CO3	**X**	**X**				**X**	**X**
CO4			**X**			**X**	**X**
CO5			**X**			**X**	**X**

CHEMISTRY OF NATURAL PRODUCTS			
Course Code	MSC403B	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- Define natural products and categorize them, with a specific focus on lipids, flavonoids, and isoflavonoids.
- Explore the biosynthetic pathways involved in the production of lipids, flavonoids, and isoflavonoids, including key enzymes and regulatory mechanisms.
- Examine the chemical structures of lipids, flavonoids, and isoflavonoids, emphasizing their functional groups and structural variations.

Module-1

Lipids: Nomenclature, classification, purification, structure and synthesis of fatty acids, phospholipids, sphingolipids. Biological importance of lipids (Lecithin, sphingolipids, oils and fats). Prostaglandins: Introduction, classification and biological importance of PG's. Constitution of PGE1. Synthesis of PGE & F series.

Module-2

Terpenoids: Introduction, classification and general methods of structural elucidation. Chemistry of pinene, camphor, caryophyllene, santonin. Biosynthesis of terpenoids.

Porphyrins: Introduction, structure and biological functions of haemin. Vitamin B12: structure and as coenzyme in molecular rearrangement reactions; Chlorophyll: structure and biological importance

Module-3

Flavonoids and Isoflavonoids: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin, Kaempferol, Quercetin, wedelolactone, Butein, Daidzein. Biosynthesis of flavonoids and isoflavonoids: Acetate Pathway and Shikimic acid Pathway. Biological importance of flavonoids and isoflavonoids

Module-4

Alkaloids: Introduction, classification, isolation and general methods of structural elucidation of alkaloids. Classification of alkaloids. Biological importance of alkaloids. Structural elucidation of nicotin, papavarine, quinine, reserpine and morphine. Biosynthesis of alkaloids (nicotin, conine and cocaine).

Module-5

Steroids: Introduction, Structural elucidation of cholesterol, bile acids, Ergosterol and its irradiation products. Sex hormones and corticosteroids: Synthesis of estrone, progesterone, androsterone, testosterone. Barton reaction for the synthesis of aldosterone. Brief discussion of homosteroids, norsteroids and oral contraceptives. Biological significance of anabolic steroids.

References

1. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
2. Organic Chemistry, Vol-II by I. L. Finar.
3. Schaum's outline of theory and problems of Organic Chemistry, Harbert Meislich, Howard Nechamkin and Jocob Sharefkin.
4. Natural products: Their chemistry and biological significance, J. Mann, R. S. Davidson, J. B. Banthorpe and J. B. Harborne.
5. Synthetic drugs, Gurdeep R. Chatwal.
6. Heterocyclic chemistry by Achison.
7. Heterocyclic chemistry by Smith and Joule. 8. Heterocyclic chemistry by Pacquete.

Course Outcomes:

CO1	Demonstrate a thorough understanding of the structure, classification, and properties of lipids, flavonoids, and isoflavonoids.
CO2	Design and conduct research projects focused on natural products, demonstrating the ability to formulate hypotheses, collect data, and analyze results.
CO3	Demonstrate an understanding of the ethical implications of using natural products in research and industry, including sustainability and biodiversity considerations.

Mapping of COs and POs

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	**X**	**X**					
CO2	**X**	**X**	**X**				
CO3	**X**	**X**	**X**			**X**	**X**

ORGANIC CHEMISTRY PRACTICAL - III			
Course Code	MSC404B	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	1:6:0	SEE Marks	50
Total Hours of Pedagogy	72	Total Marks	100
Credits	4	Exam Hours	3

Course Learning Objectives are:

- To understand synthetic methods by carrying out different experiments.
- To develop the skill for the preparation of organic compounds

MULTISTEP SYNTHESIS

1. Preparation of benzyl alcohol and benzoic acid *via* Cannizzaro reaction.
2. Oxidation of cyclohexanol to adipic acid via cyclohexanone
3. Esterification: Preparation of benzoccaine from p-nitrotoluene
4. Diazotization (Sandmeyer reaction): Preparation of p-chlorobenzoic acid from p- toluidine
5. Molecular rearrangement: Preparation of o-chlorobenzoic acid from phthalic anhydride
6. Preparation benzilic acid from benzaldehyde
7. Preparation of o-hydroxy benzophenone from phenyl benzoate via Fries rearrangement
8. Prepartion of benzanilide from benzophenone oxime via Beckmann rearrangement.
9. Synthesis of m-chloroiodobenzene from m-dinitrobenzene.
10. Synthesis if 2,4-dinitro phenyl hydrazine
11. Preparation of phenacetin from *p*-nitro phenol (*via* reduction, acetylation and ethylation)
12. Synthesis of Luminol
13. Grignard reaction: Synthesis of triphenyl carbinol from benzophenone/ethylbenzoate
14. Preparation of pyrazole from acetophenone

References

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III
3. Practical Organic Chemistry - Mann & Saunders
4. Modern Experimental Organic Chemistry by John H. Miller and E.F. Neugil, p 289.
5. An Introduction to Practical Organic Chemistry - Robert, Wingrove etc
6. Natural Products Chemistry by Raphel Ikhan
7. Experiments in organic chemistry, III edition, Louis F. Fieser.
8. Vogel's Text book of practical organic chemistry, V edition, B. B Furniss, A.J. Hannaford, P.W.G. Smith.
9. Practical Organic chemistry-Mann and saunders

Course Outcomes:

CO1	Students are involved in the multi-step synthesis of different organic compounds.
CO2	Understand the qualitative analysis of binary mixture of organic compounds through separation, identification of functional groups and preparation of some solid derivatives.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X	X	X				X
CO2	X	X	X				X