



SIES

**College of Arts,
Science &
Commerce**

RISE WITH EDUCATION

Sion (West), Mumbai – 400022.

Autonomous

Program: M.Sc.

Course: Organic Chemistry

Syllabus for M. Sc. Semester III and IV

To be implemented from 2018 - 2019

Credit Based Semester and Grading System

SEMESTER III

Contents:	
Paper I	: Theoretical organic chemistry-I
SIPSCHEO31.1	: Organic reaction mechanisms
SIPSCHEO31.2	: Pericyclic reactions
SIPSCHEO31.3	: Stereochemistry-I
SIPSCHEO31.4	: Photochemistry
Paper II	: Synthetic Organic Chemistry-I
SIPSCHEO32.1	: Name reactions with mechanism and application
SIPSCHEO32.2	: Radicals in organic synthesis
SIPSCHEO32.3	: Enamines, ylides and α -C-H functionalization
SIPSCHEO32.4	: Metals / non-metals in organic synthesis
Paper III	: Natural products and Spectroscopy
SIPSCHEO33.1	: Natural products-I
SIPSCHEO33.2	: Natural products-II
SIPSCHEO33.3	: Advanced spectroscopic techniques-I
SIPSCHEO33.4	: Advanced spectroscopic techniques-II
Paper IV	: Medicinal , Biogenesis and green chemistry
SIPSCHEOE-I-34.1	: Drug discovery, design and development
SIPSCHEOE-I-34.2	: Drug design, development and synthesis
SIPSCHEOE-I-34.3	: Biogenesis and biosynthesis of natural products
SIPSCHEOE-I-34.4	: Green chemistry
Practical	
SIPSCHEO3P1	: Separation of a solid ternary mixture using micro-scale technique
SIPSCHEO3P2	: Estimation of drugs
SIPSCHEO3P3	: Organic preparations (1.0 g scale)
SIPSCHEO3P4	: Single step organic preparation (1.0 g scale) involving, techniques of purification and green methods of synthesis

SEMESTER IV

Contents:	
Paper I	: Theoretical organic chemistry-II
SIPSCHEO41.1	: Physical organic chemistry
SIPSCHEO41.2	: Supramolecular chemistry
SIPSCHEO41.3	: Stereochemistry-II
SIPSCHEO41.4	: Asymmetric synthesis
Paper II	: Synthetic Organic Chemistry-II
SIPSCHEO42.1	: Designing organic synthesis-I
SIPSCHEO42.2	: Designing organic synthesis-II
SIPSCHEO42.3	: Electro-organic chemistry and selected methods of organic synthesis
SIPSCHEO42.4	: Transition and rare earth metals in organic synthesis
Paper III	: Natural products and heterocyclic chemistry
SIPSCHEO43.1	: Natural products-III
SIPSCHEO43.2	: Natural products-IV
SIPSCHEO43.3	: Heterocyclic compounds-I
SIPSCHEO43.4	: Heterocyclic compounds-II
Paper IV	: Intellectual property rights and cheminformatics
SIPSCHEOE-I-44.1	: Introduction to intellectual property
SIPSCHEOE-I-44.2	: Trade secrets
SIPSCHEOE-I-44.3	: Introduction to cheminformatics
SIPSCHEOE-I-44.4	: Applications
Practical	
SIPSCHEO4P1	: Separation of solid-liquid/ liquid-liquid ternary mixture using micro-scale technique
SIPSCHEO4P2	: Identification of any unknown organic compound with preparation, purification and physical constant of derivative. (minimum 8 organic compounds)
SIPSCHEO4P3	: Isolation / estimation of natural products
SIPSCHEO4P4	: Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and mass spectra).

M.Sc. Organic Chemistry Semester-III

Course Code: SIPSCHEO31

Credits: 04

Paper - I Theoretical organic chemistry-I

Learning Objectives:		
<ol style="list-style-type: none"> 1. To learn the reactive intermediates and mechanism in organic synthesis. 2. To study pericyclic reactions and their types with mechanism. 3. To understand the stereochemistry of reactants, intermediates and products. 4. To study various types of photochemical reactions with mechanism. 		
Unit 1	ORGANIC REACTION MECHANISMS	[15L]
1.1	Organic reactive intermediates, methods of generation, structure, stability and important reactions involving carbocations, nitrenes, carbenes, arynes and ketenes.	[5L]
1.2	Neighbouring group participation: Mechanism and effects of anchimeric assistance, NGP by unshared/ lone pair electrons, π -electrons, aromatic rings, σ -bonds with special reference to norbornyl and bicyclo[2.2.2]octyl cation systems (formation of non-classical carbocation)	[3L]
1.3	Role of FMOs in organic reactivity: Reactions involving hard and soft electrophiles and nucleophiles, ambident nucleophiles, ambident electrophiles and α effect.	[2L]
1.4	Pericyclic reactions: Classification of pericyclic reactions; thermal and photochemical reactions. Three approaches: Evidence for the concertedness of bond making and breaking Symmetry-Allowed and Symmetry-Forbidden Reactions – <ul style="list-style-type: none"> • The Woodward-Hoffmann Rules-Class by Class • The generalised Woodward-Hoffmann Rule Explanations for Woodward-Hoffmann Rules <ul style="list-style-type: none"> • The Aromatic Transition structures [Huckel and Mobius] • Frontier Orbitals • Correlation Diagrams, FMO and PMO approach Molecular orbital symmetry, Frontier orbital of ethylene, 1,3 butadiene, 1,3,5 hexatriene and allyl system.	[5L]
Unit 2		
PERICYCLIC REACTIONS		[15L]
2.1	Cycloaddition reactions: Supra and anta facial additions, $4n$ and $4n+2$ systems, $2+2$ additions of ketenes. Diels-Alder reactions, 1, 3-Dipolar cycloaddition and cheletropic reactions, ene reaction, retro-Diels-Alder reaction, regioselectivity, periselectivity, torquoselectivity, site selectivity and effect of substituents in Diels-Alder reactions. Other Cycloaddition Reactions- $[4+6]$ Cycloadditions, Ketene Cycloaddition, Allene Cycloadditions, Carbene Cycloaddition, Epoxidation and Related Cycloadditions. Other Pericyclic reactions: Sigmatropic Rearrangements, Electrocyclic Reactions, Alder 'Ene' Reactions.	[7L]
2.2	Electrocyclic reactions: Conrotatory and disrotatory motions, $4n\pi$ and $[4n+2]\pi$ electron and allyl systems.	[3L]

2.3	Sigmatropic rearrangements: H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations. Cope (including oxy-Cope and aza-Cope) and Claisen rearrangements. Formation of Vitamin D from 7-dehydrocholesterol, synthesis of citral using pericyclic reaction, conversion of Endiandric acid E to Endiandric acid A.	[5L]
Unit 3: STEREOCHEMISTRY-I		
3.1	Classification of point groups based on symmetry elements with examples (nonmathematical treatment).	[2L]
3.2	Conformational analysis of medium rings: Eight to ten membered rings and their unusual properties, I-strain, transannular reactions.	[3L]
3.3	Stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, perhydroanthracenes, steroids, and Bredt's rule.	[5L]
3.4	Anancomeric systems , Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism): electrophilic addition, elimination, molecular rearrangements, reduction of cyclohexanones (with LiAlH₄, selectride and MPV reduction) and oxidation of cyclohexanols.	[5L]
Unit 4 PHOTOCHEMISTRY		
4.1	Principles of photochemistry: quantum yield, electronic states and transitions, selection rules, modes of dissipation of energy (Jablonski diagram), electronic energy transfer: photosensitization and quenching process.	[3L]
4.2	Photochemistry of carbonyl compounds: $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions, Norrish-I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, photochemical rearrangements of α , β -unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction.	[8L]
4.3	Photochemistry of olefins: cis-trans isomerizations, dimerizations, hydrogen abstraction, addition and Di- π -methane rearrangement including aza-di- π -methane. Photochemical Cross-Coupling of Alkenes, Photodimerisation of alkenes.	[2L]
4.4	Photochemistry of arenes: 1, 2-, 1, 3- and 1, 4- additions. Photocycloadditions of aromatic Rings.	[1L]
4.5	Singlet oxygen and photo-oxygenation reactions. Photochemically induced Radical Reactions. Chemiluminescence.	[1L]
REFERENCES:		
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13. Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books, 2006
14. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
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18. Organic reactive intermediates, Samuel P. MacManus, Academic Press.
19. Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers, 1st Edition, Oxford University Press (2001).
20. Organic Chemistry, Seventh Edition, R.T. Morrison, R. N. Boyd & S. K. Bhattacharjee, Pearson. Advanced Organic Chemistry: Reactions & Mechanisms, second edition, B. Miller and R. Prasad, Pearson.
21. Organic reactions & their mechanisms, third revised edition, P.S. Kalsi, New Age International Publishers.
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23. Organic Chemistry, W. G. Solomons, C. B. Fryhle, 9th Edition, Wiley India Pvt. Ltd., 2009.
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25. Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
26. Pericyclic Reactions, S. Sankararaman, Wiley VCH, 2005.
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29. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
30. Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd.
31. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edit
32. Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
33. Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
34. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
35. Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
36. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
37. Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A John Wiley and Sons, Ltd., Publication).

Course Code: SIPSCHEO32

Credits: 04

Paper-II

Synthetic Organic Chemistry-I

Learning Objectives:

1. To learn various name reactions in organic synthesis.
2. To study organic free radical and their importance in organic synthesis.
3. To understand the applications of enamines, ylides and α C-H functionalization in organic synthesis.
4. To know the applications of organometallic compounds in organic synthesis.

Unit 1:	NAME REACTIONS WITH MECHANISM AND APPLICATION	[15L]
1.1	Mukaiyama esterification, Mitsunobu reaction, Darzen's Glycidic Ester synthesis, Ritter reaction, Yamaguchi esterification, Peterson olefination.	[5L]
1.2	Domino reactions: Characteristics; Nazarov cyclization	[3L]
1.3	Multicomponent reactions: Strecker Synthesis, Ugi 4CC, Biginelli synthesis, Hantzsch synthesis, Pictet-Spengler synthesis	[5L]
1.4	Click Reactions: Characteristics, Huisgen 1,3-Dipolar Cycloaddition.	[2L]
Unit 2:	RADICALS IN ORGANIC SYNTHESIS	[15L]
2.1	Introduction: Generation, stability, reactivity structural and stereochemical properties of free radicals, Persistent and charged radicals, Electrophilic and nucleophilic radicals.	[3L]
2.2	Radical Initiators: azobisisobutyronitrile (AIBN) and dibenzoyl peroxide.	[1L]
2.3	Characteristic reactions - Free radical substitution, addition to multiple bonds. Radical chain reactions, radical halogenation of hydrocarbons (Regioselectivity), radical cyclizations, autoxidations: synthesis of cumene hydroperoxide from cumene.	[4L]
2.4	Radicals in synthesis: Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol donors. Cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds. Oxidative coupling, C-C bond formation in aromatics: S _N Ar reactions.	[4L]
2.5	Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Sandmeyer reaction, Acyloin condensation.	[3L]
Unit 3:	ENAMINES, YLIDES AND α-C-H FUNCTIONALIZATION	[15]
3.1	Enamines: Generation and application in organic synthesis with mechanistic pathways, Stork enamine reaction. Reactivity, comparison between enamines and enolates. Synthetic reactions of enamines including asymmetric reactions of chiral enamines derived from chiral secondary amines.	[4L]
3.2	Phosphorus, Sulfur and Nitrogen Ylides: Preparation and their synthetic applications along with their stereochemical aspects. Wittig reaction, Horner-Wadsworth-Emmons Reaction, Barton-Kellogg olefination.	[6L]
3.3	α-C-H functionalization: By nitro, sulfoxide, sulfone and phosphonate groups: generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. Bamford-Stevens reaction, Julia olefination and its modification, Seyferth-Gilbert homologation, Steven's rearrangement.	[5L]
Unit 4:	METALS / NON-METALS IN ORGANIC SYNTHESIS	[15]
4.1	Mercury in organic synthesis: Mechanism and regiochemistry of oxymercuration and demercuration of alkenes, mercuration of aromatics, transformation of aryl mercurials to aryl halides. Organomercurials as carbene transfer reagents.	[3L]
4.2	Organoboron compounds: Mechanism and regiochemistry of hydroboration of alkenes and alkynes, asymmetric hydroboration using chiral boron reagents, 9-BBN hydroboration, oxazaborolidine (CBS catalyst) and functional group reduction by diborane.	[3L]
4.3	Organosilicons: Salient features of silicon governing the reactivity of organosilicons, preparation and important bond-forming reactions of alkyl silanes, alkenyl silanes, aryl silanes and allyl silanes. β -silyl cations as intermediates. Iodotrimethylsilane in organic synthesis.	[3L]

4.4	Silyl enol ethers: Application: As nucleophiles (Michael reaction, Mukaiyama aldol reaction), in ring contraction reactions.	[2L]
4.5	Organotin compounds: Preparation of alkenyl and allyl tin compounds; application in C-C bond formation, in replacement of halogen by H at the same C atom.	[2L]
4.6	Selenium in organic synthesis: Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and seleno acetals as α -C-H activating groups.	[2L]
REFERENCES:		
<ol style="list-style-type: none"> Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer Verlag Modern Methods of Organic Synthesis, 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004. Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam. Organic Chemistry, Clayden Greeves Warren and Wothers, Oxford Press (2001). Moder Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007). Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002). Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3rd Edn., Nelson Thornes Organic Chemistry, 7th Edn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson Strategic Applications of Name Reactions in Organic Synthesis, L. Kurti & B. Czako (2005), Elsevier Academic Press Advanced Organic Chemistry: Reactions & Mechanisms, 2nd Edn., B. Miller & R. Prasad, Pearson Organic reactions and their mechanisms, 3rd revised edition, P.S. Kalsi, New Age International Publishers Organic Synthesis: The Disconnection Approach, Stuart Warren, John Wiley & Sons, 2004 Name Reactions and Reagents in Organic Synthesis, 2nd Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience Name Reactions, Jie Jack Lie, 3rd Edn., Springer Organic Electrochemistry, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker. 		
Course Code: SIPSCHEO33 Credits: 04 Paper-III Natural products and Spectroscopy		
Learning Objectives:		
<ol style="list-style-type: none"> To learn the basic concepts involved in natural products. To study the multi-step synthesis of various natural products. To learn the advance spectroscopic technique for analysis of organic compound. To understand advance instrumental techniques for compound interpretation and identification. 		
Unit 1:	NATURAL PRODUCTS-I	[15L]
1.1	Carbohydrates: Introduction to naturally occurring sugars: Deoxysugars, aminosugars, branched sugars. Structure elucidation of lactose and D-glucosamine (synthesis not expected). Structural features and applications of inositol, starch, cellulose, chitin and heparin.	[5L]
1.2	Natural pigments: General structural features, occurrence, biological importance and applications of: carotenoids, anthocyanins, quinones, flavones, pterins and porphyrins (chlorophyll). Structure elucidation of β -carotene and Cyanin (with synthesis). Synthesis of ubiquinone from 3, 4, 5-trimethoxyacetophenone.	[5L]
1.3	Insect pheromones: General structural features and importance. Types of pheromones (aggregation, alarm, releaser, primer, territorial, trail, sex	[3L]

	pheromones etc.), advantage of pheromones over conventional pesticides. Synthesis of bombykol from acetylene, disparlure from 6-methylhept-1-ene, grandisol from 2-methyl-1, 3-butadiene.	
1.4	Alkaloids: Occurrence and physiological importance of morphine and atropine. Structure elucidation, spectral data and synthesis of coniine.	[2L]
Unit 2:	NATURAL PRODUCTS-II	[15L]
2.1	Multi-step synthesis of natural products: Synthesis of the following natural products with special reference to reagents used, stereochemistry and functional group transformations:	[8L]
	a) Woodward synthesis of Reserpine from benzoquinone	
	b) Corey synthesis of Longifoline from resorcinol	
	c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol	
	d) Corey's Synthesis of Caryophyllene from 2-Cyclohexenone and Isobutylene	
	e) Synthesis of Juvabione from Limonene	
	f) Synthesis of Taxol.	
2.2	Prostaglandins: Classification, general structure and biological importance. Structure elucidation of PGE ₁ .	[2L]
2.3	Lipids: Classification, role of lipids, Fatty acids and glycerol derived from oils and fats.	[2L]
2.4	Insect growth regulators: General idea, structures of JH ₂ and JH ₃ .	[1L]
2.5	Plant growth regulators: Structural features and applications of arylacetic acids, gibberellic acids and triacontanol. Synthesis of triacontanol (synthesis of stearyl magnesium bromide and 12-bromo-1 tetrahydropyranoyloxidodecane expected).	[2L]
Unit 3:	ADVANCED SPECTROSCOPIC TECHNIQUES-I	[15L]
3.1	Proton NMR spectroscopy: Recapitulation, chemical and magnetic equivalence of protons, first order, second order, Spin system notations (A ₂ , AB, AX, AB ₂ , AX ₂ , AMX and A ₂ B ₂ -A ₂ X ₂ spin systems with suitable examples). Long range coupling (Allylic coupling, 'W' coupling and Coupling in aromatic and heteroaromatic systems), Temperature effects, Simplification of complex spectra, nuclear magnetic double resonance, chemical shift reagents.	[7L]
3.2	¹³C –NMR spectroscopy: Recapitulation, equivalent and non-equivalent carbons (examples of aliphatic and aromatic compounds), ¹³ C- chemical shifts, calculation of ¹³ C- chemical shifts of aromatic carbons, heteronuclear coupling of carbon to ¹⁹ F and ³¹ P.	[4L]
3.3	Spectral problems based on UV, IR, ¹ HNMR and ¹³ CNMR and Mass spectroscopy.	[4L]
Unit 4:	ADVANCED SPECTROSCOPIC TECHNIQUES-II	[15L]
4.1	Advanced NMR techniques: DEPT experiment, determining number of attached hydrogens (Methyl/methylene/methine and quaternary carbons), two dimensional spectroscopic techniques, COSY and HETCOR spectra, NOE, NOESY and ROESY techniques.	[10L]
4.2	Spectral problems based on UV, IR, ¹ HNMR, ¹³ CNMR (Including 2D technique) and Mass spectroscopy	[5L]
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13. Natural Products: Chemistry and Biological Significance Interscience, J. Mann, R.S.Davidson, J.B.Hobbs, D.V. Banthrope and J. B. Harborne, Longman,Essex, 1994.
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20. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.
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27. Synthesis of (±)-4-demethoxydaunomycinone, A. V. Rama Rao , G. Venkatswamy , S. M. Javeed M. , V. H. Deshpande, B. Ramamohan Rao, J. Org. Chem., 1983, 48 (9), 1552.
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30. Medicinal Natural Products, a Biosynthetic Approach, Derick Paul, John Wiley and Sons, 2002.
31. Biosynthesis of Natural Products, Mannitto Paolo, Ellis Horwood Limited, 1981.
32. Selected Organic synthesis, Ian Fleming, John Wiley and Sons, 1973.
33. Total synthesis of Natural Products, J. Apsimon, John Wiley and Sons.
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35. Classics in Total Synthesis, K. C. Nicolaou and E. J. Sorensen, Weinheim: VCH, 1996.
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39. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974.
40. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989.
41. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987.
42. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4 th ed., .2011
43. Introduction to spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, 4 th ed., 2009.
44. Organic spectroscopic structure determination: a problem-based learning approach Douglass F. Taber, Oxford University Press, 17-Sep-2007.
45. Organic Spectroscopy: Principles And Applications, Jag Mohan, Alpha Science International Ltd., 30-Mar-2004
46. Alkaloids, V.K. Ahluwalia, Ane Books Pvt. Ltd.
47. Biotransformations in Organic Chemistry, 5 th Edition, Kurt Faber, Springer
48. Structure Determination of Organic Compounds, E. Pretsch, P. Buhlmann, C. Affolter, Springer.
Course Code: SIPSCHEOE-I-34 Credits: 04 Paper-IV Medicinal , Biogenesis and green chemistry
Learning Objectives: 1. <i>To learn the basic terminology involved in medicinal organic chemistry.</i> 2. <i>To study quantitative structure activity relationship in drug discovery, designing.</i> 3. <i>To learn primary and secondary metabolites and their importance in biogenesis.</i> 4. <i>To learn basic principles of green chemistry and its applications.</i>
Unit 1: DRUG DISCOVERY, DESIGN AND DEVELOPMENT [15L]
1.1 Introduction, important terms used in medicinal chemistry: receptor, therapeutic index, bioavailability, drug assay and drug potency. General idea of factors affecting bioactivity: Resonance, inductive effect, bioisosterism, spatial considerations. Basic pharmacokinetics: drug absorption, distribution, metabolism (biotransformation) and elimination. Physical and chemical parameters like solubility, lipophilicity, ionization, pH, redox potential, H-bonding, partition coefficient and isomerism in drug distribution and drug-receptor binding. [7L]
1.2 Procedures in drug design: Drug discovery without a lead: Penicillin, Librium. Lead discovery: random screening, non-random (or targeted) screening. Lead modification: Identification of the pharmacophore, Functional group modification. Structure-activity relationship, Structure modification to increase potency and therapeutic index: Homologation, chain branching, ring-chain transformation, bioisosterism, combinatorial synthesis (basic idea). [8L]
Unit 2: DRUG DESIGN, DEVELOPMENT AND SYNTHESIS [15L]
2.1 Introduction to quantitative structure activity relationship studies. QSAR parameters: - steric effects: The Taft and other equations; Methods used to correlate regression parameters with biological activity: Hansch analysis- A linear multiple regression analysis. [5L]

2.2	Introduction to modern methods of drug design and synthesis- computer-aided molecular graphics based drug design, drug design via enzyme inhibition (reversible and irreversible), bioinformatics and drug design.	[3L]
2.3	Concept of prodrugs and soft drugs. (a) Prodrugs: Prodrug design, types of prodrugs, functional groups in prodrugs, advantages of prodrug use. (b) Soft drugs: concept and properties.	[3L]
2.4	Synthesis and application of the following drugs: Fluoxetine, cetirizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate.	[4L]
Unit 3: BIOGENESIS AND BIOSYNTHESIS OF NATURAL PRODUCTS		[15L]
3.1	Primary and secondary metabolites and the building blocks, general pathway of amino acid biosynthesis.	[3L]
3.2	Acetate pathway: Biosynthesis of malonylCoA, saturated fatty acids, prostaglandins from arachidonic acid, aromatic polyketides.	[4L]
3.3	Shikimic Acid pathway: Biosynthesis of shikimic acid, aromatic amino acids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, flavonoids and isoflavonoids.	[4L]
3.4	Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes – geranyl cation and its derivatives, sesquiterpenes – farnesyl cation and its derivatives and diterpenes.	[4L]
Unit 4: GREEN CHEMISTRY		[15L]
4.1	Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts.	[1L]
4.2	Use of the following in green synthesis with suitable examples:	[9L]
	a) Green reagents: dimethylcarbonate, polymer supported reagents.	
	b) Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts [Aliquot 336, benzyltrimethyl ammonium chloride (TMBA), Tetra-n-butyl ammonium chloride, crown ethers], biocatalysts.	
	c) Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide.	
	d) Solid state reactions: solid phase synthesis, solid supported synthesis	
	e) Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions.	
	f) Ultrasound assisted reactions.	
4.3	Comparison of traditional processes versus green processes in the syntheses of ibuprofen, adipic acid, 4-aminodiphenylamine, p-bromotoluene and benzimidazole.	[3L]
4.4	Green Catalysts: Nanocatalyst, Types of nanocatalysts, Advantages and Disadvantages of nanocatalysts, Idea of Magnetically separable nanocatalysts.	[2L]
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1. Nelson, D. L, and Cox, M. M, (2008) Lehninger principles of Biochemistry 5 th Edition, W. H. Freeman and Company, NY., USA.		
2. Stryer, Lubert; Biochemistry; W. H. Freeman publishers.		
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26. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
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37. Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House.
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39. Chemistry of Natural Products, F. F. Bentley and F. R. Dollish, 1974.
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43. Organic synthesis in water. By Paul A. Grieco, Blackie.

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Course Code: SIPSCHEOE-II-34		Credits: 04
Paper-IV		
Bioorganic chemistry		
Learning Objectives:		
1. To know the biomolecules, their structure and importance in life. 2. To study organic biomolecular synthesis and metabolic reaction pathways. 3. To learn the importance of enzymes and co-enzymes in biological system.		
Unit 1:	BIOMOLECULES-I	[15L]
1.1	Amino acids, peptides and proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, α -helix, β -sheets, super secondary structure. Tertiary structure of protein: folding and domain structure. Quaternary structure.	[2L]
1.2	Nucleic acids: Structure and function of physiologically important nucleotides (c-AMP, ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation.	[3L]
1.3	Structure: Purine and pyrimidine bases, ribose, deoxyribose, nucleosides and nucleotides (ATP, CTP, GTP, TTP, UTP) formation of polynucleotides strand with its shorthand representation.	[3L]
1.4	RNAs (various types in prokaryotes and eukaryotes) m- RNA and r- RNA – general account , t- RNA-clover leaf model, Ribozymes.	[2L]
1.5	DNA: Physical properties – Effect of heat on physical properties of DNA (Viscosity, buoyant density and UV absorption), Hypochromism, Hyperchromism and Denaturation of DNA. Reactions of nucleic acids (with DPA and Orcinol).	[2L]
1.6	Chemical synthesis of oligonucleotides: Phosphodiester, Phosphotriester, Phosphoramidite and H- phosphonate methods including solid phase approach.	[3L]
Unit 2:	BIOMOLECULES-II	[15L]
2.1	Chemistry of enzymes: Introduction, nomenclature, classes and general types of reactions catalyzed by enzymes. Properties of enzymes: a) enzyme efficiency/ catalytic power b) enzyme specificity; Fischer's 'lock and key' and Koshland 'induced fit' hypothesis. Concept and identification of active site.	[6L]
2.2	Factors affecting enzyme kinetics: Substrate concentration, enzyme concentration, temperature, pH, product concentration etc. Reversible and irreversible inhibition.	[4L]
2.3	Mechanism of enzyme action: transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Mechanism of chymotrypsin catalyzed hydrolysis of a peptide bond.	[5L]
Unit 3:	BIOMOLECULES - III	[15L]
3.1	Chemistry of coenzymes. Structure, mechanism of action and bio-modeling studies of the following coenzymes: nicotinamide adenine dinucleotide,	[12L]

	flavin adenine dinucleotide, thiamine pyrophosphate, pyridoxal phosphate, Vitamin B12, biotin, lipoic acid, Coenzyme A.	
3.2	Oxidative phosphorylation, chemiosmosis, rotary model for ATP synthesis and role of cytochrome in oxygen activation.	[3L]
Unit 4:	BIOMOLECULES – IV	[15L]
4.1	Role of main enzymes involved in the synthesis and breakdown of glycogen.	[2L]
4.2	Enzyme catalyzed organic reactions: Hydrolysis, hydroxylation, oxidation and reduction.	[6L]
4.3	Enzymes in organic synthesis. Fermentation: Production of drugs/drug intermediates by fermentation. Production of chiral hydroxy acids, vitamins, amino acids, β -lactam antibiotics. Synthesis of chemicals via microbial transformation, synthesis of L-ephedrine. Chemical processes with isolated enzymes in free form (hydrocyanation of m-phenoxybenzaldehyde) and immobilized form (production of 6-aminopenicillanic acid).	[7L]

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1. Nelson, D. L, and Cox, M. M, (2008) Lehninger principles of Biochemistry 5th Edition, W. H. Freeman and Company, NY., USA.
2. Stryer, Lubert; Biochemistry; W. H. Freeman publishers.
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25. Biochemistry, Dr U Satyanarayan and Dr U Chakrapani, Books and Allied (P) Ltd.

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27. The Organic Chemistry of Enzyme-Catalysed Reactions, Academic Press, By Richard B. Silverman
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37. Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House.
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46. An introduction to green chemistry, V. Kumar, Vishal Publishing Co.
47. Organic synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

Course Code: SIPSCHEO3P1

Credits: 02

Practical

Paper-I

Learning Objectives:

1. To learn separation techniques of ternary mixture.
2. To identify the organic compounds and to prepare their respective derivatives.

SEPARATION OF A SOLID TERNARY MIXTURE USING MICRO-SCALE TECHNIQUE

1. Separation of solid components of a ternary mixture (water insoluble/soluble including carbohydrates) based upon differences in the physical and the chemical properties of the components.
2. Purification of the three components, measurement of their mass and determination of their physical constants.
3. Calculation of percentage yields of the individual components. (Identification of the components is not expected).

Course Code: SIPSCHEO3P2

Credits: 02

Practical

Paper-II		
Learning Objectives:		
<ol style="list-style-type: none"> 1. To estimate the actual quantity of the biologically active compound in the drugs. 2. To know the importance of spectrophotometer in quantitative analysis. 		
ESTIMATION OF DRUGS		
<ol style="list-style-type: none"> 1. Estimation of penicillin by iodometric titrations. 2. Estimation of streptomycin using uv-visible spectrophotometer. 3. Estimation of paracetamol by hydrolysis. 4. Estimation of aspirin in the given tablet using uv-visible spectrophotometer. 5. Estimation of diazepam by non-aqueous titrations. 6. Estimation of vitamin C by iodometric titrations. 		
Course Code: SIPSCHEO3P3		
Credits: 02	Paper-III	Practical
Learning Objectives:		
<ol style="list-style-type: none"> 1. To implement various organic reactions in synthetic organic chemistry. 2. To study the planning and purification techniques involved in organic synthesis. 		
ORGANIC PREPARATIONS (1.0 G SCALE)		
<ol style="list-style-type: none"> 1. Benzilic acid rearrangement: Benzilic acid from benzil 2. Sandmeyer reaction: p-Nitroiodobenzene from p-nitroaniline 3. Heterocyclic compound: 7-Hydroxy-4-methylcoumarin from resorcinol 4. Acetylation: Mannitol hexaacetate from mannitol 5. Claisen-Schmidt reaction: Dibenzalacetone from benzaldehyde 6. Oxidation: Fluorenone from fluorene 7. Acetylation: Acetylferrocene from ferrocene 		
Note:		
<p>Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.</p> <p>Students are expected to purify the product by Steam distillation / Vacuum distillation or Column chromatography, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.</p>		
Course Code: SIPSCHEO3P4		
Credits: 02	Paper-IV	Practical
Learning Objectives:		
<ol style="list-style-type: none"> 1. To know greener techniques (microwave oven) for organic compound synthesis. 		
SINGLE STEP ORGANIC PREPARATION (1.0 G SCALE) INVOLVING Techniques of purification and green methods of synthesis		
Set I: Techniques of purification:		
<ol style="list-style-type: none"> 1. Steam distillation 2. Vacuum distillation 3. Column chromatography 		
Set II: Green methods of synthesis (microwave induced)		
<ol style="list-style-type: none"> 1. Synthesis of Schiff's base from aniline and p-anisaldehyde in the presence of lime juice 2. Synthesis of coumarin by Knoevenagel reaction using salicylaldehyde, and ethyl acetoacetate in presence of a base. 		

3. Synthesis of dihydropyrimidones- Biginelli reaction: acid-catalyzed three component reaction between vanillin, ethyl acetoacetate and thiourea.
4. Synthesis of acetanilide from aniline.

Learning points:

Set I: Techniques of purification

1. Students are expected to perform a purification technique using a known mass or volume of the given substance.
2. Check the purity of the purified compound by TLC, measure its mass and physical constant.

Set II: Green methods of synthesis (Microwave induced)

Students are expected to purify the product by recrystallization, measure its mass, determine physical constant and calculate percentage yield.

References for Practicals:

1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
3. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
4. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
5. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
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8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
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12. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011.

Note:

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

Semester-IV

Course Code: SIPSCHEO41

Credits: 04

Paper - I

Theoretical organic chemistry-II

Learning Objectives:

1. To learn physical organic chemistry aspects (structural effects and reactivity) for organic chemistry.
2. To study supramolecular chemistry and its applications in organic synthesis
3. To understand the stereo-chemical aspects and its applications in organic synthesis
4. To study principles of asymmetric synthesis and chiral auxiliaries in asymmetric synthesis.

Unit 1:	PHYSICAL ORGANIC CHEMISTRY	[15L]
1.1	Structural effects and reactivity: Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation, substituent constants, theories of substituent effects, interpretation of σ -values, reaction constants ρ , Yukawa-Tsuno equation.	[7L]
1.2	Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants. The Taft model, σ_1 and σ_R scales, steric parameters E_s and β . Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's E_T parameter, Solvatochromism Z-scale, Spectroscopic Correlations, Thermodynamic Implications.	[8L]
Unit 2	SUPRAMOLECULAR CHEMISTRY	[15L]
2.1	Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes.	[3L]
2.2	Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.	[3L]
2.3	Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.	[5L]
2.4	Molecular recognition and catalysis, molecular self-assembly. Supramolecular Polymers, Gels and Fibres.	[4L]
Unit 3	STEREOCHEMISTRY - II	[15L]
3.1	Racemisation and resolution of racemates including conglomerates: Mechanism of racemisation, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds.	[3L]
3.2	Determination of enantiomer and diastereomer composition: enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR).	[3L]
3.3	Correlative method for configurational assignment: chemical, optical rotation and NMR spectroscopy.	[4L]
3.4	Molecular dissymmetry and chiroptical properties: Linearly and circularly polarized light. Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. The octant rule and the axial α -haloketone rule with applications.	[5L]
Unit 4:	ASYMMETRIC SYNTHESIS	[15L]
4.1	Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions.	[3L]
4.2	Synthesis of L-DOPA [Knowles's Monsanto process]. Asymmetric reactions with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharpless enantioselective epoxidation, hydroxylation, aminohydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.	[9L]
4.3	Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations.	[3L]

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2. A guide to mechanism in Organic Chemistry, 6th edition, 2009, Peter Sykes, Pearson education, New Delhi.
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8. Carbenes, Nitrenes and Arynes. Von T. L. Gilchrist, C. W. Rees. Th. Nelson and Sons Ltd., London 1969.
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21. Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books, 2006
22. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
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29. Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
30. Large ring compounds, J.A. Semlyen, Wiley-VCH, 1997.
31. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley- Eastern
32. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
33. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
34. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill

35. Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
 36. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
 37. Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A John Wiley and Sons, Ltd., Publication)

Course Code: SIPSCHEO42

Credits: 04

Paper - II

Synthetic organic chemistry-II

Learning Objectives:

1. To learn the synthetic planning and designing in various organic synthesis.
2. To understand the methodology, basics, and applications of electro-organic chemistry.
3. To study applications of organometallics (transition and rare earth elements) in organic synthesis.

Unit 1:	DESIGNING ORGANIC SYNTHESIS-I	[15L]
1.1	Protecting groups in Organic Synthesis: Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications.	[3L]
1.2	Concept of umpolung (Reversal of polarity): Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.	[3L]
1.3	Introduction to Retrosynthetic analysis and synthetic planning: Linear and convergent synthesis; Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions (FGI), functional group addition (FGA), functional group removal (FGR) importance of order of events in organic synthesis, one and two group C-X disconnections (1,1; 1,2; 1,3 difunctionalized compounds), selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enantioselectivity.	[9L]
Unit 2:	DESIGNING ORGANIC SYNTHESIS-II	[15L]
2.1	General strategy: Choosing a disconnection-simplification, symmetry, high yielding steps and recognisable starting material.	[3L]
2.2	One group C-C Disconnections: Alcohols (including stereoselectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.	[6L]
2.3	Two group C-C Disconnections: 1,2- 1,3- 1,4- 1,5- and 1,6-difunctionalized compounds, Diels-Alder reactions, α , β -unsaturated compounds, control in carbonyl condensations, Michael addition and Robinson annulation.	[6L]
Unit 3:	ELECTRO-ORGANIC CHEMISTRY AND SELECTED METHODS OF ORGANIC SYNTHESIS	[15L]
3.1	Electro-organic chemistry:	[7L]
3.1.1	Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes.	
3.1.2	Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitro compounds, olefins, arenes, electro-dimerization.	
3.1.3	Anodic oxidation: Oxidation of alkylbenzene, Kolbe reaction, Non-Kolbe oxidation, Shono oxidation.	
3.2	Selected Methods of Organic synthesis	[8L]
	Applications of the following in organic synthesis:	
3.2.1	Crown ethers, cryptands, micelles, cyclodextrins, catenanes.	

3.2.2	Organocatalysts: Proline, Imidazolidinone.	
3.2.3	Pd catalysed cycloaddition reactions: Stille reaction, Saeguse-Ito oxidation to enones, Negishi coupling.	
3.2.4	Use of Sc(OTf), and Yb(OTf) as water tolerant Lewis acid catalyst in aldol condensation, Michael reaction, Diels-Alder reaction, Friedel – Crafts reaction.	
Unit 4:	TRANSITION AND RARE EARTH METALS IN ORGANIC SYNTHESIS	[15L]
4.1	Introduction to basic concepts: 18 electron rule, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion.	[3L]
4.2	Palladium in organic synthesis: π -bonding of Pd with olefins, applications in C-C bond formation, carbonylation, alkene isomerisation, cross-coupling of organometallics and halides. Representative examples: Heck reaction, Suzuki-Miyaura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N, S or P atoms.	[5L]
4.3	Olefin metathesis using Grubb's catalyst.	[1L]
4.4	Application of Ni, Co, Fe, Rh, and Cr carbonyls in organic synthesis.	[4L]
4.5	Application of samarium iodide including reduction of organic halides, aldehydes and ketones, α -functionalised carbonyl and nitro compounds.	[1L]
4.6	Application of Ce (IV) in synthesis of heterocyclic quinoxaline derivatives and its role as a de-protecting agent.	[1L]
<p>REFERENCES:</p> <ol style="list-style-type: none"> Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer Verlag Modern Methods of Organic Synthesis, 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004. Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam. Organic Chemistry, Clayden Greeves Warren and Wothers, Oxford Press (2001). Moder Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007). Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002). Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3rd Edn., Nelson Thornes Organic Chemistry, 7th Edn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson Strategic Applications of Name Reactions in Organic Synthesis, L. Kurti & B. Czako (2005), Elsevier Academic Press Advanced Organic Chemistry: Reactions & Mechanisms, 2nd Edn., B. Miller & R. Prasad, Pearson Organic reactions and their mechanisms, 3rd revised edition, P.S. Kalsi, New Age International Publishers Organic Synthesis: The Disconnection Approach, Stuart Warren, John Wiley & Sons, 2004 Name Reactions and Reagents in Organic Synthesis, 2nd Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience Name Reactions, Jie Jack Lie, 3rd Edn., Springer Organic Electrochemistry, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker. 		
<p>Course Code: SIPSCHEO43 Credits: 04</p> <p>Paper - III</p> <p>Natural products and heterocyclic chemistry</p>		

Learning Objectives:		
1. To learn the importance of steroids, vitamins and terpenoids in natural products.		
2. To study the heterocyclic chemistry (3-6 membered rings) and their applications in organic synthesis.		
Unit 1:	NATURAL PRODUCTS-III	[15L]
1.1	Steroids: General structure, classification. Occurrence, biological role, important structural and stereochemical features of the following: corticosteroids, steroidal hormones, steroidal alkaloids, sterols and bile acid	[5L]
1.2	Synthesis of 16-DPA from cholesterol and plant sapogenin.	[2L]
1.3	Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone.	[5L]
1.4	Synthesis of cinerolone, jasmolone, allethrolone, exaltone and muscone.	[3L]
Unit 2:	NATURAL PRODUCTS-IV	[15L]
2.1	Vitamins: Classification, sources and biological importance of vitamin B ₁ , B ₂ , B ₆ , folic acid, B ₁₂ , C, D ₁ , E (α -tocopherol), K ₁ , K ₂ , H (β - biotin).	[5L]
	Synthesis of the following:	
	Vitamin A from β -ionone and bromoester moiety.	
	Vitamin B ₁ including synthesis of pyrimidine and thiazole moieties	
	Vitamin B ₂ from 3, 4-dimethylaniline and D(-)ribose	
	Vitamin B ₆ from: 1) ethoxyacetylacetone and cyanoacetamide, 2) ethyl ester of N-formyl-DL-alanine (Harris synthesis)	
	Vitamin E (α -tocopherol) from trimethylquinol and phytol bromide	
	Vitamin K ₁ from 2-methyl-1, 4-naphthaquinone and phytol.	
2.2	Antibiotics: Classification on the basis of activity. Structure elucidation, spectral data of penicillin-G, cephalosporin-C and chloramphenicol. Synthesis of chloramphenicol (from benzaldehyde and β -nitroethanol) penicillin-G and phenoxymethylpenicillin from D-penicillamine and t-butyl phthalimide malonaldehyde (synthesis of D-penicillamine and t-butyl phthalimide malonaldehyde expected).	[6L]
2.3	Naturally occurring insecticides: Sources, structure and biological properties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis of pyrethrin I.	[2L]
2.4	Terpenoids: Occurrence, classification, structure elucidation, stereochemistry, spectral data and synthesis of zingiberene.	[2L]
Unit 3:	HETEROCYCLIC COMPOUNDS-I	[15L]
	Heterocyclic compounds: Introduction, classification, Nomenclature of heterocyclic compounds of monocyclic (3-6 membered) (Common, systematic (Hantzsch-Widman) and replacement nomenclature)	
	Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyridazines, pyrimidine, pyrazines and oxazines.	
Unit 4:	HETEROCYCLIC COMPOUNDS-II	[15L]
	Nomenclature of heterocyclic compounds of bicyclic/tricyclic (5-6 Membered) fused heterocycles (up to three hetero atoms). (Common, systematic (Hantzsch-Widman) and replacement nomenclature)	
	Nucleophilic ring opening reactions of oxiranes, aziridines, oxetanes and azetidines.	

Structure, reactivity, synthesis and reactions of coumarins, quinoxalines, cinnolines, indole, benzimidazoles, benzoxazoles, benzothiazoles, Purines and acridines.	
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2. Natural products chemistry and applications, Sujata V. Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House, 2011.
3. Organic Chemistry Natural Products Volume-II, O. P. Agarwal, Krishna Prakashan, 2011.
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6. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co. 2008.
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12. An Introduction to the Chemistry of Heterocyclic Compounds, 2nd edition, B.M. Acheson, 1975.
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18. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers, 1998.
19. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers, 1998.
20. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.
21. Total. Synthesis of Longifolene, J. Am. Chem. Soc., E. J. Corey, M. Ohno, R. B. Mitra, and P. A. Vatakencherry. 1964, 86, 478.
22. Total. Synthesis of Longifolene, J. Am. Chem. Soc. 1961, 83, 1251.
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33. Total synthesis of Natural Products, J. Apsimon, John Wiley and Sons.

34. The Logic of Chemical Synthesis, E. J. Corey and Xue-Min Cheng, Wiley Interscience.
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48. Structure Determination of Organic Compounds, E Pretsch, P. Buhlmann, C. Affolter, Springer

Course Code: SIPSCHEOE-I-44

Credits: 04

Paper-IV

Intellectual property rights and cheminformatics

Learning Objectives:

1. To learn various terms and terminology involved in intellectual property rights
2. To study trade secrets and economic value of intellectual property.
3. To know the evolution of cheminformatics and its application.

Unit 1:	Introduction to Intellectual Property	[15L]
1.1	Introduction to Intellectual Property: Historical Perspective, Different types of IP, Importance of protecting IP.	[2L]
1.2	Patents: Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.	[5L]
1.3	Industrial Designs: Definition, how to obtain, features, International design registration.	[2L]
1.4	Copyrights: Introduction, how to obtain, Differences from Patents.	[2L]
1.5	Trade Marks Introduction, how to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.	[2L]
1.6	Geographical Indications Definition, rules for registration, prevention of illegal exploitation, importance to India.	[2L]
Unit 2:	Trade Secrets	[15L]

2.1	Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.	[2L]
2.2	IP Infringement issue and enforcement: Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.	[2L]
2.3	Economic Value of Intellectual Property: Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.	[2L]
2.4	Different International agreements: a) World Trade Organization (WTO): i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement ii) General Agreement on Trade Related Services (GATS) Madrid Protocol. iii) Berne Convention. iv) Budapest Treaty.	[5L]
	b) Paris Convention	[6L]
2.5	WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity.	
Unit III:	Cheminformatics	[15L]
3.1	Introduction to Cheminformatics: History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.	[5L]
3.2	Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.	[5L]
3.3	Searching Chemical Structures: Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.	[5L]
Unit IV:	APPLICATIONS: Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-based and Structure based Drug design, Application of Cheminformatics in Drug Design.	[15L]
REFERENCES:		
1. Andrew R. Leach & Valerie J. Gillet (2007) <i>An Introduction to Cheminformatics</i> . Springer: The Netherlands.		
2. Gasteiger, J. & Engel, T. (2003) <i>Cheminformatics: A textbook</i> . Wiley–VCH		
3. Gupta, S. P. <i>QSAR and Molecular Modeling</i> . Springer-Anamaya Pub.: New Delhi.		
Course Code: SIPSCHEOE-II-44 Credits: 04		
Paper-IV		
Research Methodology		
Learning Objectives:		
1. To learn research methodology for research data analysis and scientific writing.		
2. To study the chemical safety and ethical handling of chemicals.		
3. To learn the writing skills in scientific research project/ practical work.		

Unit 1:	SOURCES	[15L]
1.1	Print	[5L]
	Primary, Secondary and Tertiary sources.	
1.2	Journals:	
	Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.	
1.3	Digital:	[5L]
	Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus.	
1.4	Information Technology and Library Resources:	[5L]
	The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.	
Unit II:	DATA ANALYSIS	[15L]
2.1	The Investigative Approach:	
	Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.	
2.2	Analysis and Presentation of Data:	
	Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis.	
Unit III:	METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS	[15L]
	Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.	
3.1	Writing Scientific Papers:	
	Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.	
Unit IV:	CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS	[15L]
	Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressure, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.	
REFERENCES:		

<ol style="list-style-type: none"> 1. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press. OSU Safety manual 1.01 2. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), <i>Practical skills in Chemistry</i>, 2nd Ed., Prentice Hall, Harlow. 3. Hibbert, D. B. & Gooding, J. J. (2006) <i>Data Analysis for Chemistry</i> Oxford University Press. 4. Harris, D. C. (2007) <i>Quantative Chemical Analysis</i> 6th Ed., Freeman Chapters 3-5 5. Levie, R. De. (2001) <i>How to use Excel in Analytical Chemistry and in general scientific data analysis</i> Cambridge Universty Press. 6. Topping, J., (1984) <i>Errors of Observation and their Treatment</i> 4th Ed., Chapman Hill, London.
Course Code: SIPSCHEO4P1 Credits: 02 Practical Paper-I
Learning Objectives: <ol style="list-style-type: none"> 1. To learn separation techniques and miscibility criteria of ternary mixture. 2. To identify the organic compounds and to prepare their respective derivatives.
SEPARATION OF SOLID-LIQUID/ LIQUID-LIQUID TERNARY MIXTURE USING MICRO-SCALE TECHNIQUE <ol style="list-style-type: none"> 1. Separation of components of ternary mixtures (solid-liquid or liquid-liquid) based upon differences in the physical and the chemical properties of the components. 2. Purification of the three components, measurement of their mass and determination of their physical constants. 3. Calculation of percentage yield of the individual components. (Identification of the components is not expected). (Minimum 6 experiments)
Course Code: SIPSCHEO4P2 Credits: 02 Practical Paper-II
Learning Objectives: <ol style="list-style-type: none"> 1. To learn the solubility and miscibility criteria for identification of unknown organic compounds.
IDENTIFICATION OF ANY UNKNOWN ORGANIC COMPOUND WITH PREPARATION, PURIFICATION AND PHYSICAL CONSTANT OF DERIVATIVE. (MINIMUM 8 ORGANIC COMPOUNDS) (Minimum 8 experiments)
Course Code: SIPSCHEO4P3 Credits: 02 Practical Paper-III
Learning Objectives: <ol style="list-style-type: none"> 1. To learn isolation/extraction of biologically active ingredients in natural products by qualitative methods.
ISOLATION / ESTIMATION OF NATURAL PRODUCTS <ol style="list-style-type: none"> 1. Extraction of clove oil from cloves. 2. Extraction of nicotine dipicrate from tobacco. 3. Estimation of proteins by Biuret method using spectrophotometer. 4. Estimation of glucose by Folin Wu method. 5. Estimation of citral using hydroxylamine hydrochloride. 6. Estimation of saponification value of oil.
Course Code: SIPSCHEO4P4 Credits: 02 Practical

Paper-IV

Learning Objectives:

1. To learn the interpretation of the organic compounds by various spectroscopic techniques (UV, IR, PMR, CMR and Mass spectra).

INTERPRETATION OF SPECTRAL DATA OF ORGANIC COMPOUNDS (UV, IR, PMR, CMR AND MASS SPECTRA).

Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and Mass spectra). A student will be given UV, IR, PMR, CMR, and Mass spectra of a compound from which preliminary information should be reported within first half an hour of the examination without referring to any book/reference material. The complete structure of the compound may then be elucidated by referring reference material etc. (Minimum 8 spectral analysis)

Note:

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

REFERENCES FOR PRACTICALS:

1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.
2. K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
3. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
4. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
5. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
6. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
7. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
8. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.
9. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
10. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
11. Vogel's Textbook of Practical Organic Chemistry, Fifth edition, 2008, B.S.Furniss, A. J.Hannaford, P. W. G. Smith, A. R. Tatchell, Pearson Education.
12. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
13. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011.

MODALITY OF ASSESSMENT

1. The candidate is expected to submit a journal certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating

that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.

3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

Scheme of examination for M.Sc. Organic Chemistry Semester III and IV. Internal Theory examination (40 Marks)

1. One seminar based on curriculum / publication of a research paper/ presentation of a research paper in seminar or conference (to be assessed by teacher of the institution teaching PG learners).

a) Selection of the topic, introduction, write up, references.20 marks

b) Presentation. 20 marks

There will not be any internal examination for practical.

External Theory Examination (60 Marks)

Paper	Time allotted in hours	Maximum marks
Paper- I	2.5	60
Paper- II	2.5	60
Paper- III	2.5	60
Paper- IV	2.5	60

It is recommended that a total of five questions be set, based on the syllabus with due weightage to the number of lectures allotted per topic.

The candidates are expected to answer all five questions.

Question 5 will be based on all four units and the remaining questions will be based on each unit.

Semester End Practical Examination	(50 Marks)
Laboratory Work	40 Marks
Journal	05 Marks
Viva	05 Marks

The practical examination will be held for two days as described below. The candidates will be examined practically and orally on each day.

Paper	Experiments	Time duration in hours	Maximum marks
Paper- I	1	3.5	50
Paper- II	1	3.5	50
Paper- III	1	3.5	50
Paper- IV	1	3.5	50