RAMNARAIN RUIA AUTONOMOUS COLLEGE
M.Sc. Organic Chemistry
Semester – III
2024-25

Course Code	Unit	Topic	Credits	Lectures
THEORETICAL ORGANIC CHEMISTRY-I				
DSC 1	I	Stereochemistry	3	15L
	II	Pericyclic Reactions		15L
	III	Photochemistry		15L
SYNTHETIC ORGANIC CHEMISTRY-I				
DSC 2	I	Reactive intermediates in organic synthesis	3	15L
	II	Enamines, Ylides and α-C-H functionalization		15L
	III	Metals / Non-metals in organic synthesis		15L
ADVANCED SPECTROSCOPIC TECHNIQUES				
DSC 3	I	Advanced NMR Spectroscopy	3	15L
	II	2D-NMR Spectroscopy		15L
	III	Mass Spectrometry		15L
CHEMISTRY OF BIOMOLECULES AND ENZYMES				
DSE 1	I	Biomolecules	3	15L
	II	Chemistry of Enzymes		15L
	III	Chemistry of co-enzymes		15L
CHEMISTRY OF NATURAL PRODUCTS				
DSE 2	I	Synthesis and applications of carbohydrates, lipids, alkaloids and pigments	3	15L
	II	Synthesis and applications insect pheromones, insect growth regulators, plant growth regulators.		15L
	III	Biogenesis and biosynthesis of natural products.		15L
DSC1	Practical		4	
DSC2				
DSC3				
DSE1/2				

Course Code	Unit	Topic	Credits	Lectures
THEORETICAL ORGANIC CHEMISTRY-II				
DSC 1	I	Supramolecular Chemistry:	3	15L
	II	Advanced Stereochemistry		15L
	III	Asymmetric Synthesis		15L
	SYNTHETIC ORGANIC CHEMISTRY-II			
DSC 2	I	Protection-deprotection of functional groups and Introduction to Retrosynthetic Analysis	3	15L
	II	The Disconnection Approach		15L
	III	Transition and rare earth metals in organic synthesis		15L
NATURAL PRODUCTS AND HETEROCYCLIC CHEMISTRY				
DSE 1	I	Synthesis and applications of Vitamins, antibiotics, insecticides, terpenoids.	3	15L
	II	Heterocyclic Compounds -I		15L
	III	Heterocyclic compounds -II		15L
DSE 2	I	Drug discovery	3	
	II	Drug development and drug design		
	III	Drug Metabolism		
DSC1	Practical		3	
DSC2				
DSE1/2	Practical		1	

Course Code: RPSCHEO301
Discipline Specific Course-I

Theoretical organic Chemistry-I

COURSE OUTCOMES

A student completing successfully completing this course will be able to:

CO#	Description
CO1	Determine point groups based on symmetry elements and carry out conformational analysis of ring compounds.
CO2	Explain the effect of conformation on the reactivity of cyclohexanone derivatives
CO3	Predict pathways and the stereochemistry of pericyclic reactions
CO4	Explain the process of photochemical reactions with special reference to cleavage of carbonyl compounds and photochemistry of olefins.

Unit 1	**Stereochemistry**	**(15L)**
1.1	Classification of point groups based on symmetry elements with examples (nonmathematical treatment).	
1.2	Conformational analysis of medium rings: Eight to ten membered rings and their unusual properties**,** I-strain, transannular reactions.	
1.3	Stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, perhydroanthracenes, steroids, and Bredt's rule.	
1.4	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 $LiAlH_4$, selectride and MPV reduction) and oxidation of cyclohexanols.	
Unit 2:	**Pericyclic Reactions**	**(15L)**
2.1	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 – • The Woodward-Hoffmann Rules-Class by Class • The generalised Woodward-Hoffmann Rule Explanations for Woodward-Hoffmann Rules • 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.	
2.2	Cycloaddition reactions: Supra and antra 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, AlleneCycloadditions, CarbeneCycloaddition, Epoxidation and Related Cycloadditions. Other Pericyclic reactions: Sigmatropic Rearrangements, Electrocyclic Reactions, Alder 'Ene' Reactions.	
2.3	Electrocyclic reactions: Conrotatory and disrotatary motions, 4nπ and (4n+2)π electron and allyl systems.	
2.4	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.	
Unit 3	**Photochemistry**	**(15)**
3.1	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.	
3.2	Photochemistry of carbonyl compounds:$\pi \rightarrow \acute{\pi}^*$, $n \rightarrow \acute{\pi}^*$ 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.	
3.3	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.	
3.4	Photochemistry of arenes**:** 1, 2- , 1, 3- and 1, 4- additions. Photocycloadditions of aromatic Rings.	
3.5	Singlet oxygen and photo-oxygenation reactions. Photochemically induced Radical Reactions. Chemiluminescence.	
	<u>REFERENCES:</u>	
	1 Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers, 1st Edition, Oxford University Press (2001). 2 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. 3 Pericyclic Reactions, S. Sankararaman, Wiley VCH, 2005.	

	4 Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, PragatiPrakashan, 2011 5 Pericyclic reactions-A mechanistic approach, S. M. Mukherji, Macmillan Co. of India 1979. 6 Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd. 7 Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edit 8 Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd 9 Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A john Wiley and Sons, Ltd., Publication)	

Course Code: RPSCHEO302
Discipline Specific Course-II
Synthetic Organic Chemistry-I

COURSE OUTCOMES

A student completing successfully completing this course will be able to:

CO#	Description
CO1	Give the method for preparing synthetically important compounds involving radicals.
CO2	Give the method for preparing synthetically important compounds via enamines and ylides.
CO3	Understand the catalytic cycles for reaction involving various metals and non metals.
CO4	Understand and explore the application of various metals and non metals in organic synthesis.

Unit 1:	Reactive intermediates in organic synthesis	(15L)
2.1	**Introduction:** Generation, stability, reactivity and structural and stereochemical properties of free radicals, Persistent and charged radicals, Electrophilic and nucleophilic radicals.	
2.2	**Radical Initiators**: azobisisobutyronitrile (AIBN) and dibenzoyl peroxide.	
2.3	**Characteristic reactions** - Free radical substitution, addition to multiple bonds. Radical chain reactions, Radical halogenation of hydrocarbons (Regioselectivity),radicalcyclizations, autoxidations: synthesis of cumenehydroperoxide from cumene.	
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_{RN}Ar reactions.	

2.5	Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Sandmeyer reaction, Acyloin condensation.	
Unit 2:	**Enamines, Ylides and α-C-H functionalization**	**(15)**
2.1	**Enamines:** Generation & 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.	
2.2	**Phosphorus, Sulfur and Nitrogen Ylides:** Preparation and their synthetic applications along with their stereochemical aspects. Wittig reaction, Horner-Wadsworth-Emmons Reaction, Barton-Kellogg olefination.	
2.3	**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.	
Unit 3:	**Metals / Non-metals in organic synthesis**	**(15)**
3.1	**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.	
3.2	**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.	
3.3	**Organosilicons:** Salient features of silicon governing the reactivity of organosilicons, preparation and important bond-forming reactions of alkylsilanes, alkenylsilanes, aryl silanes and allylsilanes. β-silyl cations as intermediates. Iodotrimethylsilane in organic synthesis.	
3.4	**Silyl enol ethers**: Application: As nucleophiles (Michael reaction, Mukaiyamaaldol reaction), in ring contraction reactions.	
3.5	**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.	
3.6	**Selenium in organic synthesis:**Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and selenoacetals as α-C-H activating groups **REFERENCES**	
	1. Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer Verlag 2. Modern Methods of Organic Synthesis, 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.	

	3. Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam. 4. Organic Chemistry, ClaydenGreeves Warren and Wothers, Oxford Press (2001). 5. Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002). 6. Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon,3rdEdn., Nelson Thornes 7. Organic Chemistry, 7thEdn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson	

Course Code: RPSCHEO303
Discipline Specific Course-III
Advanced Spectroscopic Techniques

COURSE OUTCOMES

A student completing successfully completing this course will be able to:

CO#	Description
CO1	Explain the basic concept and applications of **^{13}C –NMR spectroscopy**
CO2	Apply 2D NMR techniques for structural elucidation.
CO3	Write the mass fragmentation for various classes of organic compounds
CO4	Develop a problem solving approach towards the structural elucidation from spectral data.

Unit 1:	**Advanced NMR Spectroscopy**	**(15)**
1.1	**ProtonNMR 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_2B_2-A_2X_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.	
1.2	**^{13}C –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.	
1.3	Spectral problems based on UV, IR, ^{1}HNMR and ^{13}CNMR and Mass spectroscopy .	

Unit 2:	**2D-NMR Spectroscopy**	**(15)**
2.1	**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 and NOESY, TOCSY, ROESY, HMQC techniques.	
2.2	Applications of NMR Spectroscopy in Determination of Configuration	
		(15)
Unit 3:	**Mass Spectrometry**	
3.1	Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, Determination of molecular formula of organic compounds based on isotopic abundance and HRMS. Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction, ortho effect.	
3.2	Structure determination involving individual or combined use of the above spectral techniques.	
	REFERENCES: 1. Spectroscopy of Organic compounds, P.S. Kalsi, New Age International Pub. Ltd. And Wiley Eastern Ltd., Second edition, 1995. 2. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987. 3. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991 4. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974. 5. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989. 6. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987. 7. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., .2011 8. Introduction to spectroscopy,Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, 4th ed., 2009. 9. Organic spectroscopic structure determination: a problem-based learning approachDouglass F. Taber, Oxford University Press, 17-Sep-2007. 10. Organic Spectroscopy: Principles And Applications,Jag Mohan, Alpha Science International Ltd., 30-Mar-2004	

Course Code:
Discipline Specific Elective-I
Chemistry of Biomolecules and Enzymes

COURSE OUTCOMES

A student completing successfully completing this course will be able to:

CO#	Description
CO1	Develop a deeper understanding in the Chemistry of Proteins and Nucleic Acids.
CO2	Infer the effect of physical parameters on the structure and function of nucleic acids.
CO3	Apply the basic concepts of organic reaction mechanism to enzyme action and the action of coenzymes.
CO4	Understand the biomimetic approach towards enzyme activity.Understand the various pathways towards the biosynthesis of important molecules and predict their pathways of synthesis.

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.	
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.	
1.3	Structure: Purine & pyrimidine bases, ribose, deoxyribose, nucleosides and nucleotides (ATP, CTP, GTP, TTP, UTP) formation of polynucleotides strand with its shorthand representation**.**	
1.4	RNAs (various types in prokaryotes and eukaryotes) m- RNA and r- RNA – general account , t- RNA-clover leaf model, Ribozymes**.**	
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).	
1.6	Chemical synthesis of oligonucleotides: Phosphodiester, Phosphotriester, Phosphoramidite and H- phosphonate methods including solid phase approach.	

Unit 2:	**Chemistry of Enzymes**	**(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.	
2.2	Factors affecting enzyme kinetics: Substrate concentration, enzyme concentration, temperature, pH, product concentration etc. Reversible and irreversible inhibition.	
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.	
Unit 3:	**Chemistry of co-enzymes**	**(15L)**
3.1	Chemistry of coenzymes. Structure, mechanism of action and bio-modeling studies of the following coenzymes: nicotinamide adenine dinucleotide, 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.	

Course Code:
Discipline Specific Elective-II
Chemistry of Natural Products

COURSE OUTCOMES

A student completing successfully completing this course will be able to:

CO#	Description
CO1	Know basic structural elucidation of carbohydrates, organic pigments and alkaloids.
CO2	Understand the synthetic strategies towards the synthesis of important biologically active molecules.
CO3	Know the basic pathways of secondary metabolism and write the biosynthesis of molecules, based on these pathways.

Unit 1:	**Synthesis and applications of natural products like carbohydrates, lipids, alkaloids and pigments**	**(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**.**	
1.2	**Lipids:** Classification, role of lipids, Fatty acids and glycerol derived from oils and fats.	
1.3	**Prostaglandins:** Classification, general structure and biological importance. Structure elucidation of **PGE_1**.	
1.4	**Alkaloids:** Occurrence and physiological importance of morphine and atropine. Structure elucidation, spectral data and synthesis of coniine.	
1.5	**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.	
Unit 2:	**Synthesis and applications of natural products like insect pheromones, insect growth regulators, plant growth regulators.**	**(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:	

	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	**Insect pheromones:** General structural features and importance. Types of pheromones (aggregation, alarm, releaser, primer, territorial, trail, sex 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**.**	
2.3	**Insect growth regulators:** General idea, structures of JH_2 and JH_3 .	
2.4	**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-tetrahydropyranyloxydodecane expected).	
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.	
3.2	Acetate pathway: Biosynthesis of malonylCoA, saturated fatty acids, prostaglandins from arachidonic acid, aromatic polyketides.	
3.3	Shikimic Acid pathway: Biosynthesis of shikimic acid, aromatic amino acids, alkaloids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, anthocyanins, flavonoids and isofalvonoids.	
3.4	Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes – geranyl cation and its derivatives, sesquiterpenes – farnesylcation and its derivatives and diterpenes.	
	REFERENCES: **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**.** 3. Voet, D. and J. G. Voet (2004) Biochemistry, 3rd Edition, John Wiley & sons, Inc. USA. 4. Enzyme catalysis in organic synthesis, 3rd edition. Edited by KarlheinzDrauz, Harold Groger, and Oliver May, Wiley-VCH Verlag GmbH & Co KgaA, 2012. 5. Natural Products Volume- 2, By O. P. Agarwal. 6. Chemistry of Natural Products, F. F. Bentley and F. R. Dollish, 1974. 7. Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S.ItoMajori and S. Nozoo, Academic Press, 1974. 8. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co.	

	9. Natural products chemistry and applications, Sujata V. Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House, 2011. 10. Total. Synthesis of Longifolene,J. Am. Chem. Soc., E. J. Corey, M. Ohno, R. B. Mitra, and P. A. Vatakencherry. 1964,86, 478. 11. Selected Organic synthesis, Ian Fleming, John Wiley and Sons, 1973. 12. Total synthesis of Natural Products, J. Apsimon, John Wiley and Sons. 13. The Logic of Chemical Synthesis, E. J. Corey and Xue-Min Cheng, Wiley Interscience. 14. Classics in Total Synthesis, K. C. Nicolaou and E. J. Sorensen, Weinhem: VCH, 1996.	
	PRACTICAL	
DSC-1 and DSC-2	**Separation of a ternary mixture of organic compounds and identification including derivative preparations using micro-scale technique** 1. Separation of a ternary mixture (S-S-S, S-S-L, S-L-L and L-L-L) (for solid mixture: water insoluble/ soluble including carbohydrates) based upon differences in the physical and the chemical properties of the components. 2. Identification of the two components (indicated by the examiner) using micro-scale technique. 3. Preparation of derivatives (any one of separated compound indicated by the examiner). (**Minimum 8 experiments**)	
DSC-3 and DSE-1/2	**Single step organic preparation involving purification by Steam distillation / Vacuum distillation or Column chromatography.** 1. Preparation of acetanilide from aniline and acetic acid using Zn dust. (Purification by column chromatography) 2. Preparation of 1-nitronaphthalene from naphthalene. (Purification by steam distillation) 3. .Preparation of acetyl ferrocene from ferrocene. (Purification by column chromatography) 4. .Preparation of 3-nitroaniline from 1,3-dinitrobenzene. (Purification by column chromatography) 5. Preparation of benzyl alcohol from benzaldehyde. (Purification by vacuum distillation). 6. Preparation of methyl salicylate from salicylic acid. (Purification by vacuum distillation). 7. .Preparation of 4-methylacetophenone from toluene. (Purification by vacuum distillation). 8. .Preparation of phenyl acetate from phenol. (Purification by vacuum distillation) 9. Preparation of 2-chlorotoluene from *o*-toluidine. (Purification by steam distillation)	

	10. Preparation of 4-nitrophenol from phenol. (Purification by steam distillation/ column chromatography) 11. Preparation of fluorenone from fluorene. (Purification by column chromatography) 12. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation) **(Minimum 8 experiments)**	
	Note: 1. 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. 2. 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.	

Semester-IV
Course Code: RPSCHEO401
Discipline Specific Course-I
Theoretical organic Chemistry-II

COURSE OUTCOMES

A student completing successfully completing this course will be able to:

CO#	Description
CO1	Correlate the effects of substituent's on a substrate with its reactivity.
CO2	Understand the concept of molecular assembly and intermolecular bond in macromolecules and their effects on their catalytic activity.
CO3	Determine enantiomeric and diastereomeric compositions using various available methods
CO4	Understand the properties of molecules by studying physical phenomenon like Circular Dichroism (CD) and and Optical Rotatory Dispersion (ORD).

Unit 1	**Supramolecular Chemistry:**	**(15L)**
1.1	Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes.	
1.2	Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.	
1.3	Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.	
1.4	Molecular recognition and catalysis, molecular self-assembly.Supramolecular Polymers, GelsandFibres.	
Unit 2:	**Advanced Stereochemistry**	**(15L)**
2.1	Racemisation and resolution of racemates including conglomerates: Mechanism of racemisation, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds.	
2.2	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).	
2.3	Correlative method for configurational assignment: chemical, optical rotation, and NMR spectroscopy.	
2.4	Molecular dissymmetry and chiroptical properties: CD and ORD Spectroscopy	

Unit 3:	Asymmetric synthesis	(15L)
3.1	Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions.	
3.2	Synthesis of L-DOPA (Knowles's Mosanto process). Asymmetric reactions with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharplessenantios electiveepoxidation, hydroxylation, aminohydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.	
3.3	Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations.	
	REFERENCES: 1. March's Advanced Organic Chemistry, Jerry March, sixth edition, 2007, John Wiley and sons 2. A guide to mechanism in Organic Chemistry, 6th edition, 2009, Peter Sykes, Pearson education, New Delhi. 3. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002). 4. Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd. 5. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edit 6. Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd 7. Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005 8. Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH. 9. Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992. 10. Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.	

Course Code: RPSCHEO402
Discipline Specific Course-II
Synthetic Organic Chemistry-II

COURSE OUTCOMES

A student completing successfully completing this course will be able to:

CO#	Description
CO1	Propose a reterosynthetic strategy for an organic compound.
CO2	Give the forward synthesis, recognizable starting material and steps involved in the synthesis of the compound.
CO3	Explore the applications of modern and greener methods of organic synthesis.
CO4	Understand the application of transition metal reagents and catalysts in organic synthesis.

Unit 1:	**Protection-deprotection of functional groups and Introduction to Retrosynthetic Analysis**	**(15L)**
1.1	**Protecting groups in Organic Synthesis:**Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications.	
1.2	**Concept of umpolung (Reversal of polarity):** Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethylsulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.	
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.	
Unit 2:	**The Disconnection Approach**	
2.1	**General strategy:** choosing a disconnection-simplification, symmetry, high yielding steps, and recognisable starting material.	
2.2	**One group C-C Disconnections:** Alcohols (including stereoslectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.	
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 annelation.	
Unit 3:	**Transition and rare earth metals in organic synthesis**	**(15L)**
3.1	**Introduction to basic concepts:** 18 electron rule, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion.	
3.2	**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-Miayura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N, S, or P atoms.	
3.3	**Olefin metathesis** using Grubb's catalyst.	
3.4	**Application of Ni, Co, Fe, Rh, and Cr carbonyls** in organic synthesis.	
3.5	**Application of samarium iodide** including reduction of organic halides, aldehydes and ketones, α-functionalised carbonyl and nitro compounds.	
3.6	**Application of Ce(IV)** in synthesis of heterocyclic quinoxaline derivatives and its role as a de-protecting agent**.**	
	REFERENCES: 1. Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer Verlag 2. Modern Methods of Organic Synthesis, 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004. 3. Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam. 4. Organic Chemistry, ClaydenGreeves Warren and Wothers, Oxford Press (2001). 5. Moder Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007). 6. Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002). 7. Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon,3rdEdn., Nelson Thornes 8. Organic Chemistry, 7thEdn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson 9. Strategic Applications of Name Reactions in Organic Synthesis, L. Kurti& B. Czako (2005), Elsevier Academic Press 10. Advanced Organic Chemistry: Reactions & Mechanisms, 2ndEdn.,B. Miller & R. Prasad, Pearson	

	11. Organic reactions and their mechanisms, 3rd revisededition, P.S. Kalsi, New Age International Publishers 12. Organic Synthesis: The Disconnection Approach, Stuart Warren, John Wiley & Sons, 2004	

Course Code:
Discipline Specific Elective-I
Natural Products and Heterocyclic Chemistry

COURSE OUTCOMES

A student completing successfully completing this course will be able to:

CO#	Description
CO1	Understand the occurrence and biological roles of steroids, vitamins, terpenoids and antibiotics.
CO2	Have an enhanced approach towards structural elucidation.
CO3	Apply the rules of IUPAC nomenclature and other methodologies towards nomenclature of heterocycles.
CO4	Understand the reactivity of various heterocyclic molecules and their importance towards synthesis of certain biologically active molecules.

Unit 1:	**Vitamins, Antibiotics, Insecticides and Terpenoids**	
1.1	**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).	
	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 phytyl bromide	
	Vitamin K_1 from 2-methyl-1, 4-naphthaquinone and phytol.	
1.2	**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 phthalimidemalonaldehyde (synthesis of D-penicillamine and t-butyl phthalimidemalonaldehyde expected).	
1.3	**Naturally occurring insecticides:** Sources, structure and biological properties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis of pyrethrin I.	
1.4	**Terpenoids**: Occurrence, classification, structure elucidation, stereochemistry, spectral data and synthesis of zingiberene .	
Unit 2:	**Heterocyclic compounds-I**	

2.1	Heterocyclic compounds: Introduction, classification, Nomenclature of heterocyclic compounds of monocyclic (3-6 membered) (Common, systematic (Hantzsch-Widman) and replacement nomenclature)	
2.2	Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyridazines, pyrimidine,pyrazines and oxazines.	
Unit 3:	**Heterocyclic compounds-II**	
3.1	Nomenclature of heterocyclic compounds of bicyclic/tricyclic (5-6 Membered) fused heterocycles (up to three hetero atoms)**.** (Common, systematic (Hantzsch-Widman) and replacement nomenclature)	
3.2	Nucleophilic ring opening reactions of oxiranes, aziridines, oxetanes and azetidines.	
3.3	Structure, reactivity, synthesis and reactions of coumarins, quinoxalines,cinnolines,indole, benzimidazoles, benzoxazoles, benzothiazoles, Purines andacridines.	
	REFERENCES: 1. Natural products chemistry and applications, Sujata V. Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House, 2011. 2. Organic Chemistry Natural Products Volume-II, O. P. Agarwal, Krishna Prakashan, 2011. 3. Chemistry of natural products, F. F. Bentley and F. R. Dollish, 1974 **4.** Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S.ItoMajori and S. Nozoo, Academic Press, 1974. 5. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co. 2008. 6. Heterocyclic chemistry, 3rd edition, Thomas L. Gilchrist, Pearson Education, 2007. 7. Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, R. K. Bansal, Wiley Eastern Ltd. 1990. 8. Heterocyclic Chemistry, J. A. Joule and G. F. Smith, ELBS, 2nd edition, 1982. 9. The Conformational Analysis of Heterocyclic Compounds, F.G. Riddell, Academic Press,1980. 10. Principles of Modern Heterocyclic Chemistry, L.A. Paquette, W.B. Benjamin, Inc., 1978. 11. An Introduction to the Chemistry of Heterocyclic Compounds, 2nd edition, B.M. Acheson, 1975. 12. Natural Products: Chemistry and Biological SignificanceInterscience, J. Mann, R.S. Davidson, J.B.Hobbs, D.V. Banthrope and J. B. Harborne, Longman,Essex, 1994. 13. Organic Chemistry, Vol 2, I.L. Finar, ELBS, 6th edition, Pearson.	

	14. Stereoselective Synthesis: A Practical Approach, M. Nogradi, Wiley-VCH, 1995. 15. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers, 1998. 16. The Alkaloids, The fundamental Chemistry A biogenetic approach, Marcel Dekker Inc. New York, 1979. 17. Comprehensive Organic Chemistry by Barton and Olis, Pergamon Press, Oxford, 1979. 18. Medicinal Natural Products, a Biosynthetic Approach, Derick Paul, John Wiley and Sons, 2002. 19. Biosynthesis of Natural Products, Mannitto Paolo, Ellis Horwoocl Limited, 1981. 20. Spectroscopy of Organic compounds, P.S. Kalsi, New Age International Pub. Ltd. And Wiley Eastern Ltd., Second edition, 1995. 21. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987. 22. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991 23. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974. 24. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989. 25. Alkaloids,V.K. Ahuluwalia,Ane Books Pvt.Ltd. 26. Biotransformations in Organic Chemistry, 5thEdition, Kurt Faber, Springer	

Course Code:
Discipline Specific Elective-II
Drug Discovery, Design and Development

COURSE OUTCOMES

A student completing successfully completing this course will be able to:

CO#	Description
CO1	Know basic terms involved in medicinal chemistry, procedures involved in drug design and factors affecting the activity and potency of a particular drug,
CO2	Understand the effect of Structure-Activity Relationship on drug function and the concept of prodrugs
CO3	Know the steps involved in drug metabolism
CO4	Understand targeted drug delivery systems.

Unit 1:	**Drug discovery**	
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.	
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, combinatiorial synthesis (basic idea).	
Unit 2:	**Drug design, development and synthesis**	
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.	

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.	
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.	
2.4	Synthesis and application of the following drugs: Fluoxetine,cetrizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate.	
Unit 3:	**Drug Metabolism**	
1.1	Introduction: Absorption, distribution, biotransformation and elimination of drug molecules.	
1.2	Reactions of Biotransformation	
1.3	Pathways of drug deactivation and elimination	
1.4	Targeted drug delivery systems	
	REFERENCES: 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**.** 3. Voet, D. and J. G. Voet (2004) Biochemistry, 3rd Edition, John Wiley & sons, Inc. USA. 4. The organic chemistry of drug design and drug action, Richard B. Silverman, 2nd edition, Academic Press 5. Medicinal chemistry, D.Sriram and P. Yogeeswari, 2nd edition, Pearson 6. An introduction to drug design-S. S. Pandeya and J. R. Dimmock (New age international) 7. Burger's medicinal chemistry and drug discovery. by Manfred E. Wolf 8. Introduction to Medicinal chemistry. by Graham Patrick 9. Medicinal chemistry-William O. Foye 10. T. B. of Organic medicinal and pharmaceutical chemistry-Wilson and Gisvold's (Ed. Robert F. Dorge) 11. An introduction to medicinal chemistry-Graham L. Patrick, OUP Oxford, 2009. 12. Principles of medicinal chemistry (Vol. I and II)-S. S. Kadam, K. R. Mahadik and K.G. Bothara ,Niraliprakashan. 13. Medicinal chemistry (Vol. I and II)-Burger 14. Strategies for organic drug synthesis and design - D. Lednicer Wiley 15. Pharmacological basis of therapeutics-Goodman and Gilman's (McGraw Hill)	

	PRACTICALS	
DSE-2 and DSC-2	Two steps preparations 1. Acetophenone →Acetophenone phenyl hydrazine → 2-phenyl indole. 2. 2-naphthol → 1-phenyl azo-2-naphthol → 1-amino-2-naphthol. 3. Cyclohexanone → cyclohexanoneoxime → Caprolactum. 4. Hydroquinone → hydroquinone diacetate → 2,5-dihydroxyacetophenone. 5. 4-nitrotoluene → 4-nitrobenzoic acid → 4-aminobenzoic acid. 6. o-nitroaniline → o-phenylenediamine → Benzimidazole. 7. Benzophenone → benzophenoneoxime → benzanilide. 8. o-chlorobenzoic acid → N-phenyl anthranilic acid → acridone. 9. Benzoin → benzil → benzilic acid. 10. Phthalic acid →phthalimide→anthranilic acid. 11. Resorcinol → 4-methyl-7-hydroxy coumarin→ 4-methyl-7-acetoxy coumarin. 12. Anthracene→anthraquinone→anthrone. (Minimum 8 experiments)	
	Note: 1. 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. 2. Students are expected to purify the product by recryllization, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.	
DSE-1/2	Session-I: Combined spectral identification: 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 to any standard values table etc (Minimum 8 spectral analysis).	
	Session-II: Project evaluation	
	References for Practicals	
	1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V. K. Ahluwalia and RenuAggarwal, 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 7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath. 8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold. 9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold. 10. 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. 11. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers. 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.	