K. J. SOMAIYA COLLEGE OF SCIENCE AND COMMERCE

AUTONOMOUS – Affiliated to University of Mumbai

Re-accredited "A' Grade by NAAC

Vidyanagar, Vidyavihar, Mumbai 400077

Syllabus for M.Sc.

Program: M.Sc. Organic Chemistry

From the academic year 2020–2021

M.Sc. – II
Organic Chemistry
Semester III
Theoretical Organic Chemistry
Course Code –– PSOCH 301

	Module I	
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_I and σ_R scales, steric parameters Es and ß. Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's E_T parameter.	**8L**
	Module – II	
2	**Photochemistry**	**15L**
2.1	Principles of photochemistry (Recapitulation): Jablonski diagram, electronic energy transfer, photosensitization and quenching process.	**1L**
2.2	Photochemistry of carbonyl compounds: σ→π*, π→π*, n→π* transitions, Norrish-I and Norrish-II cleavages, Paterno-Buchi reaction. Photo-reduction, photochemistry of enones, photochemical rearrangements of α, ß-unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction.	**8L**

2.3	Photochemistry of olefins: cis-trans isomerization, dimerization, hydrogen abstraction, addition and Di-pi methane rearrangement including aza-di-pi methane. Photochemistry of arenes**:** 1, 2- , 1, 3- and 1, 4- additions. Singlet oxygen and photo-oxygenation reactions.	**6L**
	Module– III	
3	**Stereochemistry-II**	**15L**
3.1	Dynamic stereochemistry**:** Selection of substrate, Curtin-Hammett principle, Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism): electrophilic addition, nucleophilic substitution, elimination, molecular rearrangements, reduction of cyclohexanone and oxidation of cyclohexanol**.**	**7L**
3.2	Conformational analysis of medium rings: Eight and ten membered rings and their unusual properties**,** I-strain, trans annular reactions.	**2L**
3.3	Bredt's rule, limitations and applications and stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, and steroids.	**6L**
	Module– IV	
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**.**	**2L**
4.2	Synthesis of α-amino acids (Corey's diastereoselective hydrogenation of cyclic hydrazones), synthesis of L-DOPA [Knowles's Mosanto process].	**1L**

4.3	Asymmetric reactions with mechanism: Aldol and related reactions including Cram's rule, Felkin-Ahn model for diastereoselective nucleophilic attack, Sharpless enantioselective epoxidation, hydroxylation, amino hydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.	**8L**
4.4	Use of chiral auxiliaries in diastereoselective reductions and asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines and oxazolidines in asymmetric transformations.	**4L**
	Reference Books	
	Module– I	
1	Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University Science Books, 2006.	
2	Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.	
3	Organic Reaction Mechanism, Peter Sykes, Pearson.	
	Module– II	
1	Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley- Eastern	
2	Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication, Oxford 1991.	
3	Molecular Photochemistry, N. J. Turro, W. A. Benjamin.	
4	Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill	
5	Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.	
6	Photochemistry and Pericyclic Reactions, Jagdamba Singh, Jaya Singh, New Age International Ltd., 3rd edition,2011.	
	Module III and IV	
1	Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd.	
2	Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edition.	

3	Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd.
4	Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005.
5	Binol: a versatile chiral reagent, Chem. Rev., 2007, 107 (9), pp. PR1–PR45
6	Binap: An efficient chiral element for asymmetric catalysis, Acc. Chem. Res., 1990, 23 (10), pp. 345–350

M.Sc. – II
Synthetic Organic Chemistry-I Semester III
Course Code –– PSOCH 302

	Module I	
1	**Aromaticity & Heterocyclic Compounds-I**	**15L**
1.1	**Aromaticity**: (a) Structural, thermochemical and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity. (b) Application of HMO theory to monocyclic conjugated systems. Frost-Muslin diagrams. Huckel's (4n+2) and 4n rules. (c) Aromatic and anti-aromatic compounds up to 18 carbon atoms. Aromaticity of benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, tropylium cations and homo-aromatic compounds. Craig's rule.	**7L**

1.2	**Heterocyclic Compounds-I:** Structure, reactivity and synthesis of the following heterocycles (a) Pyrrole: Paal Knorr, Hantzsch Methods (b) Thiophene: Paal Knorr, Hinsberg method (c) Furan: Paal Knorr, Fiest-Benary, Industrial Method (d) Indole: Fischer indole synthesis, Bischler synthesis, Madelung synthesis, Domino and cascade methods of indole synthesis (e) Pyridine-Hantzsch Dihydropyridine Synthesis, Chichibabin synthesis (f) Pyridine N-oxides	**8L**
	Module – II	
2	**Enamines and ylides**	**15L**
2.1	Methods of preparation of enamines: Condensation of secondary amine and aldehyde or ketone, reaction between alkynes and secondary amines. Comparison of reactivity of enamines and enolates. Synthetic reactions of enamines including asymmetric reactions of chiral enamines derived from chiral secondary amines.	**2L**
2.2	Phosphorus, sulfur and nitrogen ylides: Preparation, structure and comparison of reactivity. Reactions of phosphorus, sulfur and nitrogen ylides with carbonyl compounds, including mechanism and stereochemistry. Wittig and Wittig-Horner reaction.	**6L**
2.3	α C-H activation by nitro, sulfoxide, sulfone and phosphonate groups. Generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. Shapiro reaction, Bamford- Stevens Reaction, Julia olefination and its modification, Bestmann- Ohira Reagent, Barton-Kellogg olefination, Steven's rearrangement.	**7L**
	Module– III	

3	**Molecular Rearrangement**	**15L**
3.1	Rearrangement involving migration to electron-deficient carbon: Wagner-Meerwein, Pinacol-Pinacolone, Benzil-Benzilic acid, Wolff,	5L
	Arndt-Eistert synthesis.	
3.2	Rearrangement involving migration to electron-deficient nitrogen: Hofmann, Curtius, Lossen, Schmidt, Beckmann.	4L
3.3	Rearrangement involving migration to electron-deficient oxygen: Baeyer-Villiger oxidation, Hydro peroxide, Dakin.	2L
3.4	Other Rearrangements: Favorski, Fries, Dienone phenol, Von Richter, Steven's, Sommelet Hauser.	4L
	Module – IV	
4	**Name reactions with mechanism and applications**	**15L**
4.1	Mukaiyama esterification, Mitsunobu reaction, Baylis Hillman reaction, Suzuki coupling, Wacker process, Heck reaction, Sonogashira reaction, McMurry coupling.	**7L**
4.2	Multicomponent reactions: Domino/cascade reactions, Strecker synthesis, Biginelli synthesis, Multicomponent reactions using alkyl isocyanides: Passerini and Ugi-4-component synthesis.	**8L**
	Reference Books	
	Module – I	
1	Aromaticity , P. Garratt, McGraw Hill, New York, 1971.	
2	Carbocyclic Non-Benzenoid Aromatic Compounds. Von D. Lloyd. Elsevier Publishing Comp., Amsterdam-London-New York, 1966.	
3	March's Advanced Organic Chemistry:Reactions, Mechanisms, and Structure, Wiley publication, 7th edition, 2013.	
4	Heterocyclic chemistry, Thomas L. Gilchrist, Pearson Education, 3rdedition,	

	2007.
5	Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, R. K. Bansal, Wiley Eastern Ltd., 1990.
6	Heterocyclic Chemistry, J. A. Joule and G. F. Smith, Wiley Blackwell, 5thedition, 2010.
7	Principles of Modern Heterocyclic Chemistry, L.A. Paquette, W.B. Benjamin, Inc., 1978.
8	An Introduction to the Chemistry of Heterocyclic Compounds, B.M. Acheson, 2nd edition,1975.
	Module II
1	Advanced Organic Chemistry, Jerry March Wiley publication.
2	Advanced Organic Chemistry Part A and B, Francis A Carey and Richard Sundberg, Plenum Press.
3	Modern methods of organic synthesis, W. Carruthers and Iain Coldham, Cambridge Press, 4th edition.
4	Name Reactions. A Collection of Detailed Reaction Mechanisms, Jie Jack Li, Springer, 4th edition, 2009.
5	Organic Chemistry, Clayden, Greeves, Warren and Wothers, Oxford Press, 2001.

6	Modern Synthetic Reactions (The Organic Chemistry Monograph Series) , H.O. House.
	Module III
1	Organic Reaction Mechanisms, V.K. Ahluwalia, Rakesh Kumar Parashar, R. K. Parashar, Narosa Publication, 4th edition, 2010.
2	Name Reactions. A Collection of Detailed Reaction Mechanisms, Jie Jack Li, Springer, 4th edition, 2009.

3	March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Wiley publication, 7th edition, 2013.
	Module IV
1	Name reactions and reagents in organic synthesis, second edition, Bradford P. Mundy, Michael G. Ellard and Frank Favoloro, Jr. Wiley-Interscience .
2	Name reactions, Jie Jack Li, 3rd Edition, Springer.
3	Organic Chemistry, Clayden, Greeves, Warren and Wothers,Oxford Press, 2001.
4	Modern Synthetic Reactions (The Organic Chemistry Monograph Series), H.O. House.

M.Sc. – II
Supramolecular Chemistry, Spectroscopy and Molecular Modelling
Semester III
Course Code – PSOCH 303

	Module I	
1	**Supramolecular chemistry**	**15L**
1.1	Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes.	**3L**
1.2	Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.	**3L**
1.3	Structures, properties and applications of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes, micelles and cyclodextrins.	**6L**
1.4	Molecular recognition and catalysis, molecular self-assembly.	**3L**
	Module – II	
2	**ESR and Hyphenated techniques**	**15L**
2.1	**ESR:** principle, instrumentation, spin-spin splitting, qualitative and multiple resonance (ENDOR, ELDOR) spin labelling,	**7L**

	metallic complexes, applications.	
2.2	**Hyphenated techniques**: Need for hyphenation, possible hyphenation, interfacing devices and applications of GC-MS, GC-IR, MS-MS, LC- MS, LC-IR, LC-NMR.	**8L**
	Module – III	
3	**Mass and NMR spectroscopy**	**15L**
3.1	**Mass spectrometry:** Molecular ion peak, base peak, isotopic abundance and 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.	**7L**
3.2	**NMR spectroscopy:** (a) Application in structure elucidation. Relaxation phenomenon and relaxation time. First order, second order and higher order spectra. Methods of simplification of complex spectra. Double resonance, NOE and chemical shift reagents. Spin system notations, AB, AX, AB_2-AX_2, AMX and A_2B_2-A_2Xspin systems with suitable examples. Coupling in aromatic and heteroaromatic systems, long range coupling. Spectra of diastereotopic systems. (b) ^{19}F-NMR and ^{31}P-NMR spectroscopy: Principles and applications.	**8L**
	Module – IV	
4	**^{13}C and Two Dimensional NMR Spectroscopy**	**15L**
4.1	^{13}C –NMR spectroscopy: Introduction, ^{13}C- chemical shifts, calculation of C- chemical shifts, proton coupled ^{13}C - spectra, DEPT technique.	**4L**
4.2	Two-dimensional NMR spectroscopy: Introduction, COSY and HETCOR techniques, (including interpretation of COSY and HETCOR spectra). NOESY and ROESY techniques	**4L**
4.3	Problems based on combined use of spectroscopic techniques/ advanced techniques	**5L**

4.4	ESR spectroscopy: Principles and applications.	**2L**

	Reference Books
1	**Module I**
2	Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
3	Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
4	Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.
	Module II & III
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, 4thed., 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 approach Douglass F. Taber, Oxford University Press, 2007.
10	Organic Spectroscopy: Principles And Applications, Jag Mohan, Alpha Science International Ltd., 204.
	Module IV
1	Fundamentals of Analytical Chemistry, D .A. Skoog and D. M. West and F. J. Holler Holt- Saunders 9th Edition (2016)

2	Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann, 8th Edition(1998)
3	Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A. Settle Jr, 7th Ed CBS (1986)

M.Sc. – II
Medicinal and Bio-organic Chemistry Semester III
Course Code –– PSOCH 304

	Module I	
1	**Drug discovery, design 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 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**

	Module – II	
2	**Proteins and Nucleic acids**	**15L**

2.1	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, ß-sheets, super secondary structure. Tertiary structure of protein: folding and domain structure. Quaternary structure.	**4L**
2.2	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.	**6L**
2.3	Chemical synthesis of oligonucleotides: Phosphodiester, Phosphotriester, Phosphoramidite and H-phosphonate methods including solid phase approach.	**5L**
	Module– III	
3	**Enzyme Chemistry**	**15L**
3.1	Chemistry of enzymes: Introduction, nomenclature, classes and general types of reactions catalysed by enzymes. Properties of enzymes: i) Enzyme efficiency/catalytic power ii) Enzyme specificity; Fischer's 'lock and key' and Koshland 'induced fit' hypothesis. Concept and Identification of active site.	**6L**
3.2	Factors affecting enzyme kinetics: Substrate concentration, enzyme concentration, temperature, pH, product concentration etc. Reversible and irreversible inhibition.	**4L**
3.3	Mechanism of enzyme action: transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Mechanism of chymotrypsin catalysed hydrolysis of a peptide bond.	**5L**
	Module – IV	
4	**Chemistry of Natural Products**	**15L**

4.1	Alkaloids: Occurrence and physiological importance of morphine, coniine and papaverine. Structure elucidation and synthesis of adrenaline.	**2L**
4.2	Multi-step synthesis of natural products a) Woodward synthesis of Reserpine from benzoquinone b) Corey synthesis of Longifoline from resorcinol c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol d) Nicolaou Synthesis of Taxol .	**7L**
4.3	Prostaglandins: Classification, general structure and biological importance. Structure elucidation of PGE1 and PGF1α (synthesis not expected).	**4L**
4.4	Plant and Insect growth regulators: Structures of JH2 and JH3. Structural features and applications of gibberelic acids and triacontanol. Synthesis of triacontanol (synthesis of stearyl magnesium bromide and 12-bromo-1-tetrahydropyranyloxydodecane expected).	**2L**

Organic Chemistry Practical
Semester III

Sr. No.	Paper	Topic
1	PSOCHP301	Ternary mixture (solid-solid, Liquid-Liquid, Solid-Liquid)
2	PSOCHP302	Organic Estimation
3	PSOCHP303	Organic Preparation
4	PSOCHP304	Organic Spotting of multifunctional organic compound

	PSOCHP302 Organic Estimation
1	Estimation of Ascorbic acid by Iodometric titrations.
2	Estimation of Citral using hydroxyl amine chloride.
3	Estimation of saponification value of given sample of oil.
4	Estimation of sodium benzoate present in given sample.
5	Estimation of Aspirin by UV-visible
6	Estimation of streptomycin
7	Estimation of glucose of Folin-Wu method.
8	Estimation of protein by Buiret method.

	PSOCHP303 Organic Preparation
1	To prepare benzyllic acid from benzil.
2	Preparation of para iodonitrobenzene from para nitro benzene
3	Preparation of 7-hydroxy-4-methyl coumarin from resorcinol.
4	Preparation of dibenzyl acetone from benzaldehyde.
5	Preparation of mannitol hexaacetate from mannitol
6	Preparation of fluorenone from fluorene.
7	Preparation of acetyl ferrocene from ferrocene.
	References
1	College practical chemistry by V K Ahluwalia.
2	A I Vogel Practical Organic chemistry, 5th edition.
3	H Middleton systematic Qualitative Organic Analysis
4	University of Mumbai Practical Chemistry manual
5	Isolation, purification and estimation of organic chemistry by Bapu Thorat, Lambert Academic publication

M.Sc. – II
Synthetic Organic Chemistry-II

Semester IV
Course Code – PSOCH 401

	Module I	
1	**Designing organic synthesis-I**	**15L**
1.1	Protection and deprotection of the following functional groups: hydroxyl, carbonyl, amino and carboxyl with applications.	**6L**
1.2	Concept of umpolung, generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.	**5L**
1.3	Synthetic Strategies: Introduction, Terminology: target, synthon, synthetic equivalent, functional group interconversion, functional group addition, elimination Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemo selectivity, regioselectivity.	**4L**
	Module II	
2	**Designing organic synthesis II**	
2.1	Order of events in synthesis by retrosynthetic approach with examples. Introduction to one group C-C and C-X disconnections. One group C- C disconnections, alcohols and carbonyl compounds. One group C-X disconnections, carbonyl compounds, alcohols, ethers and sulphides. Introduction to two group C-C and C-X disconnections, two group C-X disconnections; 1,1-difunctionalised, 1,2-difunctionalised and 1,3- difunctionalised compounds. Two groups C-C disconnections; Diels- Alder reaction, 1,3-difunctrionalised compounds, 1,5- difunctionalised compounds, Michael addition and Robinson annulation. Control in carbonyl condensations. General methods of synthesis of 3-7 membered rings.	**11L**
2.2	Synthesis of some complex molecules: synthetic routes based on retrosynthetic analysis for prostaglandin A_2, atropine, camphor.	**4L**

	Module III	
3	**Metals / Non-metals in organic synthesis-II**	**15L**
3.1	Introduction, basic concepts, 18 electron rule, bonding in transition metal complexes, oxidative addition, reductive elimination, migratory insertion.	**3L**
3.2	Palladium in organic synthesis: Heck reaction, Stille, Negishi, Hiyama, Buchwald-Hartwig)	**3L**
3.3	Olefin metathesis using Grubb's catalyst, various types of metathesis and application to organic synthesis.	**2L**
3.4	Mercury in organic synthesis: oxymercuration and demercuration of alkenes, mechanism and regiochemistry, solvomercuration, mercuration of aromatics and transformation of aryl mercurials to aryl halides.	**2L**
3.5	Organotin compounds: preparation of alkenyl and allyl tin compounds	**3L**
	and their applications in C-C bond formation.	
3.6	Selenium in organic synthesis: Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and selenoacetals as a C-H activating groups.	**2L**
	Module– IV	
4	**Radicals in organic synthesis**	**15L**
4.1	General aspects: Electrophilic and nucleophilic radicals and their reactivity with π- rich/deficient olefins, Baldwin's rule for cyclisation. Inter- and intramolecular aliphatic C-C bond formation using tin hydride, carbon hydride, thio donor (Barton's reaction).	**3L**
4.2	Cleavage of C-X, C-Sn, C-Co and C-S bonds in the generation of radicals. Trapping by electron transfer reactions using manganese triacetate.	**4L**
4.3	Radical–radical processes: oxidative couplings, single	**3L**

	electron oxidation of carbanions to generate radicals, dehydrodimerization and reductive couplings.	
4.4	C-C bond formation in aromatics: Electrophilic and nucleophilic radical reactions on aromatics, radical reactions on heteroaromatics: alkylations and acylations. Hunsdiecker halo decarboxylation, autoxidation	**5L**
	Reference Books	

	Module I & II
1.	Organic synthesis: The Disconnection Approach, Stuart Warren, John Wiley & sons, 204
2.	Organic Chemistry, Clayden, Greeves, Warren and Wothers, Oxford Press (2001).
3.	Principles of Organic Synthesis, R.O.C. Norman & J.M. Coxon, 3rd Edition., Nelson Thornes
	Module III
1	G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006
2	Organo transition Metal Chemistry: Applications to Organic Synthesis, S. G. Davis, Pergamon Press, Oxford, 1982.
3	Basic Organometallic Chemistry, B. D. Gupta, A J Elias, Universities Press, Chennai, 2010 Transition Metals in the total synthesis of complex organic molecules, L. S. Hegedus, University Science Books, 1994.
	Module IV
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, Synthesis 4th Edition W.Carruthers and Iain Coldham, Cambridge University Press 204.
3	Radicals in Organic Synthesis B. Giese, Pergamon press (1986)

4	Mechanism and structure in organic chemistry, E. S. Gould.	

M.Sc. – II
Heterocyclic Chemistry and Stereochemistry Semester IV
Course Code – PSOCH 402

	Module I	
1	**Heterocyclic Chemistry-II**	
1.1	Introduction to heterocyclics and their importance. Nomenclature of ring systems (a) Trivial System (b) Fusion system (c) Hantzsch-Widman nomenclature	**3L**
1.2	Structure, reactivity and synthesis of the following three membered Heterocycles (a) Oxirane: Sharpless method, Shi epoxidation, Jacobsen epoxidation, etc (b) Thiirane (c) Aziridine	**4L**
1.3	Structure, reactivity and synthesis of the following four membered Heterocycles (a) Oxetane (b) Thietane (c) Azetine	**3L**
1.4	Structure, reactivity and synthesis of the following five membered Heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole.	**5L**
	Module – II	
2	**Unit 1: Heterocyclic compounds- III**	**15L**
2.1	Reactivity, important methods of synthesis and general reactions of the following heterocyclic: Quinoline, Isoquinoline, yridazines, pyrimidines, pyrazines, s-triazines, purines, oxazines, coumarins, isoindole, isoxazoles, benzimidazoles, benzoxazoles, benzothiazoles.	
	Module– III	
3	**Chiron approach**	**15L**
3.1	Concept of chiral pool, chiral templates, chiral precursors, rule of five, use of biomolecules as starting precursor in designing biologically active molecules	**3L**
3.2	Basic concepts-carbohydrates, amino acids, hydroxyl acids &	**3L**

	terpenes.	
3.3	The concept of chiral template and chiron wherein the carbon skeleton is the chiral precursor.	**4L**
3.4	Utilization of the basic concept for retrosynthetic strategy and synthesis of the following: (S)-propane diol, (R) & (S) epichlorohydrin, L- alanine, 11- oxaprostaglandin $F_{2\alpha}$, (-) multistratin, (-) pentinomycin, (-) shikimic acid, carbonolide B.	**5L**
	Module – IV	
4	**Racemization, Resolution and Chiroptical Properties**	**15L**
4.1	Racemisation and resolution: Mechanism of racemisation, methods of resolution: chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds.	**3L**
4.2	Determination of enantiomer and diastereomer composition: Isotope dilution method, enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatisingagents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR).	**3L**
4.3	Correlative methods for configurational assignment: chemical, optical rotation, quasi-racemate and NMR spectroscopy.	**4L**
4.4	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**
	Reference Books	
	Module – I& II	
1	Heterocyclic chemistry, Thomas L. Gilchrist, Pearson Education, 3rdedition, 2007.	
2	Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, R. K. Bansal, Wiley Eastern Ltd., 1990.	

3	Heterocyclic Chemistry, J. A. Joule and G. F. Smith, Wiley Blackwell, 5th edition, 2010.	
4.	Principles of Modern Heterocyclic Chemistry, L.A. Paquette, W.B. Benjamin, Inc., 1978.	
5.	An Introduction to the Chemistry of Heterocyclic Compounds, B.M. Acheson, 2nd edition, 1975.	
	Module III	
1	Chiron approach in organic synthesis – S. Hanessian (Relevant chapters For Chirons)	
2	Advanced Organic Chemistry Part A and Part B: Reaction and Synthesis, Francis A Carey, Richard J Sundberg, 5th edition, Springer Verlag.	
3	Organic chemistry by I.L.Finar	
4	Organic Chemistry, 7th Edn. R.T. Morrison, R.N. Boyd & S.K.Bhattacharjee, Pearson.	
	Module IV	
1	Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd.	
2	Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edition.	

M.Sc. – II
Medicinal and Bio-organic chemistry-II
Semester IV
Course Code –– PSOCH 403

	Module I	
1	**Drug design, development and synthesis:**	**15L**

1.1	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**
1.2	Computers Aided Drug Design: Basic concept of computational chemistry like quantum mechanics, molecular mechanics, force fields, energy minimization, conformational search, molecular dynamics, 3D pharmacophore identification.	**3L**
1.3	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**
1.4	Synthesis and application of the following drugs: Fluoxetine, oxyphenbutazone, cetrizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate.	**4L**
	Module – II	
2	**Biogenesis and biosynthesis of natural products**	**15L**
2.1	Biogenesis: Precursors, primary and secondary metabolites. Acetate hypothesis. Mevalonate and Shikimic acid pathways.	**7L**
2.2	General principles involved in the biosynthesis of amino acids, alkaloids, steroids and terpenoids	**3L**
2.3	Biosynthesis of selected natural products: L-tryptophan, cholesterol, ephedrine, citronellol.	**5L**
	Module– III	
3	**Chemistry of Steroids**	**15L**
3.1	Steroids: General structure, nomenclature, classification. Occurrence, biological role, important structural and stereochemical features of the following: corticosteroids, steroidal hormones, steroidal alkaloids, sterols (structural elucidation of cholesterol) and bile acids, calciferols and sapogenins. Synthesis of 16-DPA from cholesterol and plant sapogenin.	**9L**

3.2	Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestadiol, oestriol, and progesterone.	**6L**
	Module – IV	
4	**Vitamins, Antibiotics and Insecticides**	**15L**
4.1	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).	**2L**
4.2	Synthesis of the following: 1) Vitamin B1 including synthesis of pyrimidine and thiazole moieties 2) Vitamin B2 from 4,5-Dimethyl-2-nitro aniline and D(-)ribose , 3) Vitamin B6 from: i) ethoxyacetylacetone and cyanoacetamide (Harris synthesis) and ii) ethyl ester of N-formyl-DL-alanine, 4) Vitamin E (α-tocopherol) from trimethylquinol and phytyl bromide 5) Vitamin K1 and K2 from napthalene and phytol.	**4L**
4.3	Antibiotics: Classification on the basis of activity. Structure elucidation of penicillin-G and cephalosporin-C. Synthesis of penicillin-G and phenoxymethylpenicillin from D-penicillamine and t- butyl phthalimidemalonaldehyde (synthesis of D-penicillamine and t- butyl phthalimidemalonaldehyde expected).	**4L**
4.4	Naturally occurring insecticides: Sources, structure and biological properties of pyrethrums (pyrethrin I), rotenoids (rotenone), azadirachtin. Synthesis of pyrethrin I.	**3L**
4.5	Synthesis of insecticides and perfumeric chemicals: cinerolone, jasmolone, allethrolone, exaltone and muscone	**2L**

	Reference Books	
	Module I	
1	An Introduction to Medicinal Chemistry- 2nd Edn. Patrick (Oxford 2001)	
2	Molecular Modeling, Principles and applications -Andrew Leach (Longman) 1998.	
3	Organic Chemistry of drug design and drug action-RB. Silverman (1993) Acad. Press.	
4	A Text book of Drug design and development, 2nd edition. Povl.Krogsgaard-Larsen, Tommy L. and U Madsen (1996) Harwood Acad. Publishers.	
5	Organic Chemistry of Drug synthesis-D Lednicer and L.A. Mitcher, Vol I to III , Wiley 2007	
6	Burger's medicinal chemistry and drug discovery, Wiley, 2003.	
	Module II	
1	Natural product chemistry, A mechanistic, biosynthetic and ecological approach, Kurt B.G. Torssel Apotekarsocieteten – Swedish pharmaceutical press.	
2	Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House	
3	Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co	
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.	
6	Organic Chemistry, 7th Edition, R.T. Morrison, R.N.Boyd & S.K. Bhattacharjee, Pearson	
7	Medicinal Natural Products: A Biosynthetic Approach, 3rd Edition Paul M. Dewick	

	Module III	
1	Natural product chemistry, A mechanistic, biosynthetic and ecological approach, Kurt B.G. Torssell Apotekarsocieteten – Swedish pharmaceutical press.	
2	Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House	
3	Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co	
4	Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S.Ito Majori and S. Nozoo, Academic Press, 1974.	
5	Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co.	
6	Chemistry of Natural Products Sujata V. Bhat, Bhimsen A. Nagasampagi, Meenakshi Sivakumar Hardcover, 840 Pages First Edition - 2005. ISBN: 3-540-40669-7	
	Module IV	
1	Natural product chemistry, A mechanistic, biosynthetic and ecological approach, Kurt B.G. Torssell, Apotekarsocieteten – Swedish pharmaceutical press.	
2	Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House	
3	Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co	
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.	
6	Chemistry of Natural Products, Sujata V. Bhat, Bhimsen A. Nagasampagi, Meenakshi Sivakumar Hardcover, 840 Pages First Edition - 2005. ISBN: 3-540-40669- 7	
7	Total Synthesis of Natural Products: At the Frontiers of Organic Chemistry by Jie Jack Li, E. J. Corey Hardcover, 279 Pages 1st Edition, 2012 ISBN: 978-3-642-34065-9, Springer.	
8	Classics in Total Synthesis ,K. C. Nicolaou, Eric J. Sorensen Paperback, 798 Pages,1st Edition, 1996, ISBN: 3-527-29231-4,Wiley- VCH.	

M.Sc. – II

Chemistry Semester IV

Course Code – PSA/I/P/OCH 404

Environmental and Green Chemistry

	Environmental chemistry	
1	**Module –I: Air and Water Pollution**	**15L**
	Air pollution:	**7L**
1.1	Natural and anthropogenic sources of pollution, primary and secondary pollutants, transport and diffusion of pollutants, gas laws governing the behaviour of the pollutants in the atmosphere.	
1.2	Sampling and analysis of: particulate matter, aerosols, SO_2, H_2O, NO_x, CO, NH_3, organic vapours.	
1.3	Effect of pollutants on human beings, plants, animals, materials and on climates.	
	Water pollution:	**8L**
1.4	Sources of water pollution, basic chemistry of water pollutants, effects and control.	
1.5	Determination of water pollution parameters and their significance.	
1.6	Physical parameters: colour, pH, Temperature, odour, turbidity, density, TOS, TSS, TS.	
1.7	Chemical parameters- acidity, alkalinity, hardness, DO, COD, BOD, TOC, THOD, MPN, biological parameters.	
1.8	Heavy metal pollutants like Hg, Pb, Cd, As, Cu, Cr with respect to their sources, distribution, speciation, toxic effect, control, treatment.	
2	**Module II: Pollution control technology**	**15L**

	Air pollution control technologies: methods to control air pollution in the environment, Limestone injection and fluidised bed combustion, desulphurisation, catalytic convertor and control of vehicular emission, gravity setting chamber, fabric filters.	**5L**
2.1	**Solid Waste disposal**: solid waste disposal methods- open dumps, ocean dumping, land-fills, incineration, recycling and reuse, organic pollutants and hazardous waste disposal and management, non-destructive solid waste, biomedical waste.	**5L**
2.2	**Sewage and waste water treatment system**: primary, secondary and tertiary treatments, measurements of treatment efficiencies. biological treatments-aerobic verses anaerobic treatments, bio augmentation and bio stimulation, biofilms in treatments.	**5L**
3	**Module III: Non renewable energy sources**	**15L**
3.1	Concept and demand of energy, Growing energy needs, Renewable and non renewable sources of energy.	**2L**
3.2	Use of alternate energy sources, Wind energy, Solar energy, Nuclear energy, Tidal energy. Water as source of energy,.	**6L**
3.3	Biofuels production, use and sustainability, use and over exploitation of energy sources and associated problems	**4L**
3.4	Role of an individual in conservation of natural resources. Equitable use resources for sustainable lifestyles	**3L**
4	**Module–IV: Environmental policies, Regulation, Assessment and Green chemistry**	**15L**
4.1	Important environmental laws in India: Article 48A, Article 51 A, and other laws for environmental management. Role of HOEF and pollution control boards in pollution control- role of international environmental agency- UNEP, GEF, UNFCC and IPCC.	**3L**
4.2	Environmental impact assessment (EIM): need of EIA, scope, objectives, types of environmental impacts, steps involved in conducting the EIA studies, techniques- Ad-hoc method, checklist method, overlay mapping method, merits and demerits of EIA	**4L**

	studies.	
4.3	Environmental audit: types, objectives, benefits practice and procedures.	**3L**
4.4	Principle and concept of green chemistry, environmental benign solutions, solvent free systems, SCF, ionic liquids as catalysts and solvents, photochemical reactions, chemistry using microwave, sonochemistry, electrochemical synthesis, Designing greener processes- inherently safer designs (ISD), process intensification (PI) in process monitoring. Porous phase reactions, heterogeneous catalysis, bio-catalysis, greener methods.	**5L**
	References: 1. Environmental Pollution Analysis, S. M. Khopkar, New Age International publication (2011). 2. Water and water pollution (hand book) Ed., Seonard'l Ciacere, Vol I to IV, Marcel Dekkerinc. N.Y.(1972) 3. Water pollution, Arvind Kumar, APH publishing (2004) 4. Introduction to Potable Water Treatment Processes Simon Parsons, Bruce Jefferson, Paperback publication. 5. Guidelines for drinking-water quality, third edition, (incorporating first and second addenda). WHO report. 6. Solid waste management, K Sasikumar and Sanoop Gopi Krishna PHI publication (2009) 7. Solid waste management, Surendrakumar Northen Book Center (2009) 8. Handbook of chemical technology and pollution control 3rd Edn Martin Hocking AP Publication (2005). 9. Fundamental Concepts of Environmental Chemistry, Second Edition	
	G. S. Sodhi , Alpha Science, 2005. 10. Chemical analysis of metals ; Sampling and analysis of metal bearing ores: American Society for Testing and Materials 1980 - Technology & Engineering.	

	11. Manual of Procedures for Chemical and Instrumental Analysis of Ores, Minerals, and Ore Dressing Products. Government of India Ministry of Steel & Mines, Indian Bureau of Mines, 1979. 12. Alloying: understanding the basics, edited by Joseph R. Davis, ASM International (2001). 13. Zone refining and allied techniques, Norman L. Parr, G. Newnes Technology & Engineering (1960).	

M.Sc. – II
Organic Chemistry Practical
Semester IV

Project and Dissertation

In semester IV the student will not have any practical courses instead students will be undertaking project work of duration 4 months in the college laboratories.

Project work goals:

- The students will learn the skills required to succeed in industry or professional school.
- The students will learn and will be exposed to a breadth of experimental techniques using modern instrumentation.
- The student will learn the laboratory skills needed to design, safely conduct and interpret chemical research.
- The student will acquire a foundation of chemistry of sufficient breadth and depth to enable them to understand and critically interpret the primary chemical literature.
- The student will develop the ability to effectively communicate scientific information and research results in written and oral formats.
- The student will learn professionalism, including the ability to work in teams and apply basic ethical principles.