Vivekanand Education Society's

College of Arts, Science and Commerce

(Autonomous)

Sindhi Society, Chembur, Mumbai, Maharashtra – 400 071.

Accredited by NAAC "A Grade" in 3rd Cycle - 2017

Best College Award – Urban Area, University of Mumbai (2012-13)

Recipient of FIST Grant (DST) and STAR College Grant (DBT)

Affiliated to the

University of Mumbai

Syllabus for

Program: M.Sc. (Organic Chemistry)

(Program code: VESPSCHO)

As per Choice Based Semester and Grading System (CBSGS)
with effect from Academic Year 2023 - 2024

Program Outcomes (PO):

A leaner completing M.Sc. Chemistry will be able to:

PO1 Exercise their critical thinking in creating new knowledge leading to innovation, entrepreneurship and employability

PO2 Make choices based on the values upheld by the college, and have the readiness and know-how to preserve the environment and work towards sustainable growth and development.

PO3 Demonstrate professional behaviour of being unbiased, and truthful in all aspects of work as an individual as well as team.

PO4 Develop an ethical view of life, and have a broader (global) perspective transcending the provincial outlook.

PO5 Explore new knowledge independently for the development of the nation and the world and are able to engage in a lifelong learning process.

PO6 Have developed their critical reasoning, judgment and communication skills.

PO7 inculcate logical thinking to address a problem and become result oriented with a positive attitude.

Program Specific Outcomes (PSO's)

On completion of M.Sc. Chemistry program, learners will be enriched with knowledge and be able to

PSO1 Improve theoretical and practical knowledge in the field of Organic chemistry

PSO2 Explain the basic scientific concepts effectively and solve the problems systematically and analytically related to organic chemistry

PSO3 Apply the principles of chemistry in industry, agriculture, medicine and Environment.

PSO4 Design projects in different fields of organic chemistry and develop research aptitude.

PSO5 Apply their understanding in Chemistry to design solutions to unfamiliar problems in Chemistry and those involving other related disciplines

PSO6 understand various reactions and rearrangements.

PSO7 understand and write mechanism of reactions and their applications.

PSO8 understand how to convert one molecule into another by using oxidising and reducing, reagents.

PSO10 Demonstrate an awareness of the relevance of chemistry in a wider multi-disciplinary context.

PSO11 understand different purification techniques in organic chemistry like recrystallization, distillation, steam distillation and extraction

PSO12 Have developed their critical reasoning, judgment and communication skills

PSO13 Ability to identify, design and conduct appropriate experiments, interpret data

obtained, draw pertinent conclusions and communicate all these effectively.

PSO14 Augment the recent developments in the field of green and eco-friendly reactions, pharmaceutical, Bioorganic Chemistry and relevant fields of research and development.

PSO15 get awareness of safety techniques and handling of chemicals.
PSO16 become aware of green chemistry and role of green chemistry in pollution reduction
PSO17 know meaning of safety signs on container of chemicals, safety in handling of chemicals, MSDS sheets. know use of safety goggles, shoes and gloves, fire extinguisher and its use and action to be taken in accidental cases
PSO18 know handling of glass wares and care to be taken, handling of organic flammable as well as toxic solvents in laboratory
PSO19 know use of safety goggles, shoes and gloves, fire extinguisher and its use and action to be taken in accidental cases
PSO20 understand the Principles of IR, NMR, C13 NMR spectroscopy
PSO22 apply the techniques for structure determination of organic molecules.
PSO23 draw various organic reactive intermediates with stereochemistry
PSO24 Industrial applications of organometallic compounds in organic reactions.
PSO25 understand various Pericyclic and photochemical reactions and rearrangements.

M.Sc. (ORGANIC CHEMISTRY)
(SEMESTER III)

Course Code	Title	Credits & Lectures per Semester	Lectures per Week
VESPSCHO301	**Paper 01 Theoretical organic chemistry-I**	**60**	**4**
	Unit I: Organic reaction mechanisms	**15 Lectures**	
	Unit II: Pericyclic reactions	**15 Lectures**	
	Unit III: Stereochemistry-I	**15 Lectures**	
	Unit IV: Photochemistry	**15 Lectures**	
VESPSCHO302	**Paper 02 Synthetic Organic Chemistry-I**	**60**	**4**
	Unit I: Name reactions with mechanism and application	**15 Lectures**	
	Unit II: Radicals in organic synthesis	**15 Lectures**	
	Unit III: Enamines, ylides and α-C-H functionalization	**15 Lectures**	
	Unit IV: Metals / non-metals in organic synthesis	**15 Lectures**	

VESPSCHO303	**Paper 03 Natural products and Spectroscopy**	**60**	**4**
	Unit I: Natural products-I	**15 Lectures**	
	Unit II: Natural products-II	**15 Lectures**	
	Unit III: Advanced spectroscopic techniques-I	**15 Lectures**	
	Unit IV: Advanced spectroscopic techniques-II	**15 Lectures**	
VESPSCHOEC-I 304	**Paper 04 Medicinal, Biogenesis and green chemistry**	**60**	**4**
	Unit I: Drug discovery, design and development	**15 Lectures**	
	Unit II: Drug design, development and synthesis	**15 Lectures**	
	Unit III: Biogenesis and biosynthesis of natural products	**15 Lectures**	
	Unit IV: Green chemistry	**15 Lectures**	
VESPSCHOEC-II 304	**Paper 04 Bioorganic chemistry**	**60**	**4**
	Unit I: Biomolecules-I	**15 Lectures**	
	Unit II: Biomolecules-II	**15 Lectures**	
	Unit III: Biomolecules - III	**15 Lectures**	
	Unit IV: Biomolecules – IV	**15 Lectures**	
VESPSCHO3P1	**Paper 01 Theoretical Organic Chemistry-I**		
VESPSCHO3P2	**Paper 02 Synthetic Organic Chemistry-I**		
VESPSCHO3P3	**Paper 03 Natural products and Spectroscopy-I**		
VESPSCHO3P4A	**Paper 04 Medicinal, Biogenesis and green chemistry**		

Detailed Syllabus: Unit wise with number of lectures
Course title: Paper 01 Theoretical organic Chemistry-I
Course code: VESPSCHO 301
Objective: To understand and develop competence in use of Theoretical organic chemistry
Learning Outcomes (LO):

On successful completion of this course students will be able to:

LO1 **Learning Objectives:**
To learn the reactive intermediates and mechanism in organic synthesis.
LO2 To understand the stereochemistry of reactants, intermediates and products.
LO3 To study pericyclic reactions and their types with mechanism.
LO4 To study various types of photochemical reactions with mechanism

Course title: Organic Chemistry Paper 1 Theoretical organic Chemistry-I

Course code: VESPSCHO301

Unit no.	Details of topics	No of lectures
1	**Organic reaction mechanisms** 1.1 Organic reactive intermediates, methods of generation, structure, stability and important reactions involving carbocations, nitrenes, carbenes, arynes and ketenes. 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) 1.3 Role of FMOs in organic reactivity: Reactions involving hard and soft electrophiles and nucleophiles, ambident nucleophiles, ambident electrophiles, the α effect. 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 – • 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.	15 Lectures
2	**Pericyclic reactions** 2.1 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, Allene Cycloadditions, Carbene Cycloaddition, Epoxidation and Related Cycloadditions. Other Pericyclic reactions: Sigmatropic Rearrangements, Electrocyclic Reactions, Alder 'Ene' Reactions. 2.2 Electrocyclic reactions: Conrotatory and disrotatary motions, 4nπ and (4n+2)π electron and allyl systems. 2.3 Sigmatropic rearrangements: H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations. Cope (including oxyCope 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.	15 Lectures
3	Stereochemistry-I 3.1 Classification of point groups based on symmetry elements with example 3.2 Conformational analysis of medium rings: Eight to ten membered rings and their unusual properties, I-strain, transannular reactions.	15 Lectures

	3.3 Stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, perhydroanthracenes, steroids, and Bredt's rule. 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.	
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. 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. 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. 4.4 Photochemistry of arenes: 1, 2- , 1, 3- and 1, 4- additions. Photocycloadditions of aromatic Rings. 4.5 Singlet oxygen and photo-oxygenation reactions. Photochemically induced Radical Reactions. Chemiluminescence.	15 Lectures

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3. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002).
4. Mechanism and theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.
5. Organic Reaction Mechanism, 4th edition, V. K. Ahluvalia, R. K. Parashar, Narosa Publication.
6. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan Publishers, India.
7. Organic Chemistry, Part A and B, Fifth edition,2007, Francis A.Carey and Richard J. Sundberg, Springer.
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9. Organic reactive intermediates, Samuel P. MacManus, Academic Press.
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11. Organic Chemistry, Seventh Edition, R.T. Morrison, R. N. Boyd & S. K.

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12. Organic reactions & their mechanisms, third revised edition, P.S. Kalsi, New Age International Publishers.
13. Organic Chemistry: Structure and Function, P. Volhardt and N. Schore, 5th Edition, 2012
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15. Pericyclic Reactions, S. Sankararaman, Wiley VCH, 2005.
16. Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
17. Pericyclic reactions, Ian Fleming, Oxford university press, 1999.
18. Pericyclic reactions-A mechanistic approach, S. M. Mukherji, Macmillan Co. of India 1979.
19. Organic chemistry, 8th edition, John McMurry
20. Modern methods of Organic Synthesis, 4th Edition W. Carruthers and Iain Coldham, Cambridge University Press 2004
21. Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books,2006
22. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
23. Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd.
24. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edit
25. Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
26. Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
27. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
28. Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
29. Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
30. Large ring compounds, J.A.Semlyen, Wiley-VCH, 19977.
31. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, WileyEastern
32. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific Publication.
33. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
34. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hil
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)

Detailed Syllabus: Unit wise with number of lectures
Course title: Paper 02 Synthetic Organic Chemistry-I
Course code: VESPSCHO 302
Objective: To understand and develop competence in use of Basic of Synthetic Organic chemistry

Learning Outcomes (LO):

On successful completion of this course students will be able to:
LO1 To learn various name reactions in organic synthesis.
LO2 To study organic free radical and their importance in organic synthesis.

LO3 To understand the applications of enamines, ylides and α C-H functionalization in organicsynthesis.

LO4 To know the applications of organometallic compounds in organic synthesis.

Course title: Paper 02 Synthetic Organic Chemistry-I

Course code: VESPSCHO302

Unit no.	**Details of topics**	**No of lectures**
1	Name reactions with mechanism and application 1.1 Mukaiyama esterification, Mitsonobu reaction, Darzen's Glycidic Ester syntheis, Ritter reaction, Yamaguchi esterification, Peterson olefination. 1.2 Domino reactions: Characteristics; Nazerov cyclization 1.3 Multicomponent reactions: Strecker Synthesis, Ugi 4CC, Biginelli synthesis, Hantzsch synthesis, Pictet-Spengler synthesis. 1.4 Click Reactions: Characteristics; Huisgen 1,3-Dipolar Cycloaddition	15 Lectures
2	Radicals in organic synthesis. 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),radical cyclizations, autoxidations: synthesis of cumene hydroperoxide 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: SRNAr reactions. 2.5 Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Sandmeyer reaction, Acyloin condensation.	15 Lectures
3	Enamines, Ylides and α-C-H functionalization 3.1 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. 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. 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.	15 Lectures
4	Metals / Non-metals in organic synthesis 4.1 Mercury in organic synthesis: Mechanism and regiochemistry of oxymercuration and demercuration of alkenes, mercuration of aromatics,	15 Lectures

	transformation of aryl mercurials to aryl halides. Organomercurials as carbene transfer reagents. 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. 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. 4.4 Silyl enol ethers: Application: As nucleophiles (Michael reaction, Mukaiyama aldol reaction), in ring contraction reactions. 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. 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	

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2. Modern Methods of Organic Synthesis, 4 th 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, Clayden Greeves Warren and Wothers, Oxford Press (2001).
5. Modern Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).
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7. Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3 rd Edn., Nelson Thornes
8. Organic Chemistry, 7 th Edn, 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
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11. Organic reactions and their mechanisms, 3 rd revisededition, P.S. Kalsi, New Age International Publishers
12. Organic Synthesis: The Disconnection Approach, Stuart Warren, John Wiley & Sons, 2004
13. Name Reactions and Reagents in Organic Synthesis, 2 nd Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
14. Name Reactions, Jie Jack Lie, 3rd Edn., Springer
15. Organic Electrochemistry, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

Detailed Syllabus: Unit wise with number of lectures
Course title: Paper 03 Natural products and Spectroscopy
Course code: VESPSCHO303
Objective: To understand synthesis and biologically active natural products.
To understand spectroscopy of organic componds.

Learning Outcomes (LO):

On successful completion of this course students will be able to:

LO1 To learn the basic concepts involved in natural products.
LO2 To study the multi-step synthesis of various natural products.
LO3 To learn the advance spectroscopic technique for analysis of organic compound.
LO4 To understand advance instrumental techniques for compound interpretation and identification

Course title: Paper 03 Natural products and Spectroscopy
Course code: VESPSCHO303

Unit no.	**Details of topics**	**No of lectures**
1	Natural products-I 1.1 Carbohydrates: Introduction to naturally occurring sugars: Deoxysugars, aminosugars, branched sugars. Structure elucidation of lactose and Dglucosamine (synthesis not expected).Structural features and applications of inositol, starch, cellulose, chitin and heparin. 1.2 Natural pigments: General structural features, occurrence, biological importance and applications of: carotenoids, anthocyanins, quinones, flavones, pterins and porphyrins (chlorophyll). Structure elucidation of βcarotene and Cyanin (with synthesis). Synthesis of ubiquinone from 3, 4, 5- trimethoxyacetophenone. 1.3 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. Alkaloids: Occurrence and physiological importance of morphine and atropine. Structure elucidation, spectral data and synthesis of coniine.	15 Lectures
2	Natural products-II 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 Prostaglandins: Classification, general structure and biological importance. Structure elucidation of PGE1. 2.3 Lipids: Classification, role of lipids, Fatty acids and glycerol derived	15 Lectures

	from oils and fats. 2.4 Insect growth regulators: General idea, structures of JH2 and JH3. 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-tetrahydropyranyloxydodecane expected).	
3	Advanced spectroscopic techniques-I 3.1 Proton NMR spectroscopy: Recapitulation, chemical and magnetic equivalence of protons, First order, second order, Spin system notations (A2, AB, AX, AB2, AX2, AMX and A2B2-A2X2 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, nu clear magnetic double resonance, chemical shift reagents. 3.2 13C –NMR spectroscopy: Recapitulation, equivalent and non-equivalent carbons (examples of aliphatic and aromatic compounds), 13C- chemical shifts, calculation of 13C- chemical shifts of aromatic carbons, heteronuclear coupling of carbon to 19F and 31P. 3.3 Spectral problems based on UV, IR, 1HNMR and 13CNMR and Mass spectroscopy .	15 Lectures
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 and NOESY techniques. [10L] 4.2 Spectral problems based on UV, IR, 1HNMR, 13CNMR (Including 2D technique) and Mass spectroscopy	15 Lectures

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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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Longman,Essex, 1994. 14. Organic Chemistry, Vol 2, I.L. Finar, ELBS, 6th edition, Pearson.
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23. The structure and total synthesis of 5-Vetivone, J. A. Marshall and P. C. Johnson, J. Org. Chem., 35, 192 (1970).
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39. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974.
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47. Biotransformations in Organic Chemistry, 5thEdition, Kurt Faber, Springer
48. Structure Determination of Organic Compounds, EPretsch, P. Buhlmann, C.Affolter, Springer

Detailed Syllabus: Unit wise with number of lectures
Course title: Paper 04 Medicinal, Biogenesis and Green chemistry
Course code: VESPSCHOEC-I 304
Objective: To understand and develop competence in use of medicinal, biogenesis and green synthesis.
Learning Outcomes (LO):
On successful completion of this course students will be able to:

LO1 To learn the basic terminology involved in medicinal organic chemistry.
LO2 To study quantitative structure activity relationship in drug discovery, designing.
LO3 To learn primary and secondary metabolites and their importance in biogenesis.
LO4 To learn basic principles of green chemistry and its applications.

Course title: Paper 04 Medicinal, Biogenesis and green chemistry
Course code: VESPSCHOEC-I 304

Unit no.	Details of topics	No of lectures
1	Drug discovery, design and development 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).	15 Lectures
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- computeraided molecular graphics based drug design, drug design via enzyme inhibition (reversible and irreversible), bioinformatics and drug	15 Lectures

	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.	
3	Biogenesis and biosynthesis of natural products 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, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, flavonoids and isofalvonoids. 3.4 Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes – geranyl cation and its derivatives, sesquiterpenes – farnesyl cation and its derivatives and diterpenes.	15 Lectures
4	Green chemistry 4.1 Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts. 4.2 Use of the following in green synthesis with suitable examples: a) Green reagents: dimethylcarbonate, polymer supported reagents. b) Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts [Aliquat 336, benzyltrimethyl ammonium chloride (TMBA), Tetra-n-butyl ammonium chloride, crown ethers], biocatalysts.c) Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxided) 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. 4.4 Green Cataysts : Nanocatalyst, Types of nanoctalysts, Advantages and Disadvantages of Nanocatalysts, Idea of Magnetically separable nanocatalysts.	15 Lectures

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Unit I

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2. Stryer, Lubert; Biochemistry; W. H. Freeman publishers.

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12. The organic chemistry of drug design and drug action, Richard B. Silverman, 2nd edition, Academic Press

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15. Burger's medicinal chemistry and drug discovery. by Manfred E. Wolf

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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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30. Bioorganic Chemistry- A practical approach to Enzyme action, H. Dugas and C. Penny. Springer Verlag, 1931

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32. Concepts in biotechnology by D. Balasubrarnanian & others

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44. Green chemistry, Theory and Practical, Paul T. Anastas and John C. Warner. 45. New trends in green chemistry By V. K. Ahulwalia and M. Kidwai, 2nd edition, Anamaya Publishers, New Delhi.

46. An introduction to green chemistry, V. Kumar, Vishal Publishing Co.

47. Organic synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

Detailed Syllabus: Unit wise with number of lectures
Course title: Chemistry Paper 04 Bioorganic chemistry
Course code: VESPSCHOEC-II 304
Objective: To understand and develop competence in use of Bioorganic chemistry
Learning Outcomes (LO):
On successful completion of this course students will be able to:

LO1 To know the biomolecules, their structure and importance in life.

LO2 To study organic biomolecular synthesis and metabolic reaction pathways.

LO3 To learn the importance of enzymes and co-enzymes in biological system.

Course title: Chemistry Paper 04 Bioorganic chemistry
Course code: VESPSCHOEC-II 304

Unit no.	Details of topics	No of lectures
1	Biomolecules-I 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, βsheets, 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	15 Lectures

	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.	
2	Biomolecules-II 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.	15 Lectures
3	Biomolecules – III 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	15 Lectures
4	Biomolecules – IV 4.1 Role of main enzymes involved in the synthesis and breakdown of glycogen. 4.2 Enzyme catalyzed organic reactions: Hydrolysis, hydroxylation, oxidation and reduction. 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 mphenoxybenzaldehyde) and immobilized form (production of 6- aminopenicillanic acid).	15 Lectures

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2. Stryer, Lubert; Biochemistry; W. H. Freeman publishers.

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Rev. 2011, 111, 3036-3075;

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25. Biochemistry, Dr U Satyanarayan and Dr U Chakrapani, Books and Allied (P) Ltd.

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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.

M.Sc. (CHEMISTRY)
(SEMESTER III) PRACTICAL

Course code: VESPSCHO3P1
Separation of a ternary mixture of organic compounds and identification including derivative preparations using micro-scale technique.

LO1 To learn separation techniques of ternary mixture.
LO2 To identify the organic compounds and to prepare their respective derivatives.

Unit no.	Details of topics	No of lectures
	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).	

Course code: VESPSCHO3P2
Single step organic preparation (1.0 g scale) involving purification by Steam distillation / Vacuum distillation or Column chromatography.
LO1 To implement various organic reactions in synthetic organic chemistry.
LO2 To study the planning and purification techniques involved in organic synthesis.

Unit no.	Details of topics	No of lectures
	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)	

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12. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011.

M.Sc. ORGANIC CHEMISTRY
(SEMESTER IV)

Course Code	Title	Credits & Lectures per Semester	Lectures per week
VESPSCHO401	**Paper 01** Theoretical organic chemistry-II	**60**	**4**
	Unit I: Physical organic chemistry	**15 Lectures**	
	Unit II: Supramolecular chemistry	**15 Lectures**	
	Unit III: Stereochemistry- II	**15 Lectures**	
	Unit IV: Asymmetric synthesis	**15 Lectures**	
VESPSCHO402	**Paper 02** Synthetic organic chemistry-II	**60**	**4**
	Unit I: Designing Organic Synthesis-I	**15 Lectures**	
	Unit II: Designing Organic Synthesis-II	**15 Lectures**	
	Unit III: Electro-organic chemistry and Selected methods of Organic synthesis	**15 Lectures**	
	Unit IV: Transition and rare earth metals in organic synthesis	**15 Lectures**	
VESPSCHO403	**Paper 03** Natural products and heterocyclic chemistry	**60**	**4**
	Unit I: Natural products-III	**15 Lectures**	
	Unit II: Natural products-IV	**15 Lectures**	
	Unit III: Heterocyclic compounds-I	**15 Lectures**	
	Unit IV: Heterocyclic compounds-II	**15 Lectures**	
VESPSCHOOC-I 404	**Paper 04** INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS)	**60**	**4**
	Unit I: Introduction to Intellectual Property: Patents: Industrial Designs: Copyrights: Trade Marks: Geographical Indications:	**15 Lectures**	

	Unit II: Trade Secrets: IP Infringement issue and enforcement: Economic Value of Intellectual Property: Different International agreements: (a) World Trade Organization (WTO): (b) Paris Convention WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity	**15 Lectures**	
	Unit III: Introduction to Cheminformatics Representation of molecules and chemical reactions: Searching Chemical Structures:	**15 Lectures**	
	Unit IV: Applications	**15 Lectures**	
VESPSCHOOC-II 404 RESEARCH METHODOLOGY	**Paper 04** RESEARCH METHODOLOGY	**60**	**4**
	Unit I: Print: Journals Digital: Information Technology and Library Resources:	**15 Lectures**	
	Unit II: DATA ANALYSIS: The Investigative Approach: Analysis and Presentation of Data	**15 Lectures**	
	Unit III: METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS Writing Scientific Papers	**15 Lectures**	
	Unit IV: CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS	**15 Lectures**	
VESPSCHO4P1	**Paper 01** Theoretical organic chemistry-II		
VESPSCHO4P2	**Paper 02** Synthetic organic chemistry-II		
VESPSCHO4P3	**Paper 03** Natural products and heterocyclic chemistry		
VESPSCHO4P4B	**Paper 04** Research Methodology		

Detailed Syllabus: Unit wise with number of lectures
Course title: Chemistry Paper 01 Theoretical organic chemistry-II
Course code: VESPSCHO401
Objective: To understand and develop competence in use of Theoretical organic chemistry

LO1 To learn physical organic chemistry aspects (structural effects and reactivity) for organicchemistry.
LO2 To study supramolecular chemistry and its applications in organic synthesis
LO3 To understand the stereo-chemical aspects and its applications in organic synthesis
LO4 To study principles of asymmetric synthesis and chiral auxiliaries in asymmetric synthesis

Unit no.	Details of topics	No of lectures
1	Physical organic chemistry 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 σvalues, 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, σI and σR scales, steric parameters Es and β. Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's ET parameter, Solvatochromism Zscale, Spectroscopic Correlations, Thermodynamic Implications.	15 Lectures
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. 2.4 Molecular recognition and catalysis, molecular selfassembly.Supramolecular Polymers, Gelsand Fibres	15 Lectures
3	Stereochemistry- II 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. 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). 3.3 Correlative method for configurational assignment: chemical, optical rotation, and NMR spectroscopy.	15 Lectures

	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	
4	Asymmetric synthesis 4.1 Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions. 4.2 Synthesis of L-DOPA [Knowles's Mosanto 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. 4.3 Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations.	15 Lectures

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31 Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, WileyEastern 32 Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific 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)

Detailed Syllabus: Unit wise with number of lectures
Course title: Chemistry Paper 02 Synthetic organic Chemistry-II
Course code: VESPSCHO402
Objective: To understand and develop competence in use of Synthetic organic chemistry

LO1 To learn the synthetic planning and designing in various organic synthesis.

LO2 To understand the methodology, basics, and applications of electro-organic chemistry.

LO3 To study applications of organometallics (transition and rare earth elements) in organicsynthesis.

LO4 To learn the synthetic planning and designing in various organic synthesis.

Unit no.	Details of topics	No of lectures

1	Designing Organic Synthesis-I 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 thiomethyl sulfoxides, 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.	15 Lectures
2	Designing Organic Synthesis-II 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.	15 Lectures
3	Electro-organic chemistry and Selected methods of Organic synthesis [15L] 3.1 Electro-organic chemistry: 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 alkylbezene, 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.	15 Lectures

4	Transition and rare earth metals in organic synthesis 4.1 Introduction to basic concepts: 18 electron rule, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion. 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-Miayura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N, S, or P atoms. 4.3 Olefin metathesis using Grubb's catalyst. 4.4 Application of Ni, Co, Fe, Rh, and Cr carbonyls in organic synthesis. 4.5 Application of samarium iodide including reduction of organic halides, aldehydes and ketones, α-functionalised carbonyl and nitro compounds. 4.6 Application of Ce(IV) in synthesis of heterocyclic quinoxaline derivatives and its role as a de-protecting agent.	15 Lectures

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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.
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5. Modern Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).
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8. Organic Chemistry, 7th Edn, 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, 2nd Edn., B. Miller & R. Prasad,Pearson
11. Organic reactions and their mechanisms, 3rd revisededition, P.S. Kalsi, New AgeInternational Publishers
12. Organic Synthesis: The Disconnection Approach, Stuart Warren, John Wiley & Sons, 2004
13. Name Reactions and Reagents in Organic Synthesis, 2nd Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
14. Name Reactions, Jie Jack Lie, 3rd Edn., Springer
15. Organic Electrochemistry, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker

Detailed Syllabus: Unit wise with number of lectures

Course title: Chemistry Paper 03 Natural products and heterocyclic chemistry

Course code: VESPSCHO403

Objective: To understand and develop competence in use of natural products and heterocyclic compounds.

LO1 To learn the importance of steroids, vitamins and terpenoids in natural products.

LO2 To study the heterocyclic chemistry (3-6 membered rings) and their applications in organicsynthesis.

Unit no.	Details of topics	No of lectures
1	Natural products-III 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 acids. 1.2 Synthesis of 16-DPA from cholesterol and plant sapogenin. 1.3 Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone. 1.4 Synthesis of cinerolone, jasmolone, allethrolone, exaltone and muscone.	15 Lectures
2	Natural products-IV 2.1 Vitamins: Classification, sources and biological importance of vitamin B1, B2, B6, folic acid, B12, C, D1, E (α-tocopherol), K1, K2, H (β- biotin). 2.2 Synthesis of the following: Vitamin A from β-ionone and bromoester moiety. Vitamin B1 including synthesis of pyrimidine and thiazole moieties Vitamin B2 from 3, 4-dimethylaniline and D(-)ribose Vitamin B6 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 K1 from 2-methyl-1, 4-naphthaquinone and one and phytol. 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). 2.3 Naturally occurring insecticides: Sources, structure and biological properties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis of pyrethrin I. 2.4 Terpenoids: Occurrence, classification, structure elucidation, stereochemistry, spectral data and synthesis of zingiberene .	15 Lectures
3	Heterocyclic compounds-I 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., conjugated polyenes (cyclic and acyclic), carbonyl and unsaturated carbonyl compounds, substituted aromatic compounds. Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, and solvent polarity. Calculation of absorption maxima for above classes of compounds by Woodward-Fieser rules (using Woodward-Fieser tables for values for substituents). 3.2.2. Infrared spectroscopy: Fundamental, overtone and combination bands, vibrational coupling, factors affecting vibrational frequency (atomic weight, conjugation, ring size, solvent and hydrogen bonding). Characteristic vibrational frequencies for alkanes, alkenes, alkynes, aromatics, alcohols, ethers, phenols, amines, nitriles and nitro compounds. Detailed study of vibrational frequencies of carbonyl compounds, aldehydes, ketones, esters, amides, acids, acid halides,	15 Lectures

	anhydrides, lactones, lactams and conjugated carbonyl compounds.	
4	Heterocyclic compounds-II 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.	15 Lectures

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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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7. Heterocyclic chemistry, 3rd edition, Thomas L. Gilchrist, Pearson Education, 2007.
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32. Selected Organic synthesis, Ian Fleming, John Wiley and Sons, 1973.
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35. Classics in Total Synthesis , K. C. Nicolaou and E. J. Sorensen, Weinhem: VCH, 1996.
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37. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987.
38. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991
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40. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989.
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Detailed Syllabus: Unit wise with number of lectures
Course title: Chemistry Paper 04 INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS
Course code: VESPSCHOOC-I 404
Objective: To understand and develop intellectual property rights and cheminformatics.

LO1 To learn various terms and terminology involved in intellectual property rights
LO2 To study trade secrets and economic value of intellectual property.
LO3 To know the evolution of cheminformatics and its application.

Unit no.	Details of topics	No of lectures
1	Introduction to Intellectual Property: Historical Perspective, Different types of IP, Importance of protecting IP. Patents: Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing	15 Lectures

	promoting innovation with public health, Software patents and their importance for India. Industrial Designs: Definition, How to obtain, features, International design registration. Copyrights: Introduction, How to obtain, Differences from Patents. Trade Marks: Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc. Geographical Indications: Definition, rules for registration, prevention of illegal exploitation, importance to India.	
2	Trade Secrets: Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection. IP Infringement issue and enforcement: Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. Economic Value of Intellectual Property: Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer. 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 (b) Paris Convention [6L] WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity	15 Lectures
3	Introduction to Cheminformatics: History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation. 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. 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.	15 Lectures
4	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, Ligandbased and Structure based Drug design, Application of Cheminformatics in Drug Design.	15 Lectures

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Detailed Syllabus: Unit wise with number of lectures
Course title: RESEARCH METHODOLOGY
Course code: VESPSCHOOC-II 404
Objective: To understand research methodology and develop scientific attitude
LO1 To learn research methodology for research data analysis and scientific writing.
LO2 To study the chemical safety and ethical handling of chemicals.
LO3 To learn the writing skills in scientific research project/ practical work

Unit no.	Details of topics	No of lectures
1	Unit 1: Print: Primary, Secondary and Tertiary sources. 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 Digital: 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. Information Technology and Library Resources: The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.	15 Lectures
2	The Investigative Approach: Making and recording Measurements, SI units and their use, Scientific methods and design of experiments. 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.	15 Lectures
3	METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation. 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.	15 Lectures
4	CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS 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.	15 Lectures

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M.Sc. (CHEMISTRY)
(SEMESTER IV) PRACTICALS

Course code: VESPSCHO4P1

LO1 To learn two step preparation techniques and find out the yield of the product.

Unit no.	Details of topics	No of lectures
	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 → cyclohexanone oxime → Caprolactum. 4. Hydroquinone → hydroquinone diacetate → 2,5-dihydroxyacetophenone. 5. 4-nitrotoluene → 4-nitrobenzoic acid → 4-aminobenzoic acid. 6. o-nitroaniline → o-phenylene diamine → Benzimidazole. 7. Benzophenone → benzophenone oxime → 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 method. 12. Anthracene → anthraquinone → anthrone.	

Course code: **VESPSCHO4P2** **Semester IV**

LO1 To learn the interpretation of the organic compounds by various spectroscopic techniques (UV,IR, PMR, CMR and Mass spectra).

Unit no.	Details of topics	No of lectures
	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 text-book/reference material etc	
	Session-II: Project evaluation	

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
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.

Modality of assessment

The performance of the learners shall be evaluated into two parts. The learner's performance shall be assessed by Internal Assessment with 40% marks in the first part & by conducting the Semester End Examinations with 60% marks in the second part. Practical Examination will consist of End Sem examination.

Student will have to score 40% of marks in Internal assessment as well as End Sem examination to pass the course.

The allocation of marks for the Internal Assessment and Semester End Examinations are as shown below:-

Internal Assessment: It is defined as the assessment of the learners on the basis of internal evaluation as envisaged in the Credit & Choice based system by way of participation of learners in various academic and correlated activities in the given semester of the programme.

Semester End Assessment : It is defined as the assessment of the learners on the basis of Performance in the semester end Theory/ written/ Practical examination.

A. Theory - Internal assessment 40% **40 marks**

Sr No	Evaluation type	Marks
1.	Seminar presentation/internship/project	40

B. Theory - External examination - 60% **60 marks**

Semester End Theory Assessment **Semester End Theory Assessment**

Duration - Each paper shall be of 2.5 hours' duration.

1. Theory question paper pattern as per the university pattern : -
   a. There shall be FIVE compulsory questions.
   b. Question No 1, 2, 3 and 4 will be based upon Unit 01, Unit 02, Unit 03 and Unit 04 respectively.
   c. Question No 05 will be based on Unit 01, 02 ,03 and 04 two questions from each unit.

Question no.	**Details**	**Marks**
Q1.	**(Unit 01)**	12M
	Attempt **any three of the six** A) /B) / C) /D) /E) /F)	
Q2.	**(Unit 02)**	12M
	Attempt **any three of the six** A**)/** B)/C)/D)/E)/F)	
Q3.	**(Unit 03)**	12M
	Attempt **any three of the six** A)/B)/C)/D)/E)/F)	
Q4	**(Unit 04)**	12M
	Attempt **any three of the six** A**)/**B)/C)/D)/E)/F)	

Q5	**(Unit 01, 02 ,03 and 04)**	12M
	Attempt **any four out of eight** A)/B)/C)/D)/E)/F)/G)/H)	

C. For Each Semester Practical Assessment

	Section 1 Based on Paper 02	**Marks**
A	Experimental work	40
B	Viva	05
C	Journal	05
		50 Marks

PRACTICAL BOOK/JOURNAL

The students are required to present a duly certified journal for appearing at the practical examination, failing which they will not be allowed to appear for the examination.

In case of loss of Journal and/ or Report, a Lost Certificate should be obtained from Head/ Coordinator / In-charge of the department ; failing which the student will not be allowed to appear for the practical examination.

Overall Examination and Marks Distribution Pattern

SEMESTER III

Course	**VESPSCHO301**	**VESPSCHO302**	**VESPSCHO303**	**VESPSCHOEC I-304**	**Grand Total**
Theory	**100**	**100**	**100**	**100**	**400**
Course	**VESPSCHO3P1**	**VESPSCHO3P2**	**VESPSCHO3P3**	**VESPSCHO3P4**	**Grand Total**
Practical	**50**	**50**	**50**	**50**	**200**

SEMESTER IV

Course	**VESPSCHO401**	**VESPSCHO402**	**VESPSCHO403**	**VESPSCHOOC -II 404**	**Grand Total**
Theory	**100**	**100**	**100**	**100**	**400**
Course	**VESPSCHO4P1**	**VESPSCHO4P2**	**VESPSCHO4P3**	**VESPSCHO4P4**	**Grand Total**
Practical	**50**	**50**	**50**	**50**	**200**