



The Kelkar Education Trust's  
**Vinayak Ganesh Vaze College of Arts, Science & Commerce**  
**AUTONOMOUS**

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**Syllabus for M. Sc. Part-II Programme**

**Chemistry (Specialization Organic Chemistry)**

Syllabus as per Choice Based Credit System (NEP-2020)

**(June 2024 Onwards)**

**Submitted by**

**Department of Chemistry**

**Vinayak Ganesh Vaze College of Arts, Science and Commerce**

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❖ Syllabus as per Choice Based Credit System (NEP 2020)

**Syllabus for Approval**

**Chemistry (Specialization Organic Chemistry)**

Sr. No.	Heading	Particulars
1	Title of Programme	M.Sc. Chemistry:Semester IIIand IV
2	Eligibility for Admission	The B.Sc. degree examination of this university with chemistry 6 units or degree of anyother university recognized as equivalent thereto.
3	Passing marks	Minimum D Grade or equivalent minimum marks for passing at the Graduation level.
4	Ordinances/Regulations (if any)	---
5	No. of Years/Semesters	One year/Two semester
6	Level	P.G. part-II : Level-6.5
7	Pattern	Semester
8	Status	Revised
9	To be implemented from Academic year	2024-2025

Date: 22/03/2024

Signature:

BOS Chairperson: Prof. Suresh S. Shendage

## Post Graduate Program in Chemistry (Organic Chemistry Specialization)

Year (2 Yr PG)	Level	Sem. (2 Yr)	Major		RM	OJT / FP	RP	Cum. Credits	Degree
			Mandatory*	Electives Anyone					
2	6.5	Sem-III	For Organic Chemistry Specialization						PG Degree After 3- Yr UG
			<b>Credits 14 (4+4+4+2)</b> Course 1 Credits 4 :Theoretical organic Chemistry-I Course 2 Credits 4 :Synthetic Organic Chemistry-I Course 3 Credits 4 :Natural products and Spectroscopy Course 4 Credits 2 : <b>Practicals</b> (Separation of a ternary mixture & Combined Spectral Interpretation & Identification Organic Compounds)	<b>Credits 4 (2+2)</b> <b>Course 1:</b> Medicinal Chemistry & <b>Practicals :</b> Single Step Organic Preparation OR <b>Course 2:</b> Biogenesis and Green Chemistry & <b>Practicals :</b> Single Step Organic Preparation	--	--	04	22	
		Sem-IV	For Organic Chemistry Specialization						
			<b>Credits 12 (4+4+4)</b> Course 1 Credits 4 : Theoretical organic Chemistry-II Course 2 Credits 4 : Synthetic Organic Chemistry-II Course 3 Credits 4 : Natural Products and Heterocyclic Chemistry	<b>Credits 4 (2+2)</b> <b>Course 1:</b> Intellectual Property Rights and <b>Practical :</b> Two Step Organic Preparations OR <b>Course 2:</b> Cheminformatics and <b>Practical :</b> Two Step Organic Preparations	--	--	06	22	
<b>Cum. Cr. for 2 Year PG Degree</b>			<b>54</b>	<b>16</b>	<b>4</b>	<b>4</b>	<b>10</b>	<b>88</b>	
<b>2 Years - 4 Sem. PG Degree (80-88) credits after 3 Years UG Degree</b>									

## Programme Educational Objectives

<b>PEO1</b>	Achievement of mastery of chemistry in a foundational level to the current knowledge
<b>PEO2</b>	Development of cognitive research skills at a level required to pursue higher education
<b>PEO3</b>	Understanding of experimentation, observation and data analysis suitable for any Chemistry based industry
<b>PEO4</b>	Familiarity with available instrumentation for conducting specific scientific research
<b>PEO5</b>	To communicate effectively, verbally and written, for the purposes of conveying chemical information to both professional scientists and to the public

## Programme Outcomes

<b>PO1</b>	To understand the application of the classical subjects in modern chemistry
<b>PO2</b>	To master factual and experimental knowledge across the principal areas of chemistry
<b>PO3</b>	To demonstrate competence in solving industrial scientific problems through experimental, computational and/or data analysis models
<b>PO4</b>	To indulge in deeper learning of the principles of Organic, Inorganic and Physical Chemistry
<b>PO5</b>	To learn modern analytical and spectroscopic tools and their applications to different disciplines of chemistry
<b>PO6</b>	To design and conduct experiments as well as to analyse and interpret the data
<b>PO7</b>	To work effectively both as an individual and as a collaborative team member
<b>PO8</b>	To learn the interdisciplinary nature of chemistry and to integrate the knowledge with a variety of chemical problems
<b>PO9</b>	To appreciate the importance of goal-setting and to recognize the need for life-long reflective learning.
<b>PO10</b>	To learn, design and demonstrate sustainable industrial reactions within realistic constraints such as economic, environmental, social, ethical, health, safety and productivity

## Curriculum

The total minimum credits required for completing the M.Sc. in Chemistry is **66**

<b>SEMESTER -III</b>					
<b>Code</b>	<b>Course of Study</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
VGVP SMCH301	Theoretical organic Chemistry-I	4	-	-	4
VGVP SMCH302	Synthetic Organic Chemistry-I	4	-	-	4
VGVP SMCH303	Natural products and Spectroscopy	4	-	-	4
VGVP SMCHP301	<b>Practicals</b> : (Separation of a ternary mixture & Combined spectral Interpretation )	-	-	4	2
	<b>Electives</b>				
VGVP SELCH301	Medicinal Chemistry	2	-	-	2
VGVP SELCHP301	Practicals : Single Step Organic Preparation	-	-	4	2
VGVP SELCH302	Biogenesis and Green Chemistry	2	-	-	2
VGVP SELCHP302	Practicals : Single Step Organic Preparation	-	-	4	2
VGVP SRPCH301	<b>Research Project (RP)</b>	-	-	8	4
		-	-	-	<b>22</b>

\*\*\*\*\* **Note:** Students are allowed to select one elective out of two electives given in curriculum

<b>SEMESTER - IV</b>					
<b>Code</b>	<b>Course of Study</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
VGVPSMCH401	Theoretical organic Chemistry-II	4	-	-	4
VGVPSMCH402	Synthetic Organic Chemistry-II	4	-	-	4
VGVPSMCH403	Natural Products and Heterocyclic Chemistry	4	-	-	4
VGVPSMCHP401	<b>Practicals :</b>	-	-	-	-
	<b>Electives</b>				
VGVPSELCH401	Intellectual Property Rights	2	-	-	2
VGVPSELCHP401	Practicals : Two Step Organic Preparations	-	-	4	2
VGVPSELCH402	Cheminformatics	2	-	-	2
VGVPSELCHP402	Practicals : Two Step Organic Preparations	-	-	4	2
VGVPSRPCH401	<b>Research Project (RP)</b>	-	-	12	6
		-	-	-	<b>44</b>

\*\*\*\*\* **Note:** Students are allowed to select one elective out of two electives given in curriculum

### Evaluation Pattern

<b>Continuous Internal Assessment (CIA)</b> 40 marks					<b>End Semester Examination</b> 60 Marks		<b>Total Marks</b>
<b>Course</b>	<b>Credit</b>	<b>CIA-1</b>	<b>CIA-2</b>	<b>CIA-3</b>	<b>Theory</b>	<b>Practical</b>	
Mandatory	4.0	15	15	10	60	100	100
Electives	2.0	15	15	10	60	100	100
Practicals	2.0	-	-	-	-	100	100
Research Project (RP)	4.0/ 6.0	-	-	-	-	100	100

**Proposed Draft Syllabus for M.Sc. Chemistry Semester III and IV**  
**(Organic Chemistry Specialization)**  
**Choice Based Credit System (NEP 2020)**  
(To be implemented from the academic year, 2024-2025)

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**Semester – III**

**Paper I**

**Course Code: VGVPSMCH301**

**Credits: 4**

**Theoretical Organic Chemistry-I**

**Course Learning Objectives**

Upon completion of the course the student will be able to understand

- The basics of reaction mechanism and the mechanistic concepts
- The fundamentals of substitution reactions and reactive intermediates
- The mechanism of elimination reactions and important redox reagents
- The concept of Pericyclic reactions
- Stereochemistry of different types of compounds and reactions
- To introduce the students regarding the fundamentals of photochemistry and various photochemical reactions in detail

**Course Outcome**

Upon completing the course the student will be able to understand

<b>CO1</b>	The basics of reaction mechanism and the mechanistic concepts
<b>CO2</b>	Understand the various types of rearrangement reactions and their mechanism.
<b>CO3</b>	The Concept of Pericyclic reactions and their applications
<b>CO4</b>	Understand the stereochemistry of organic molecules in detail.
<b>CO5</b>	Solve various problems on photochemical transformations.

**COURSE CONTENT**

<b>Unit 1</b>	<b>Organic reaction mechanisms</b>	<b>15H</b>
	<b>1.1</b> Organic reactive intermediates, methods of generation, structure, stability and important reactions involving carbocations, nitrenes, carbenes, arynes and ketenes.	<b>05H</b>
	<b>1.2</b> Neighbouring group participation: Mechanism and effects of anchimeric assistance, NGP by unshared/ lone pair electrons, $\pi$ -electrons, aromatic rings, $\sigma$ -bonds with special reference to norbornyl and <b>bicyclo[2.2.2]octyl cation</b> systems (formation of non-classical carbocation)	<b>03H</b>
	<b>1.3</b> Role of FMOs in organic reactivity: Reactions involving hard and soft electrophiles and nucleophiles, ambident nucleophiles, ambident electrophiles, the $\alpha$ effect.	<b>02H</b>
	<b>1.4</b> Pericyclic reactions: Classification of pericyclic reactions; thermal and photochemical reactions. Three approaches: Evidence for the concernedness of bond making and breaking Symmetry-Allowed and Symmetry-Forbidden	<b>05H</b>
	<b>Reactions –</b> <ul style="list-style-type: none"><li>• The Woodward-Hoffmann Rules-Class by Class</li><li>• The generalized Woodward-Hoffmann Rule Explanations for Woodward-</li></ul>	

	<p>Hoffmann Rules</p> <ul style="list-style-type: none"> <li>• The Aromatic Transition structures [Huckel and Mobius]</li> <li>• Frontier Orbitals</li> <li>• Correlation Diagrams, FMO and PMO approach Molecular orbital symmetry, Frontier orbital of ethylene, 1,3 butadiene, 1,3,5-hexatriene and allyl system.</li> </ul>	
<b>Unit 2</b>	<b>Pericyclic Reactions</b>	<b>15H</b>
	<p><b>2.1 Cycloaddition reactions:</b> Supra and antarafacial additions, <math>4n</math> and <math>4n+2</math> 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.</p> <p><b>Other Cycloaddition Reactions-</b> [4+6] Cycloadditions, Ketene Cycloaddition, Allene Cycloadditions, Carbene Cycloaddition, Epoxidation and Related Cycloadditions. Other Pericyclic reactions: Sigmatropic Rearrangements, Electrocyclic Reactions, Alder 'Ene' Reactions.</p>	<b>07H</b>
	<p><b>2.2 Electrocyclic reactions:</b> Conrotatory and disrotatory motions, <math>4n\pi</math> and <math>(4n+2)\pi</math> electron and allyl systems.</p>	<b>03H</b>
	<p><b>2.3 Sigmatropic rearrangements:</b> H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations. Cope (including oxy-Cope and aza-Cope) and Claisen rearrangements. Formation of Vitamin D from 7-dehydro cholesterol, synthesis of citral using pericyclic reaction, conversion of Endiandric acid E to Endiandric acid A.</p>	<b>05H</b>
<b>Unit3</b>	<b>Stereochemistry-I</b>	<b>15H</b>
	<p><b>3.1</b> Classification of point groups based on symmetry elements with examples (Nonmathematical treatment).</p>	<b>02H</b>
	<p><b>3.2</b> Conformational analysis of medium rings: Eight to ten membered rings and their unusual properties, I-strain, transannular reactions.</p>	<b>03H</b>
	<p><b>3.3</b> Stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, perhydroanthracenes, steroids, and Bredt's rule.</p>	<b>05H</b>
	<p><b>3.4 Anancomeric systems,</b> Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism): electrophilic addition, elimination, molecular rearrangements, reduction of cyclohexanones (<b>with LiAlH<sub>4</sub>, selectride and MPV reduction</b>) and oxidation of cyclohexanols.</p>	<b>05H</b>
<b>Unit 4</b>	<b>Photochemistry</b>	<b>15H</b>
	<p><b>4.1 Principles of photochemistry:</b> quantum yield, electronic states and transitions, selection rules, modes of dissipation of energy (Jablonski diagram), electronic energy transfer: photosensitization and quenching process.</p>	<b>03H</b>
	<p><b>4.2 Photochemistry of carbonyl compounds:</b> <math>\pi \rightarrow \pi^*</math>, <math>n \rightarrow \pi^*</math> transitions, Norrish-I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, photochemical rearrangements of <math>\alpha</math>, <math>\beta</math>-unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction.</p>	<b>08H</b>

	<b>4.3 Photochemistry of olefins:</b> cis-trans isomerizations, dimerizations, hydrogen abstraction, addition and Di- $\pi$ -methane rearrangement including aza-di- $\pi$ -methane. Photochemical Cross-Coupling of Alkenes, Photodimerisation of alkenes.	<b>02H</b>
	<b>4.4 Photochemistry of arenes:</b> 1, 2-, 1, 3- and 1, 4- additions. Photocycloadditions of aromatic Rings.	<b>01H</b>
	<b>4.5 Singlet oxygen and photo-oxygenation reactions.</b> Photochemically induced Radical Reactions. Chemiluminescence.	<b>01H</b>

#### Reference Books:

1. March's Advanced Organic Chemistry, Jerry March, sixth edition, 2007, John Wiley and sons.
2. A guide to mechanism in Organic Chemistry, 6th edition, 2009, Peter Sykes, Pearson education, New Delhi.
3. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002).
4. 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.
8. Carbenes, Nitrenes and Arynes. Von T. L. Gilchrist, C. W. Rees. Th.Nelson and Sons Ltd., London
9. Organic reactive intermediates, Samuel P. MacManus, AcademicPress.
10. Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers,1st Edition, Oxford University Press (2001).
11. Organic Chemistry, Seventh Edition, R.T. Morrison, R. N. Boyd &S. K. Bhattacharjee, Pearson. Advanced Organic Chemistry: Reactions & Mechanisms, second edition, B. Miller and R. Prasad, Pearson.
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
14. Organic Chemistry, W. G. Solomons, C. B. Fryhle, , 9th Edition, Wiley India Pvt. Ltd.,2009.
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 edn, 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, 1997.
  31. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley-Eastern
  32. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
  33. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
  34. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
  35. Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
  36. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
  37. Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A John Wiley and Sons, Ltd., Publication)
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**Semester – III**  
**Paper II**  
**Course Code: VGVPSMCH302**  
**Credits: 4**  
**Synthetic Organic Chemistry-I**

**Course Outcome**

Upon completing the course, the student will be able to understand

<b>CO1</b>	the concept of retrosynthesis and the terms involved
<b>CO2</b>	about one group and two group disconnections
<b>CO3</b>	the various protection and deprotection of important functional groups
<b>CO4</b>	the use of important reagents in organic synthesis
<b>CO5</b>	about selected name reactions in Organic synthesis

**Course Content**

<b>Unit-1</b>	<b>Name reactions with mechanism and application</b>	<b>15 H</b>
	<b>1.1</b> Mukaiyama esterification, Mitsunobu reaction, Darzen's Glycidic Esters synthesis, Ritter reaction, Yamaguchi esterification, Peterson olefination.	<b>05 H</b>
	<b>1.2 Domino reactions:</b> Characteristics; Nazarov cyclization	<b>03 H</b>
	<b>1.3 Multicomponent reactions:</b> Strecker Synthesis, Ugi 4CC, Biginelli synthesis, Hantzsch synthesis, Pictet-Spengler synthesis	<b>05 H</b>
	<b>1.4 Click Reactions:</b> Characteristics; Huisgen 1,3-Dipolar Cycloaddition	<b>02H</b>
<b>Unit-2</b>	<b>Radicals in organic synthesis</b>	<b>15 H</b>
	<b>2.1 Introduction:</b> Generation, stability, reactivity and structural and stereochemical properties of free radicals, Persistent and charged radicals, Electrophilic and nucleophilic radicals.	<b>03 H</b>
	<b>2.2 Radical Initiators:</b> azobisisobutyronitrile (AIBN) and dibenzoyl peroxide.	<b>01 H</b>
	<b>2.3 Characteristic reactions</b> - Free radical substitution, addition to multiple bonds. Radical chain reactions, Radical halogenation of hydrocarbons (Regioselectivity), radical cyclization, autoxidations: synthesis of cumene hydroperoxide from cumene.	<b>04 H</b>
	<b>2.4 Radicals in synthesis:</b> Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol donors. Cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds. Oxidative coupling, C-C bond formation in aromatics: $S_{RN}Ar$ reactions.	<b>04H</b>
	<b>2.5</b> Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Sandmeyer reaction, Acyloin condensation.	<b>03H</b>
<b>Unit-3</b>	<b>Enamines, Ylides and <math>\alpha</math>-C-H functionalization</b>	<b>15 H</b>
	<b>3.1 Enamines:</b> 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.	<b>04 H</b>

	3.2 <b>Phosphorus, Sulphur and Nitrogen Ylides:</b> Preparation and their synthetic applications along with their stereochemical aspects. Wittig reaction, Horner-Wadsworth-Emmons Reaction, Barton-Kellogg olefination.	<b>06 H</b>
	3.3 <b><math>\alpha</math>-C-H functionalization:</b> 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-Stephen's reaction, Julia olefination and its modification, Seyferth-Gilbert homologation, Steven's rearrangement.	<b>05H</b>
<b>Unit-4</b>	<b>Metals / Non-metals in organic synthesis</b>	<b>15 H</b>
	4.1 <b>Mercury in organic synthesis:</b> Mechanism and regiochemistry of oxymercuration and demercuration of alkenes, mercuration of aromatics, transformation of aryl mercurials to aryl halides. Organomercurials as carbene transfer reagents.	<b>03 H</b>
	4.2 <b>Organoboron compounds:</b> 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.	<b>03 H</b>
	4.3 <b>Organosilicons:</b> Salient features of silicon governing the reactivity of organosilicons, preparation and important bond-forming reactions of alkylsilanes, alkenyl silanes, aryl silanes and allyl silanes. $\beta$ -silyl cations as intermediates. Iodotrimethyl silane in organic synthesis.	<b>03 H</b>
	4.4 <b>Silyl enol ethers:</b> Application: As nucleophiles (Michael reaction, Mukaiyama aldol reaction), in ring contraction reactions.	<b>02H</b>
	4.5 <b>Organotin compounds:</b> Preparation of alkenyl and allyl tin compounds; application in C-C bond formation, in replacement of halogen by H at same C atom	<b>02H</b>
	4.6 <b>Selenium in organic synthesis:</b> Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and seleno acetals as $\alpha$ -C-H activating groups	<b>02H</b>

#### Reference Books:

- Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5<sup>th</sup> Edition, Springer Verlag
  - Modern Methods of Organic Synthesis, 4<sup>th</sup> Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
  - Organic Chemistry, Clayden Greeves Warren and Wothers, Oxford Press (2001).
  - Moder Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).
  - Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002).
  - Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3<sup>rd</sup> Edn., Nelson Thornes
  - Organic Chemistry, 7<sup>th</sup> Edn, R. T. Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson
  - Advanced Organic Chemistry: Reactions & Mechanisms, 2<sup>nd</sup> Edn., B. Miller & R. Prasad, Pearson
  - Organic Synthesis: The Disconnection Approach, Stuart Warren, John Wiley & Sons, 2004
  - Name Reactions and Reagents in Organic Synthesis, 2<sup>nd</sup> Edn.,
  - Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
  - Name Reactions, Jie Jack Lie, 3<sup>rd</sup> Edn., Springer
  - Organic Electrochemistry, H. Lund, and M. Baizer, 3<sup>rd</sup> Edn., Marcel Dekker.
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**Semester – III**  
**Paper III**  
**Course Code: VGVPSMCH303**  
**Credits: 4**  
**(Natural products and Spectroscopy)**

**COURSE OUTCOME**

Upon completing the course the student will be able to

<b>CO1</b>	Have a detailed understanding about General structural features, occurrence, biological importance and applications of different Natural products
<b>CO2</b>	Learn about the Multi-step synthesis of different natural products
<b>CO3</b>	Learn about the different pulse sequences and applications of <sup>1</sup> H-NMR spectroscopy and <sup>13</sup> C – NMR spectroscopy to the structural characterization of molecules
<b>CO4</b>	Advanced spectroscopic techniques
<b>CO5</b>	Combined Spectroscopic approach for problem solving and structural analysis

**COURSE CONTENT**

<b>Unit-1</b>	<b>Natural products-I</b>	<b>15 H</b>
	<p><b>1.1 Carbohydrates:</b> Introduction to naturally occurring sugars: Deoxysugars, aminosugars, branched sugars. Structure elucidation of lactose and D-glucosamine (Synthesis not expected). Structural features and applications of inositol, starch, cellulose, chitin and heparin.</p> <p><b>1.2 Natural pigments:</b> General structural features, occurrence, biological importance and applications of: carotenoids, anthocyanins, quinones, flavones, pterins and porphyrins (chlorophyll). Structure elucidation of β-carotene and Cyanin (with synthesis). Synthesis of ubiquinone from 3, 4, 5-trimethoxy acetophenone.</p> <p><b>1.3 Insect pheromones:</b> 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.</p> <p><b>1.4 Alkaloids:</b> Occurrence and physiological importance of morphine and atropine. Structure elucidation, spectral data and synthesis of coniine.</p>	<p><b>05 H</b></p> <p><b>05 H</b></p> <p><b>03H</b></p> <p><b>02H</b></p>
<b>Unit-2</b>	<b>Natural products-II</b>	<b>15 H</b>
	<p><b>2.1 Multi-step synthesis of natural products:</b> Synthesis of the following natural products with special reference to reagents used, stereochemistry and functional group transformations:</p> <p>a) Woodward synthesis of Reserpine from benzoquinone</p> <p>b) Corey synthesis of Longifoline from resorcinol</p> <p>c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol</p> <p>d) Corey's Synthesis of Caryophyllene from 2-Cyclohexenone and Isobutylene</p> <p>e) Synthesis of Juvabione from Limonene</p> <p>f) Synthesis of Taxol.</p>	<b>08 H</b>

	2.2 <b>Prostaglandins:</b> Classification, general structure and biological importance. Structure elucidation of <b>PGE<sub>1</sub></b> .	<b>02 H</b>
	2.3 <b>Lipids:</b> Classification, role of lipids, Fatty acids and glycerol derived from oils and fats.	<b>02 H</b>
	2.4 <b>Insect growth regulators:</b> General idea, structures of JH <sub>2</sub> and JH <sub>3</sub>	<b>03H</b>
	2.5 <b>Plant growth regulators:</b> 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).	
<b>Unit-3</b>	<b>Advanced spectroscopic techniques-I</b>	<b>15 H</b>
	<b>3.1 Proton NMR spectroscopy:</b> Recapitulation, chemical and magnetic equivalence of protons, First order, second order, Spin system notations (A <sub>2</sub> , AB, AX, AB <sub>2</sub> , AX <sub>2</sub> , AMX and A <sub>2</sub> B <sub>2</sub> -A <sub>2</sub> X <sub>2</sub> spin systems with suitable examples). Long range coupling (Allylic coupling, 'W' coupling and coupling in aromatic and hetero-aromatic systems), Temperature effects, Simplification of complex spectra, nuclear magnetic double resonance, chemical shift reagents.	<b>07 H</b>
	<b>3.2 <sup>13</sup>C –NMR spectroscopy:</b> Recapitulation, equivalent and non-equivalent carbons (Examples of aliphatic and aromatic compounds), <sup>13</sup> C- chemical shifts, calculation of <sup>13</sup> C- chemical shifts of aromatic carbons, hetero-nuclear coupling of carbon to <sup>19</sup> F and <sup>31</sup> P.	<b>04 H</b>
	<b>3.3 Spectral problems based on UV, IR, <sup>1</sup>HNMR and <sup>13</sup>CNMR and Mass spectroscopy.</b>	<b>04 H</b>
<b>Unit-4</b>	<b>Advanced Spectroscopic Techniques-II</b>	<b>15 H</b>
	<b>4.1 Advanced NMR techniques:</b> 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.	<b>10 H</b>
	<b>4.2 Spectral problems based on UV, IR, <sup>1</sup>HNMR, <sup>13</sup>CNMR (Including 2D technique) and Mass spectroscopy</b>	<b>05 H</b>

### Reference Books:

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, 2011.
3. Organic Chemistry Natural Products Volume-II, O. P. Agarwal, Krishna Prakashan, 2011.
4. Chemistry of natural products, F. F. Bentley and F. R. Dollish, 1974
5. Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S.ItoMajori and S. Nozoo, Academic Press, 1974.
6. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co. 2008.
7. Heterocyclic chemistry, 3rd edition, Thomas L. Gilchrist, Pearson Education, 2007.
8. Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, R.K. Bansal, Wiley Eastern Ltd.,
9. Heterocyclic Chemistry, J. A. Joule and G. F. Smith, ELBS, 2<sup>nd</sup> edition, 1982.

10. The Conformational Analysis of Heterocyclic Compounds, F.G.Riddell, Academic Press, 1980.
  11. Principles of Modern Heterocyclic Chemistry, L.A. Paquette, W.B. Benjamin, Inc., 1978.
  12. An Introduction to the Chemistry of Heterocyclic Compounds, 2<sup>nd</sup> edition, B.M. Acheson, 1975.
  13. Natural Products: Chemistry and Biological Significance Interscience, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J. B. Harborne, Longman, Essex, 1994.
  14. Organic Chemistry, Vol 2, I.L. Finar, ELBS, 6th edition, Pearson.
  15. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
  16. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers, 1998.
  17. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers, 1998.
  18. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.
  19. The Total Synthesis of Reserpine, Woodward, R. B.; Bader, F. E.; Bickel, H., Frey, A. J.; Kierstead, R. W. Tetrahedron 1958, 2, 1-57.
  20. Total synthesis of Griseofulvin, Stork, G.; Tomasz, M. J. Am. Chem. Soc. 1962, 84, 310.
  21. Synthesis of ( $\pm$ )-4-demethoxydaunomycinone, A. V. Rama Rao, G. Venkatswamy, S. M. Javeed M., V. H. Deshpande, B.
  22. Ramamohan Rao, J. Org. Chem., 1983, 48 (9), 1552.
  23. The Alkaloids, The fundamental Chemistry A biogenetic approach, Marcel Dekker Inc. New York,
  24. Comprehensive Organic Chemistry by Barton and Ollis, Pergamon Press, Oxford, 1979.
  25. Medicinal Natural Products, a Biosynthetic Approach, Derick Paul, John Wiley and Sons, 2002.
  26. Biosynthesis of Natural Products, Mannitto Paolo, Ellis Horwood Limited, 1981.
  27. Selected Organic synthesis, Ian Fleming, John Wiley and Sons, 1973.
  28. Total synthesis of Natural Products, J. Apsimon, John Wiley and Sons.
  29. The Logic of Chemical Synthesis, E. J. Corey and Xue-Min Cheng, Wiley Interscience.
  30. Classics in Total Synthesis, K. C. Nicolaou and E. J. Sorensen, Weinheim: VCH, 1996.
  31. Spectroscopy of Organic compounds, P.S. Kalsi, New Age International Pub. Ltd. And Wiley Eastern Ltd., Second edition, 1995.
  32. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India,
  33. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991
  34. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974.
  35. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989.
  36. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987.
  37. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., . 3122
  38. Introduction to spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, 4th ed., 2009.
  39. Organic spectroscopic structure determination: a problem-based learning approach Douglass F. Taber, Oxford University Press, 17-Sep-2007.
  40. Organic Spectroscopy: Principles and Applications, Jag Mohan, Alpha Science International Ltd., 30-Mar-2004
  41. Alkaloids, V. K. Ahluwalia, Ane Books Pvt. Ltd.
  42. Biotransformations in Organic Chemistry, 5th Edition, Kurt Faber, Springer
  43. Structure Determination of Organic Compounds, EPretsch, P. Buhlmann, C. Affolter, Springer
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## ELECTIVE COURSE

Semester – III

Paper IV: Electives-1

Course Code: VGVPSSELCH301

Credits: 2

(Medicinal Chemistry)

### COURSE OUTCOME

Upon completing the course the student will be able to

<b>CO1</b>	Know the history and fundamentals of medicinal chemistry
<b>CO2</b>	Classify the drugs and relationship between structure and activity.
<b>CO3</b>	Understand the bio-mechanism of the antibiotics along with their synthetic routes
<b>CO4</b>	Know the structure of enzymes, their activity and different types of interactions in bio-molecules

### COURSE CONTENT

<b>Unit-1</b>	<b>Drug discovery, design and development</b>	<b>15 H</b>
	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.	<b>07 H</b>
	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).	<b>08 H</b>
<b>Unit-2</b>	<b>Drug design, development and synthesis</b>	<b>15 H</b>
	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.	<b>05 H</b>
	2.2 Introduction to modern methods of drug design and synthesis- computer aided molecular graphics-based drug design, drug design via enzyme inhibition (reversible and irreversible), bioinformatics and drug design.	<b>03 H</b>
	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.	<b>03 H</b>

	2.4 Synthesis and application of the following drugs: Fluoxetine, cetirizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate.	<b>04 H</b>
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### Reference Books:

1. Nelson, D. L, and Cox, M. M, (2008) Lehninger principles of Biochemistry 5<sup>th</sup> Edition, W. H. Freeman and Company, NY., USA.
2. The organic chemistry of drug design and drug action, Richard B. Silverman, 2<sup>nd</sup> edition, Academic Press
3. An introduction to drug design-S. S. Pandeya and J. R. Dimmock (Newage international)
4. Introduction to Medicinal chemistry. by Graham Patrick
5. Principles of medicinal chemistry (Vol. I and II)-S. S. Kadam, K. R.
6. Medicinal chemistry (Vol. I and II)-Burger
7. Strategies for organic drug synthesis and design - D. Lednicer Wiley
8. Pharmacological basis of therapeutics-Goodman and Gilman's (McGraw Hill)
9. Biochemistry, Dr U Satyanarayan and Dr U Chakrapani, Books and Allied (P) Ltd.
10. The Organic Chemistry of Enzyme-Catalysed Reactions, Academic Press, By Richard B. Silverman
11. The Organic Chemistry of Biological Pathways by John McMurry, Tadhg Begley by Robert and company publishers
12. Biochemistry: The chemical reactions in living cells, by E. Metzler. Academic Press.
13. Medicinal Natural Products: A Biosynthetic Approach by Paul M. Dewick. 3<sup>rd</sup> Edition, Wiley.
14. Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House.
15. Natural Products Volume- 2, By O. P. Agarwal.
16. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co.

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**Semester – III**  
**Paper IV: Electives-2**  
**Course Code: VGVPSSELCH302**  
**Credits: 2**  
**(Biogenesis and Green Chemistry)**

### Course Outcome

Upon completing the course the student will be able to understand

<b>CO1</b>	to learn Biogenesis and biosynthesis of natural products
<b>CO2</b>	the Primary and secondary metabolites and the building blocks with synthesis pathways like Acetate pathway, Shikimic Acid pathway, Mevalonate pathway of amino acid biosynthesis
<b>CO3</b>	basic fundamentals of Green chemistry including basic principles of green chemistry and Designing a green synthesis
<b>CO4</b>	comparison of traditional processes versus green processes in the syntheses



## COURSE CONTENT

Unit-1	Biogenesis and biosynthesis of natural products	15 H
	3.1 Primary and secondary metabolites and the building blocks, general pathway of amino acid biosynthesis.	03 H
	3.2 <b>Acetate pathway:</b> Biosynthesis of malonyl CoA, saturated fatty acids, prostaglandins from arachidonic acid, aromatic polyketides.	04H
	3.3 <b>Shikimic Acid pathway:</b> Biosynthesis of shikimic acid, aromatic amino acids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, flavonoids and isoflavonoids.	04 H
	3.4 <b>Mevalonate pathway:</b> Biosynthesis of mevalonic acid, monoterpenes –geranyl cation and its derivatives, sesquiterpenes – farnesyl cation and its derivatives and diterpenes.	04 H
Unit-2	Green chemistry	15 H
	4.1 Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts.	01 H
	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 CO <sub>2</sub> . d) Solid state reactions: solid phase synthesis, solid supported synthesis e) Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions. f) Ultrasound assisted reactions.	09 H
	4.3 Comparison of traditional processes versus green processes in the syntheses of ibuprofen, adipic acid, 4-aminodiphenylamine, p-bromotoluene and benzimidazole.	03 H
	4.4 <b>Green Catalysts</b> :Nanocatalyst, Types of nanocatalysts, Advantages and Disadvantages of Nanocatalysts, Idea of Magnetically separable nanocatalysts.	02 H

### Reference Books:

1. Nelson, D. L, and Cox, M. M, (2008) Lehninger principles of Biochemistry 5th Edition, W. H. Freeman and Company, NY., USA.
2. Voet, D. and J. G. Voet (2004) Biochemistry, 3rd Edition, John Wiley & sons, Inc. USA.
3. K. Philippot and P. Serp, Nanomaterials in catalysis, First Edition. Edited by P. Serp and K. Philippot;
4. C. N. R. Roa, A. Muller and A. K. Cheetham, The chemistry of Nanomaterials, Wiley-VCH Verlag GmbH & Co. KGaA, 2005, 1-11;
5. The organic chemistry of drug design and drug action, Richard B.Silverman, 2nd edition, Academic Press
6. Medicinal chemistry, D. Sriram and P. Yogeewari, 2nd edition, Pearson

7. An introduction to drug design-S. S. Pandeya and J. R. Dimmock (New age international)
  8. Burger's medicinal chemistry and drug discovery. by Manfred E. Wolf
  9. Medicinal chemistry-William O. Foye
  10. An introduction to medicinal chemistry-Graham L. Patrick, OUP Oxford, 2009.
  11. Principles of medicinal chemistry (Vol. I and II)-S. S. Kadam, K. R.Mahadik and K.G. Bothara , Nirali prakashan.
  12. Medicinal chemistry (Vol. I and II)-Burger
  13. Strategies for organic drug synthesis and design - D. Lednicer Wiley
  14. Enzyme catalysis in organic synthesis, 3rd edition. Edited by Karlheinz Drauz, Harold Groger, and Oliver May, Wiley-VCH Verlag GmbH & Co KgaA, 2012.
  15. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
  16. The Organic Chemistry of Enzyme-Catalysed Reactions, Academic Press, By Richard B. Silverman
  17. The Organic Chemistry of Biological Pathways by John McMurry, Tadhg Begley by Robert and company publishers
  18. Concepts in biotechnology by D. Balasubramanian & others
  19. Principles of biochemistry by Horton & others.
  20. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
  21. Medicinal Natural Products: A Biosynthetic Approach by Paul M. Dewick. 3rd Edition, Wiley.
  22. Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House.
  23. Natural Products Volume- 2, By O. P. Agarwal.
  24. Chemistry of Natural Products, F. F. Bentley and F. R. Dollish, 1974.
  25. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co.
  26. Green Chemistry: An Introductory Text, 2nd Edition, Published by Royal Society of Chemistry, Authored by Mike Lancater.
  27. New trends in green chemistry By V. K. Ahulwalia and M. Kidwai, 2<sup>nd</sup> edition, Anamaya Publishers, New Delhi.
  28. An introduction to green chemistry, V. Kumar, Vishal Publishing Co.
  29. Organic synthesis: Special techniques. V.K. Ahulwalia and Renu Aggarwal.
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### **Semester – III**

#### **Practicals- Mandatory**

**Course Code: VGVPSMCHP301**

**Credits: 2**

**(Separation of a ternary mixture of organic compounds)**

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#### **Organic Chemistry Practical Paper**

##### **A) Separation of a ternary mixture of organic compounds and their purification**

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. Separation of all three components and their Purification using **Distillation** or **Recrystallization** methods using appropriate solvent.
3. To find the yield of purified components and report their physical constants.  
(**Minimum 6 experiments**)

#### Learning points:

1. Separation of different components of organic mixture based on the difference in their physical and chemical properties, and safety aspects including MSDS should be learnt.
2. Purification of the product by crystallization or distillation and purity of the product should be checked by TLC
3. Report mass and melting point of the isolated components.

### B) 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.

(**Minimum 8 spectral analysis**)

#### Learning points:

1. Students should know how to predict the preliminary information from the UV, IR, PMR, CMR, and Mass spectra of a organic compound.
2. Students are expected to interpret the various spectra and draw reliable information from it using reference material/books.
3. To deduce and confirm the structure of organic compound

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#### Reference:

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, 3rd Edn, 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. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.
  7. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
  8. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
  9. 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.
  10. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
  11. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011.
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**Semester – III**  
**Practicals - Elective 1 and 2**  
**Course Code: VGVPSSELCHP301**  
**Credits: 2**  
**(Single Step Organic Preparation)**

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**Single step organic preparation (1.0 g scale) involving purification by Steam distillation / Vacuum distillation or Column chromatography**

1. Preparation of acetanilide from aniline and acetic acid using Zn dust. (Purification by column chromatography)
  2. Preparation of 1-nitronaphthalene from naphthalene. (Purification by steam distillation)
  3. Preparation of acetyl ferrocene from ferrocene. (Purification by column chromatography)
  4. Preparation of 3-nitroaniline from 1,3-dinitrobenzene. (Purification by column chromatography)
  5. Preparation of benzyl alcohol from benzaldehyde. (Purification by vacuum distillation).
  6. Preparation of methyl salicylate from salicylic acid. (Purification by vacuum distillation).
  7. Preparation of 4-methylacetophenone from toluene. (Purification by vacuum distillation).
  8. Preparation of phenyl acetate from phenol. (Purification by vacuum distillation)
  9. Preparation of 2-chlorotoluene from *o*-toluidine. (Purification by steam distillation)
  10. Preparation of 4-nitrophenol from phenol. (Purification by steam distillation/ column chromatography)
  11. Preparation of fluorenone from fluorene. (Purification by column chromatography)
  12. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation)
- (Minimum 8 experiments)**

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**Learning points:**

1. Students are expected to know
  - The planning of synthesis, effect of reaction parameters including stoichiometry, and **safety Aspects including MSDS**
  - The possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
2. Students are expected to purify the product by Steam distillation / Vacuum distillation or Column chromatography, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

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**Reference Books:**

1. Comprehensive Practical Organic Chemistry: Preparation and
2. Quantitative Analysis- V.K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
3. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
4. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
5. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
6. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.

8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
  9. 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.
  10. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
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### **Semester-III: Research Project-RP**

**Code : VGVPSRPCH301**

**(Research Project)**

**Credits: 4**

- A student will undertake a research project related to **Mandatory Courses** in the final year of their M. Sc. Programme which will be of **120 hrs** duration. Students can carry out their research work either at Industry Laboratories under the supervision of an expert from the concern industry as an External Supervisor and practical Incharge as an Internal Supervisor.
- Students should prepare a detailed project report duly signed by both the supervisors and submit to the chemistry department.
- Students will be evaluated through Presentation of their research work followed by Viva by examiner during Semester-III practical examination.

#### **Note :-**

1. At the end of the second semester, the Head of Department will assign the supervisors for the project.
2. **In semester –III** student would collect literature related to an assigned area, understand the lacunae in the literature, and analyze the literature and present suitable guidelines for carrying out experimental work of the assigned project.
3. Student would propose a defined plan for the research and write a neat report following the guidelines prescribed by the department.
4. *Students can do their partial project work in Semester-III and present during Practical Exam, Semester-III.*
5. **It should be noted that the same project would be continued in semester-IV.**
6. The students will do the experimental work on the project and submit the thesis before the prescribed date, which will be a date before the last date of the **Semester - IV**.
7. The thesis shall be submitted in the format prescribed.
8. The thesis will be evaluated by the supervisor along with one other external referee as per the norms.

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#### **Course Outcomes:**

- Student would be able to collect literature related to an assigned area
  - Student would be able to understand the lacunae in the literature
  - Student would be able to analyze the literature and present suitable guidelines
  - Student would be able to write a neat report following the guidelines
  - Student would be able to propose a defined plan for the research
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## Guidelines for Writing a Project Report :

**Typically, the report should contain the following:**

**(a) Introduction:** 2 pages maximum,

**(b) Exhaustive review of literature (including figures):** 10 – 12 pages: 50% Weightage

**(c) Critical analysis of the literature and comments:**

1. Critical analysis should also contain quantitative comparison of observations, results, and conclusion amongst the various papers.
2. Two typed copies of the report on thesis size bond paper A4 (297 mm x 210 mm) are to be submitted to Incharge on - time to be decided by the Practical Incharge. In addition, soft copy of the report should be submitted to the department. The detailed timetable for the presentation would be communicated.
3. The report should be prepared using the Times Roman font (size 12) using 1.5 spacing leaving 1-inch margin on all sides producing approximately 29 lines per page. The report should be typed on one side of the paper and need not be bound in a hard cover binding. Figures and tables should be shown as a part of the running text. Each figure should be drawn inside a rectangular box of 12 cm width and 10 cm height. The figures must be sufficiently clear and hand drawn figures will be acceptable. Particular care must be taken if a figure is photocopied from source. Each figure must have a sequence number and caption below. Each table must have a sequence number and title at the top.
4. **Name of the student, title of the problem and year of examination** must be indicated on the top cover. **THE NAME OF THE SUPERVISOR (ONLY INITIALS) MUST APPEAR ON THE BOTTOM RIGHT CORNER OF THE TOP COVER.**
5. The report must be precise. All important aspects of the topic should be considered and reported. The total number of pages, including tables, figures, and references should not exceed 75. Chapters or subsections need not be started on new pages, while getting the report typed.
6. Typographical errors in the report must be corrected by the student. The student will be discredited for any omission in the report. All the symbols used in the text should be arranged in an alphabetical order and given separately after conclusions.
7. The list of references should be arranged in alphabetical order of the names of authors. In the text, the reference should be cited with author's name and year. (Author – date style) For example:
  - (i) The flow pattern in gas-liquid-solid fluidized bed has been reported in the published literature (Murooka et al., 1982).

OR

- (ii) Murooka et al. (1982) have measured flow patterns in gas-liquid-solid fluidized beds. The title of the article should also be included. The references must be given in the following standard format.
  - (a) Format for listing references of articles from periodicals: Murooka S., Uchida K. And Kato Y., "Recirculation Turbulent Flow of Liquid in Gas-Liquid-Solid Fluidised Bed", J. Chem. Engg. Japan, 15, 29-34 (1982).
  - (b) Format for listing references of Books:  
Constant R.F., "Crystallization, Academic Press, New York, pp. 89-90, 1968.
  - (c) Format for listing Thesis:  
Niranjan K., "Hydrodynamic and Mass Transfer Characteristics of Packed Columns", Ph.D. (Tech.) Thesis, University of Mumbai, 1983.
  - (d) Format for listing references of Patents in Chemical Abstracts: Cananaush R.M., U.S.Patent 2,647,141, Cf. C.A. 48, 82636 (1954).
  - (e) Format for listing Handbooks, Tables, Symposia etc.:

Kumar R and Kuloor N.R., "Formation of Drops and Bubbles", in Advances in Chemical Engineering, Vol.8, T.B.Drew et.al. (Eds.) New York, Academic Press, pp.256-364 (1970).

(f) Format for listing Private Communications and other categories: Sharma, M.M., Private Communication (1984).

8. Consistency of units should be maintained in the written report. SI systems should be used. [For SI system – Ref: Ind. Chem. Engr., 24, 32, 3 (1983)]. Units used in the literature (if not SI) should be correctly converted.
9. The time allotted for the oral presentation is 20 minutes: additional 10 minutes are provided for questions and answers.

**10. INCOMPLETE AND CARELESSLY WRITTEN REPORT IS LIABLE TO BE REJECTED.**

11. The last date for submission will NOT be extended on any grounds whatsoever.
12. There must not be any acknowledgment about the guidance by the faculty in the report.
13. The report will be evaluated on the basis of
  - i) Rational approach to the problem,
  - ii) Correctness and completeness of the written text and
  - iii) Performance in the oral presentation.
14. Word-to-word copying from the published article is not permitted. Flowery language is not to be used



# SEMESTER : IV

## Course content - Semester IV

### Semester – IV

#### Paper I

Course Code: VGVPSMCH401

Credits: 4

### Theoretical organic Chemistry-I

#### Course Outcome

Upon completing the course the student will be able to understand

CO1	structural effects and reactivity and Linear free energy relationship (LFER) in determination of organic reaction mechanism,
CO2	principles of molecular associations and organizations in biological macromolecules like nucleic acids, proteins and enzymes.
CO3	structures, properties, synthesis and applications of crown ethers
CO4	racemization and resolution of racemates including conglomerates
CO5	principles of asymmetric synthesis and Asymmetric reactions with mechanism

#### Course Content

Unit 1	<b>Physical organic chemistry</b>	<b>15 H</b>
	<b>1.1</b> 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 $\sigma$ - values, reaction constants $\rho$ , Yukawa-Tsuno equation.	<b>07 H</b>
	<b>1.2</b> Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants. The Taft model, $\sigma_I$ and $\sigma_R$ scales, steric parameters $E_s$ and $\beta$ . Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's ET parameter, Solvatochromism Z-scale, Spectroscopic Correlations, Thermodynamic Implications.	<b>08 H</b>
Unit 2	<b>Supramolecular chemistry</b>	<b>15 H</b>
	<b>2.1</b> Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes.	<b>3H</b>
	<b>2.2</b> Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.	<b>3H</b>
	<b>2.3</b> Structures and properties of crown ethers, cryptands, cyclophanes, alixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.	<b>5H</b>
	<b>2.4</b> Molecular recognition and catalysis, molecular self-assembly. Supramolecular Polymers, Gels and Fibres.	<b>4H</b>



<b>Unit 3</b>	<b>Stereochemistry-I</b>	<b>15 H</b>
	<b>3.1 Racemization and resolution of racemates including conglomerates:</b> Mechanism of racemization, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds.	<b>03 H</b>
	<b>3.2 Determination of enantiomer and diastereomer composition:</b> enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR).	<b>03 H</b>
	<b>3.3 Correlative method for configurational assignment:</b> chemical, optical rotation, and NMR spectroscopy.	<b>04 H</b>
	<b>3.4 Molecular dissymmetry and chiroptical properties:</b> 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 $\alpha$ -haloketone rule with applications.	<b>05 H</b>
<b>Unit 4</b>	<b>Asymmetric synthesis</b>	<b>15 H</b>
	<b>4.1 Principles of asymmetric synthesis:</b> Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst-controlled reactions.	<b>03 H</b>
	<b>4.2 Synthesis of L-DOPA [Knowles's Monsanto process].</b> <b>Asymmetric reactions with mechanism:</b> Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharpless enantio selective epoxidation, hydroxylation, aminohydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.	<b>09 H</b>
	<b>4.3 Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification.</b> Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations.	<b>03 H</b>

### Reference Books:

- 1) March's Advanced Organic Chemistry, Jerry March, sixth edition, 2007, John Wiley and sons.
- 2) A guide to mechanism in Organic Chemistry, 6<sup>th</sup> edition, 2009, Peter Sykes, Pearson education, New Delhi.
- 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, 4<sup>th</sup> 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.
- 8) Carbenes, Nitrenes and Arynes. Von T. L. Gilchrist, C. W. Rees. Th. Nelson and Sons Ltd., London
- 9) Organic reactive intermediates, Samuel P. MacManus, Academic Press.
- 10) Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers, 1st Edition, Oxford University Press (2001).
- 11) Organic Chemistry, Seventh Edition, R.T. Morrison, R.N. Boyd & S. K. Bhattacharjee, Pearson.
- 12) Advanced Organic Chemistry: Reactions & Mechanisms, second edition, B. Miller and R. Prasad, Pearson.

- 17) Organic reactions & their mechanisms, third revised edition, P.S. Kalsi, New Age International Publishers.
  - 18) Organic Chemistry: Structure and Function, P. Volhardt and N. Schore, 5th Edition, 2012
  - 19) Organic Chemistry, W. G. Solomons, C. B. Fryhle, 9th Edition, Wiley India Pvt. Ltd., 2009.
  - 20) Pericyclic Reactions, S. Sankararaman, Wiley VCH, 2005.
  - 21) Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
  - 22) Pericyclic reactions, Ian Fleming, Oxford University Press, 1999.
  - 23) Pericyclic reactions-A mechanistic approach, S. M. Mukherji, Macmillan Co. of India 1979.
  - 24) Organic chemistry, 8<sup>th</sup> edition, John McMurry
  - 25) Modern methods of Organic Synthesis, 4<sup>th</sup> Edition W. Carruthers and Iain Coldham, Cambridge University Press 2004
  - 26) Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University Science Books, 2006
  - 27) Physical Organic Chemistry, N.S. Isaacs, ELBS/Longman
  - 28) Stereochemistry of Carbon Compounds: Principles and Applications, D. Nasipuri, 3<sup>rd</sup> edition, New Age International Ltd.
  - 29) Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edit
  - 30) Stereochemistry, P.S. Kalsi, 4<sup>th</sup> edition, New Age International Ltd.
  - 31) Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
  - 32) Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
  - 33) Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
  - 34) Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
  - 35) Larger ring compounds, J.A. Semlyen, Wiley-VCH, 1997.
  - 36) Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley- Eastern
  - 37) Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
  - 38) Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
  - 39) Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
  - 40) Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
  - 41) Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
  - 42) Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A John Wiley and Sons, Ltd., Publication).
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**Semester – IV**  
**Paper II**  
**Course Code: VGVPSMCH402**  
**Credits: 4**  
**Synthetic Organic Chemistry-II**

**Course Outcome**

Upon completing the course the student will be able to understand

<b>CO1</b>	designing organic synthesis and protecting groups in organic synthesis
<b>CO2</b>	concept of umpolung and retrosynthetic analysis of organic compounds
<b>CO3</b>	synthetic planning with general strategy, one/two group C-C disconnections
<b>CO4</b>	applications of metals in organic synthesis using selected methods
<b>CO5</b>	the concept olefin metathesis using Grubb's catalyst

**COURSE CONENT**

<b>Unit-1</b>	<b>Designing Organic Synthesis-I</b>	<b>15 H</b>
	<b>1.1 Protecting groups in Organic Synthesis:</b> Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications.	<b>03 H</b>
	<b>1.2 Concept of umpolung (Reversal of polarity):</b> Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.	<b>03 H</b>
	<b>1.3 Introduction to Retrosynthetic analysis and synthetic planning:</b> 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.	<b>09 H</b>
<b>Unit-2</b>	<b>Designing Organic Synthesis-II</b>	<b>15 H</b>
	<b>2.1 General strategy:</b> choosing a disconnection-simplification, symmetry, high yielding steps, and recognizable starting material.	<b>03 H</b>
	<b>2.2 One group C-C Disconnections:</b> Alcohols (including stereoselectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.	<b>06 H</b>
	<b>2.3 Two group C-C Disconnections:</b> 1,2- 1,3- 1,4- 1,5- and 1,6-difunctionalized compounds, Diels-Alder reactions, $\alpha$ , $\beta$ -unsaturated compounds, control in carbonyl condensations, Michael addition and Robinson annelation.	<b>06 H</b>
<b>Unit-3</b>	<b>Electro-organic chemistry and Selected methods of Organic synthesis</b>	<b>15 H</b>
	<b>3.1 Electro-organic chemistry:</b> Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes. Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitro compounds, olefins, arenes, electro-dimerization. Anodic oxidation: Oxidation of alkylbenzene, Kolbe reaction, Non-Kolbe oxidation, Shono oxidation.	<b>07 H</b>
	<b>3.2 Selected Methods of Organic synthesis:</b> Applications of the following in organic synthesis: Crown ethers, cryptands, micelles, cyclodextrins, catenanes.	<b>08 H</b>

	Organo catalysts: Proline, Imidazolidinone. <b>Pd catalysed cycloaddition reactions:</b> Stille reaction, Saeguse-Ito oxidation to enones, Negishi coupling. Use of Sc(OTf) <sub>3</sub> and Yb(OTf) <sub>3</sub> as water tolerant Lewis acid catalyst in aldol condensation, Michael reaction, Diels-Alder reaction, Friedel – Crafts reaction.	
<b>Unit-4</b>	<b>Transition and rare earth metals inorganic synthesis</b>	<b>15 H</b>
	<b>4.1 Introduction to basic concepts:</b> 18 electron rules, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion.	<b>03 H</b>
	<b>4.2 Palladium in organic synthesis:</b> $\pi$ -bonding of Pd with olefins, applications in C-C bond formation, carbonylation, alkene isomerization, cross-coupling of organometallic and halides. Representative examples: Heck reaction, Suzuki-Miyaura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N, S, or P atoms.	<b>05H</b>
	<b>4.3 Olefin metathesis</b> using Grubb's catalyst.	<b>01 H</b>
	<b>4.4 Application of Ni, Co, Fe, Rh, and Cr carbonyls</b> in organic synthesis.	<b>04H</b>
	<b>4.5 Application of samarium iodide</b> including reduction of organic halides, aldehydes and ketones, $\alpha$ -functionalised carbonyl and nitro compounds.	<b>01H</b>
	<b>4.6 Application of Ce(IV)</b> in synthesis of heterocyclic quinoxaline derivatives and its role as a de-protecting agent.	<b>01H</b>

#### Reference Books:

- Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5<sup>th</sup> Edition, Springer Verlag.
- Modern Methods of Organic Synthesis, 4<sup>th</sup> Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
- Chem. Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L.Lam.
- Organic Chemistry, Clayden Greeves Warren and Wothers, Oxford Press (2001).
- Modern Organic Synthesis: An Introduction, G.S. Zweifel and M.H.Nantz, W.H. Freeman and Company, (2007).
- Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002).
- Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3<sup>rd</sup> Edn., Nelson Thornes.
- Organic Chemistry, 7<sup>th</sup> Edn, R. T. Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson.
- Strategic Applications of Name Reactions in Organic Synthesis, L. Kurti & B. Czako (2005), Elsevier Academic Press.
- Advanced Organic Chemistry: Reactions & Mechanisms, 2<sup>nd</sup> Edn., B. Miller & R. Prasad, Pearson
- Organic reactions and their mechanisms, 3<sup>rd</sup> revised edition, P.S. Kalsi, New Age International Publishers.
- Organic Synthesis: The Disconnection Approach, Stuart Warren, John Wiley & Sons, 2004.
- Name Reactions and Reagents in Organic Synthesis, 2<sup>nd</sup> Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
- Name Reactions, Jie Jack Lie, 3<sup>rd</sup> Edn., Springer.
- Organic Electrochemistry, H. Lund, and M. Baizer, 3<sup>rd</sup> Edn., Marcel Dekker.

**Semester – IV****Paper III****Course Code: VGVPSMCH403****Credits: 4****(Natural products and heterocyclic chemistry)****Course Outcome**

Upon completing the course the student will be able to understand

<b>CO1</b>	general structural features, occurrence, biological role, important structural and stereochemical features of steroids
<b>CO2</b>	sources and biological importance of vitamins, antibiotics, naturally occurring insecticides and terpenoids
<b>CO3</b>	classification, nomenclature of heterocyclic compounds of monocyclic (3-6 membered)
<b>CO4</b>	nucleophilic ring opening reactions of oxiranes, aziridines, oxetanes and azetidines.
<b>CO5</b>	structure, reactivity, synthesis and reactions of coumarins, quinoxalines, cinnolines, indole, benzimidazoles heterocycles

**Course Content**

<b>Unit-1</b>	<b>Natural Products-III</b>	<b>15 H</b>
	<b>1.1 Steroids:</b> General structure, classification. Occurrence, biological role, important structural and stereochemical features of the following: Corticosteroids, steroidal hormones, steroidal alkaloids, sterols and bile acids.	<b>05 H</b>
	<b>1.2</b> Synthesis of 16-DPA from cholesterol and plants apogenin.	<b>02 H</b>
	<b>1.3</b> Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone.	<b>05 H</b>
	<b>1.4</b> Synthesis of cinerolone, jasmolone, allethrolone, exaltone and muscone.	<b>03 H</b>
<b>Unit-2</b>	<b>Natural Products- IV</b>	<b>15 H</b>
	<b>2.1 Vitamins:</b> Classification, sources and biological importance of vitamin B1, B2, B6, folic acid, B12, C, D1, E ( $\alpha$ -tocopherol), K1, K2, H ( $\beta$ - biotin). Synthesis of the following: Vitamin A from $\beta$ -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) ethoxyacetyl acetone and cyanoacetamide, 2) ethyl ester of N-formyl-DL-alanine (Harris synthesis) Vitamin E( $\alpha$ -tocopherol) from trimethylquinol and phytolbromide Vitamin K1 from 2-methyl-1,4-naphthaquinone and phytol.	<b>05 H</b>
	<b>2.2 Antibiotics:</b> Classification on the basis of activity. Structure elucidation, spectral data of penicillin-G, cephalosporin-C and chloramphenicol. Synthesis of chloramphenicol (from benzaldehyde and $\beta$ -nitroethanol) penicillin-G and phenoxymethyl penicillin from D-penicillamine and t-butyl phthalimide malonaldehyde.	<b>06 H</b>
	<b>2.3 Naturally occurring insecticides:</b> Sources, structure and biological Properties of pyrethrums (Pyrethrin I), rotenoids (rotenone). Synthesis of Pyrethrin I.	<b>02H</b>
	<b>2.4 Terpenoids:</b> Occurrence, classification, structure elucidation, stereochemistry, spectral data and synthesis of zingiberene.	<b>02H</b>

<b>Unit-3</b>	<b>Heterocyclic Compounds-I</b>	<b>15 H</b>
	<b>Heterocyclic compounds:</b> 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.	<b>15 H</b>
<b>Unit-4</b>	<b>Heterocyclic compounds-II</b>	<b>15 H</b>
	Nomenclature of heterocyclic compounds of bicyclic/tricyclic (5-6Membered) fused heterocycles (up to three heteroatoms). (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.	

### Reference Books:

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, 2011.
3. Organic Chemistry Natural Products Volume-II, O. P. Agarwal, Krishna Prakashan, 2011.
4. Chemistry of natural products, F.F. Bentley and F.R. Dollish, 1974.
5. Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S.Ito Majori and S. Nozoo, Academic Press, 1974.
6. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co. 2008.
7. Heterocyclic chemistry, 3<sup>rd</sup> edition, Thomas L. Gilchrist, Pearson Education, 2007.
8. Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, R. K. Bansal, Wiley Eastern Ltd.,
9. Heterocyclic Chemistry, J.A. Joule and G.F. Smith, ELBS, 2<sup>nd</sup> edition, 1982.
10. The Conformational Analysis of Heterocyclic Compounds, F.G. Riddell, Academic Press, 1980.
11. Principles of Modern Heterocyclic Chemistry, L.A. Paquette, W.B. Benjamin, Inc., 1978.
12. An Introduction to the Chemistry of Heterocyclic Compounds, 2<sup>nd</sup> edition, B.M. Acheson, 1975.
13. Natural Products: Chemistry and Biological Significance Interscience, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J. B. Harborne, Longman, Essex, 1994.
14. Organic Chemistry, Vol 2, I.L. Finar, ELBS, 6<sup>th</sup> edition, Pearson.
15. Stereoselective Synthesis: A Practical Approach, M. Nogradi, Wiley-VCH, 1995.
16. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
17. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
18. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers, 1998.
19. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers, 1998.
20. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.
21. Total Synthesis of Longifolene, J. Am. Chem. Soc., E. J. Corey, M. Ohno, R. B. Mitra, and P. A. Vatakencherry. 1964, 86, 478.
22. Total Synthesis of Longifolene, J. Am. Chem. Soc. 1961, 83, 1251.

23. The structure and total synthesis of 5-Vetivone, J. A. Marshall and P. C. Johnson, *J. Org. Chem.*, 35, 192 (1970).
24. Total synthesis of spirovetivanes, *J. Am. Chem. Soc.* 1967, 89, 2750.
25. The Total Synthesis of Reserpine, Woodward, R. B.; Bader, F. E.; Bickel, H., Frey, A. J.; Kierstead, R. W. *Tetrahedron* 1958, 2, 1-57.
26. Total synthesis of Griseofulvin, Stork, G.; Tomasz, M. *J. Am. Chem. Soc.* 1962, 84, 310.
27. Synthesis of ( $\pm$ )-4-demethoxydaunomycinone, A.V. RamaRao, G. Venkatswamy, S. M. Javeed M., V. H. Deshpande, B. Ramamohan Rao, *J. Org. Chem.*, 1983, 48 (9), 1552.
28. *The Alkaloids, The fundamental Chemistry A biogenetic approach*, Marcel Dekker Inc. New York,
29. *Comprehensive Organic Chemistry by Barton and Ollis*, Pergamon Press, Oxford, 1979.
30. *Medicinal Natural Products, a Biosynthetic Approach*, Derick Paul, John Wiley and Sons, 2002.
31. *Biosynthesis of Natural Products*, Mannitto Paolo, Ellis Horwood Limited, 1981.
32. *Selected Organic synthesis*, Ian Fleming, John Wiley and Sons, 1973.
33. *Total synthesis of Natural Products*, J. Apsimon, John Wiley and Sons.
34. *The Logic of Chemical Synthesis*, E.J. Corey and Xue-Min Cheng, Wiley Interscience.
35. *Classics in Total Synthesis*, K. C. Nicolaou and E. J. Sorensen, Weinheim: VCH, 1996.
36. *Spectroscopy of Organic compounds*, P.S. Kalsi, New Age International Pub. Ltd. And Wiley Eastern Ltd., Second edition, 1995.
37. *Applications of Absorption Spectroscopy of Organic compounds*, J. R. Dyer, Prentice Hall of India,
38. *Spectrometric Identification of Organic compounds*, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991.
39. *Absorption spectroscopy of organic Molecules*, V.M. Parikh, 1974.
40. *Spectroscopic methods in organic chemistry*, Williams and Fleming, Tata McGraw Hill, 4th ed,
41. *Organic spectroscopy*, William Kemp, ELBS, 3<sup>rd</sup> ed., 1987.
42. *Organic structures from spectra*, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4<sup>th</sup> ed., .3122
43. *Introduction to spectroscopy*, Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, 4<sup>th</sup> ed., 2009.
44. *Organic spectroscopic structure determination: a problem-based learning approach* Douglass F. Taber, Oxford University Press, 17- Sep-2007.
45. *Organic Spectroscopy: Principles and Applications*, Jag Mohan, Alpha Science International Ltd., 30-Mar-2004
46. *Alkaloids*, V.K. Ahluwalia, Ane Books Pvt. Ltd.
47. *Biotransformations in Organic Chemistry*, 5<sup>th</sup> Edition, Kurt Faber, Springer
48. *Structure Determination of Organic Compounds*, E. Pretsch, P. Bühlmann, C. Affolter, Springer.

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# ELECTIVE COURSE

Semester – IV

Paper IV: **Electives-3**

Course Code: VGVPSSELCH401

Credits: 2

**(Intellectual Property Rights)**

## Course Outcome

Upon completing the course the student will be able to understand

CO1	the detail concept of Intellectual Property, Patents, Industrial Designs, Copyrights, Trade Marks and Geographical Indications
CO2	the Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection
CO3	the details of different International agreements like <b>WTO, GATT, TRIPS</b> , etc.
CO4	how to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc

## Course Contents

<b>Unit-1</b>	<b>Introduction to Intellectual Property:</b>	<b>15 H</b>
	<b>Introduction to Intellectual Property:</b> Historical Perspective, Different types of IP, Importance of protecting IP.	<b>02 H</b>
	<b>Patents:</b> Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.	<b>05 H</b>
	<b>Industrial Designs:</b> Definition, How to obtain, features, International design registration.	<b>02 H</b>
	<b>Copyrights:</b> Introduction, How to obtain, Differences from Patents.	<b>02 H</b>
	<b>Trade Marks:</b> Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.	<b>02 H</b>
	<b>Geographical Indications:</b> Definition, rules for registration, prevention of illegal exploitation, importance to India	<b>02 H</b>
<b>Unit-2</b>	<b>Trade Secrets:</b>	<b>15 H</b>
	<b>Trade Secrets:</b> Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.	<b>02 H</b>
	<b>IP Infringement issue and enforcement:</b> Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.	<b>02 H</b>
	<b>Economic Value of Intellectual Property:</b>	



	Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.	<b>02H</b>
	<b>Different International agreements:</b>	
	<b>(a) World Trade Organization (WTO):</b>	<b>05 H</b>
	(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>(b) Paris Convention</b>	<b>04 H</b>
	WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity	

### Reference Books:

1. Andrew R. Leach & Valerie J. Gillet (2007) An Introduction to Cheminformatics. Springer: The Netherlands
2. Gasteiger, J. & Engel, T. (2003) Cheminformatics: A textbook. Wiley–VCH
3. Gupta, S. P. QSAR and Molecular Modeling. Springer-Anamaya Pub.: New Delhi.

**Semester – IV**  
**Paper IV: Electives-4**  
**Course Code: VGVPSSELCH402**  
**Credits: 2**  
**(Introduction to Cheminformatics)**

### Course Outcome

Upon completing the course the student will be able to understand

<b>CO1</b>	history and evolution of cheminformatics and applications of cheminformatics
<b>CO2</b>	molecular modeling and structure elucidation using cheminformatics
<b>CO3</b>	three-dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization, etc.
<b>CO4</b>	computer assisted Synthesis Design, drug design, Target Identification and Validation, etc.

### Course Content

<b>Unit-1</b>	<b>Introduction to Cheminformatics:</b>	<b>15 H</b>
	<b>Introduction to Cheminformatics:</b> History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.	<b>05 H</b>

	<p><b>Representation of molecules and chemical reactions:</b> Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and tool kits, Different electronic effects, Reaction classification.</p>	<b>05 H</b>
	<p><b>Searching Chemical Structures:</b> 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.</p>	<b>05 H</b>
<b>Unit-2</b>	<b>Applications:</b>	<b>15 H</b>
	<p>Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-based and Structure based Drug design, Application of Cheminformatics in Drug Design</p>	

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## Semester – IV

### Practicals- Elective - 3 or 4

**Course Code: VGVPSSELCHP401/2**

**Credits: 2**

**(Two steps preparations)**

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### Two steps preparations

1. Acetophenone → Acetophenone phenyl hydrazine → 2-phenylindole.
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-acetoxycoumarin.
12. Anthracene → anthraquinone → anthrone.

**(Minimum 8 experiments)**

**Learning points:**

1. Students are expected to know
    - (i) The planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS
    - (ii) The possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
  2. Students are expected to purify the product by recrystallization, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.
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**Instructions:**

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

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. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.
  7. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
  8. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Edward Arnold.
  9. 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.
  10. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
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## Semester – IV

Course Code: VGVPSRPCH401

### Semester-IV: Research Project-RP

(Research Project – II)

Credits: 6

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- A student will undertake a research project related to **Mandatory Courses** which will be of **180 hrs** duration. Students can carry out their research work either at Industry Laboratories under the supervision of an expert from the concern industry as an External Supervisor and practical Incharge as an Internal Supervisor.
  - Students should prepare a detailed project report duly signed by both the supervisors and submit to the chemistry department.
  - Students will be evaluated through Presentation of their research work followed by Viva by examiner during Semester-IV practical examination.

- ❖ This would be concerned with the continuation of the research project executed in the **Semester-III** and the exact work plan will be decided in consultation with the research guide.
- ❖ At the end of the project, the candidate is expected to submit a report as per similar guidelines provided for Semester-3 (Project-I) which will be evaluated by the research guide and an external examiner from the Department/Industry based on the presentation made by the candidate.
- ❖ A suitable combination of the marks for report and presentation will be considered for the final evaluation.

