



Shri Vile Parle Kelavani Mandal's  
**MITHIBAI COLLEGE OF ARTS, CHAUHAN INSTITUTE OF SCIENCE &  
AMRUTBEN JIVANLAL COLLEGE OF COMMERCE AND ECONOMICS  
(AUTONOMOUS)**

*NAAC Reaccredited 'A' grade, CGPA: 3.57 (February 2016),  
Granted under RUSA, FIST-DST & -Star College Scheme of DBT, Government of  
India,  
Best College (2016-17), University of Mumbai*

Affiliated to the  
**UNIVERSITY OF MUMBAI**

**Program: M.Sc.**

**Course: Organic Chemistry**

**Semester III**

**Credit Based Choice System (CBCS) with effect from the  
Academic year 2020-21**

## **PROGRAMME SPECIFIC OUTCOMES (PSO'S)**

On completion of the **M.Sc.-Organic Chemistry**, the learners should be enriched with knowledge and be able to-

- PSO1:** gain complete knowledge about all fundamental aspects of all the elements of organic chemistry.
- PSO2:** develop analytical thinking and apply the same for the understanding of underlining principles, proposing mechanism, problem solving, identification of chemical species and arriving to logical conclusion.
- PSO3:** understands the background of organic reaction mechanisms, complex chemical structure, and molecular rearrangements.
- PSO4:** gain knowledge in classical laboratory techniques and be able to use modern instrumentation, so that they can perform new experiments, obtain experimental data and its spectral interpretation through theoretical principals.
- PSO5:** integrate knowledge learned in chemistry to various industry and pharmaceutical needs.
- PSO6:** learn about the potential uses of medicinal chemistry and green chemistry.
- PSO7:** carry out experiments in the area of organic analysis, estimation, separation, derivative process.
- PSO8:** access, search and use the chemical literature for research article review and research project work.

### **Preamble**

The purpose of post-graduate education in science is to create highly skilled manpower in specific areas, which will lead to generation of new knowledge and creation of wealth for the country. Chemistry is a fundamental science and has contributed immensely to the improvement of the life of human beings by providing many of human requirements and essentialities. The credit system has been adopted for all these courses, which would allow students to develop a strong foundation in the fundamentals and specialize in the disciplines of his/her liking and abilities. The courses are designed so that the students pursuing these courses will obtain fundamental knowledge about the subject in the respective specialization. The students are also expected to get corresponding experimental training during the practical courses.

### **Evaluation Pattern**

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The performance of the learner will be evaluated in two components. The first component will be a Continuous Assessment with a weightage of 25% of total marks per course. The second component will be a Semester end Examination with a weightage of 75% of the total marks per course. The allocation of marks for the Continuous Assessment and Semester end Examinations is as shown below:

**a) Details of Continuous Assessment (CA)**

25% of the total marks per course:

<b>Continuous Assessment</b>	<b>Details</b>	<b>Marks</b>
<b>Component 1 (CA-1)</b>	Test	15 marks
<b>Component 2 (CA-2)</b>	Assignment	10 marks

**b) Details of Semester End Examination**

75% of the total marks per course. Duration of examination will be two and half hours.

<b>Question Number</b>	<b>Description</b>	<b>Marks</b>	<b>Total Marks</b>
1	Attempt any Three out of Five	15 Marks	15 Marks
2	Attempt any Three out of Five	15 Marks	15 Marks
4	Attempt any Three out of Five	15 Marks	15 Marks
4	Attempt any Three out of Five	15 Marks	15 Marks
5	Attempt any Three out of Four	15 Marks	15 Marks
<b>Total Marks</b>			<b>75</b>

Signature

Signature

Signature

HOD

Approved by Vice –Principal

Approved by Principal

<b>Program: M.Sc. Organic Chemistry</b>	<b>Semester: III</b>
<b>Course: Theoretical organic chemistry-I</b>	<b>Course Code: PSMACHO301</b>

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Teaching Scheme				Evaluation Scheme	
Lecture (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks - 25)	Semester End Examinations (SEE) (Marks- 75 in Question Paper)
4	4	N/A	4 + 2	15 +10	75
<b>Learning Objectives:</b>					
The objective of the course is to introduce students to					
1. Reactive intermediates such carbocation, carbanion, free radicals etc.					
2. Pericyclic chemistry, interesting approaches of molecular synthesis, advanced stereochemistry and essentials of reactive organic intermediates and photochemistry					
<b>Course Outcomes:</b>					
After completion of the course, learners would be able to:					
<b>CO1:</b> In depth knowledge of reactive organic intermediates.					
<b>CO2:</b> Gain theoretical understanding of pericyclic chemistry, photochemistry, stereochemistry,					
<b>CO3:</b> Get an overview of interesting approaches for molecular synthesis					
<b>Outline of Syllabus: (per session plan)</b>					
Module	Description				No of Hours
1	Organic reaction mechanism and interesting approaches of molecular synthesis				15 L
2	Pericyclic Chemistry I				15 L
3	Pericyclic Chemistry – II & Photochemistry				15 L
4	Stereochemistry - I				15 L
	Total				60 L
<b>PRACTICALS</b>					

*To develop scientific temper and interest by exposure through industrial visits and study/educational tours is recommended in each semester*

## PRACTICAL I

Course code: PSMACHO3P1

Unit	Topic	No. of Hours/Credits
<b>Module 1</b>	<b>Organic reaction mechanism and interesting approaches of molecular synthesis</b>	<b>15</b>
	<p><b>1.1 Organic reactive intermediates (7L)</b> Methods of generation, structure, stability and important reactions involving carbocations, nitrenes, carbenes, arynes, ketenes and carbanion.</p> <p><b>1.2 Neighbouring group participation (2L)</b> Mechanism and effects of anchimeric assistance, NGP by unshared/ lone pair electrons, <math>\pi</math>-electrons, aromatic rings, <math>\sigma</math>-bonds with special reference to norbornyl and bicyclo[2.2.2]octylcation systems (formation of non-classical carbocation)</p> <p><b>1.3 Role of FMOs in organic reactivity (1L)</b> Reactions involving hard and soft electrophiles and nucleophiles, ambident nucleophiles, ambident electrophiles, the <math>\alpha</math> effect</p> <p><b>1.4 Interesting approaches of molecular synthesis (5L)</b> Click Chemistry, Hybrid chemistry, Cascade reactions, Biomimetic synthesis Artificial Intelligence.</p>	
<b>Module 2</b>	<b>Pericyclic Chemistry - I</b>	<b>15 L</b>
	<p><b>2.1 Introduction (2L)</b> Definition and classification of pericyclic reactions, Molecular orbitals of ethylene, butadiene, hexatriene, propenyl and pentadienyl systems.</p> <p><b>2.2 Electrocyclic Reactions (4L)</b> Definition, classification and stereochemistry of electrocyclic reactions, Woodward Hoffmann rules of electrocyclic reactions, Analysis of electrocyclic reactions by: Frontier orbital method, Orbital symmetry correlation diagram, Transition state aromaticity method Few illustrative examples of electrocyclic reactions in synthesis: Stereoselective synthesis of estrone by Vollhardt, Photocyclization of cis – stilbene, Thermal electrocyclic reactions of fulvalene.</p> <p><b>2.3 Cycloaddition reactions (9L)</b> Definition, classification and stereochemistry, Woodward Hoffmann rules of cycloaddition reactions, Analysis of electrocyclic reactions by: Frontier orbital method, Orbital symmetry correlation diagram, Transition state aromaticity method Some important cycloaddition reactions: <math>(2\pi + 2\pi)</math> cycloaddition reaction (Photochemical and thermal); <math>(4\pi + 2\pi)</math> cycloaddition reactions: Diels Alder reaction: Dienes, dienophiles, 'Cis' rule,</p>	

	<p>'endo' rule, regioselectivity, heterodienes and dienophiles, inverse electron demand Diels Alder reaction (IEDDA), Intramolecular Diels Alder reactions (IDA), catalysis of Diels Alder reaction; 1,3 – Dipolar cycloaddition reactions: Mechanism, few illustrative examples of cycloadditions of nitron, azomethine and nitrile oxide.</p> <p>Few illustrative examples of cycloaddition reactions in synthesis: Synthesis of barralene by Lucchi, Synthesis of [2.2] paracyclophane by Hopf, Synthesis of triptycene, Synthesis of dihydroazulene.</p>	
<b>Module 3</b>	<b>Pericyclic Chemistry – II &amp; Photochemistry</b>	<b>15 L</b>
	<p><b>3.1 Sigmatropic rearrangements (8 L)</b> Definition, classification and stereochemistry, Woodward Hoffmann rules of cycloaddition reactions, Analysis of electrocyclic reactions by: Frontier orbital method, Transition state aromaticity method Some illustrative sigmatropic rearrangement reactions [1,3] sigmatropic rearrangements, [1,5] sigmatropic rearrangements, [3,3] sigmatropic rearrangements e.g. Cope and Claisen rearrangement, [2,3] sigmatropic rearrangements e.g. sulphurylid, Sommelet Houser rearrangement, Wittig rearrangement, [5,5] sigmatropic rearrangements e.g. benzidine rearrangement, Chelotropic and group transfer reactions with selective examples, Ene reaction</p> <p><b>3.2 Photochemistry (7L)</b> 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, Photochemistry of carbonyl compounds: <math>\pi \rightarrow \pi^*</math>, <math>n \rightarrow \pi^*</math> transitions, Norrish- I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, photochemistry of enones, photochemical rearrangements of <math>\alpha</math>, <math>\beta</math>-unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction, Photochemistry of olefins, cis-trans isomerizations, dimerizations, Di- <math>\pi</math>- methane rearrangement including aza-di- <math>\pi</math> -methane, Photochemistry of arenes, Chemiluminescence.</p>	
<b>Module 4</b>	<b>Stereochemistry I</b>	<b>15 L</b>
	<p>4.1 Classification of point groups based on symmetry elements with examples (nonmathematical treatment). (2L)</p> <p>4.2 Conformational analysis of medium rings: Eight to ten membered rings and their unusual properties, I-strain, transannular reactions. (3L)</p> <p>4.3 Stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, perhydroanthracenes, steroids, and Bredt's rule. (5L)</p> <p>4.4 Anancomeric systems, Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism): electrophilic addition, elimination, molecular</p>	

	rearrangements, reduction of cyclohexanones (with $\text{LiAlH}_4$ , selectride and MPV reduction) and oxidation of cyclohexanols. (5L)	
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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 alcohol from ketone/aldehyde by sodium borohydride (Column)
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. Benzyl/THP protection of alcohol (Column).
12. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation)

**(Minimum 8 experiments)**

**Note:**

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

**Suggested Readings**

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.

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8. Carbenes, Nitrenes and Arynes. Von T. L. Gilchrist, C. W. Rees. Th. Nelson and Sons Ltd., London 1969.
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. 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, PragatiPrakashan, 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.
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, 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).

<b>Program: M.Sc. Organic Chemistry</b>		<b>Semester: III</b>	
<b>Course: Synthetic Organic Chemistry-I</b>		<b>Course Code: PSMACHO302</b>	
<b>Teaching Scheme</b>		<b>Evaluation Scheme</b>	



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Lecture (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks - 25)	Semester End Examinations (SEE) (Marks- 75 in Question Paper)
4	4	N/A	4 + 2	15 +10	75

**Learning Objectives:**

The objective of the course is to introduce students to importance of,

1. Various multicomponent reaction, domino reaction and click reaction.
2. Chemistry of radicals.
3. Enamines and ylides chemistry.
4. Role of metals and non-metals in organic synthesis.

**Course Outcomes:**

After completion of the course, learners would be able to:

**CO1:** Mechanism and applications of various multicomponent reaction, domino reaction and click reaction.

**CO2:** Introduction to radicals, Radical Initiators: azobisisobutyronitrile (AIBN) and dibenzoyl peroxide.

**CO3:** Generation of Enamines and its application in organic synthesis, Chemistry of Phosphorus, Sulfur and Nitrogen Ylides.

**CO4:** Role of mercury, organoboron, organosilicon, organotin compounds, selenium in organic synthesis.

**CO5:** Application of silylenol ether in organic synthesis.

**Outline of Syllabus: (per session plan)**

Module	Description	No of Hours
1	Name reactions with mechanism and application	15 L
2	Radicals in organic synthesis	15 L
3	Enamines, Ylides and $\alpha$ -C-H functionalization	15 L
4	Metals /Non-metals in organic synthesis	15 L
	<b>Total</b>	<b>60L</b>
<b>PRACTICALS</b>		

*To develop scientific temper and interest by exposure through industrial visits and study/educational tours is recommended in each semester*

**PRACTICAL II**

**Course code: PSMACHO3P2**

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<b>Unit</b>	<b>Topic</b>	<b>No. of Hours/Credits</b>
<b>Module 1</b>	<b>Name reactions with mechanism and application</b>	<b>15L</b>
	1.1 Name reactions: Mukaiyama esterification, Mitsunobu reaction, Ritter reaction, Yamaguchi esterification, Peterson olefination. 1.2 Domino reactions: Characteristics; Nazarov cyclization 1.3 Multicomponent reactions: Strecker Synthesis, Passerini and Ugi 4-component synthesis, Biginelli synthesis, Pictet-Spengler synthesis 1.4 Click Reactions: Characteristics; Huisgen 1,3-Dipolar Cycloaddition	
<b>Module 2</b>	<b>Radicals in organic synthesis</b>	<b>15 L</b>
	2.1 Introduction: Generation, stability, reactivity and structural and stereochemical properties of free radicals, Persistent and charged radicals, Electrophilic and nucleophilic radicals, Radical Initiators: azobisisobutyronitrile (AIBN) and dibenzoyl peroxide 2.2 Characteristic reactions - Free radical substitution, addition to multiple bonds. Radical chain reactions, Radical halogenation of hydrocarbons (Regioselectivity), radical cyclizations, autoxidations: synthesis of cumenehydroperoxide from cumene. 2.3 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. 2.4 Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Acyloin condensation.	
<b>Module 3</b>	<b>Enamines, Ylides and <math>\alpha</math>-C-H functionalization</b>	<b>15 L</b>
	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 $\alpha$ -C-H activation: By nitro, sulfoxide, sulfone and phosphonate groups: generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. Bamford-Stevens reaction, Julia olefination and its modification, Seyferth-Gilbert homologation, Steven's rearrangement.	
<b>Module 4</b>	<b>Metals / Non-metals in organic synthesis</b>	

	<p><b>4.1 Organotin compounds:</b> Preparation of alkenyl and allyl tin compounds; application in C-C bond formation, in replacement of halogen by H at the same C atom.</p> <p><b>4.2 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.</p> <p><b>4.3 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.</p> <p><b>4.4 Organosilicons:</b> Salient features of silicon governing the reactivity of organosilicons, preparation and important bond-forming reactions of alkylsilanes, alkenylsilanes, aryl silanes and allylsilanes. <math>\beta</math>-silylcations as intermediates. Iodotrimethylsilane in organic synthesis.</p> <p><b>4.5 Silylenol ethers:</b> Application: As nucleophiles (Michael reaction, Mukaiyamaaldol reaction), in ring contraction reactions.</p> <p><b>4.6 Selenium in organic synthesis:</b> Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and selenoacetals as <math>\alpha</math>-C-H activating groups.</p>	
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After the preparation of organic compounds in paper-I practical, student will do the purification of prepared compound by techniques such as Steam distillation/Vacuum distillation or Column chromatography and check its purity with TLC and physical constant in Paper-II practical.

**Note:**

1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS** (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.

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.

**Suggested Readings**

1. Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer Verlag
2. Modern Methods of Organic Synthesis, 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
3. Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam.
4. Organic Chemistry, Clayden Greeves Warren and Wothers, Oxford Press (2001).
5. Moder Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).
6. Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002).
7. Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3rd Edn., Nelson Thornes
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).

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Elsevier Academic Press

10. Advanced Organic Chemistry: Reactions & Mechanisms, 2nd Edn., B. Miller & R. Prasad, Pearson

11. Organic reactions and their mechanisms, 3rd revised edition, 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, 2nd Edn.,

14. Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience

15. Name Reactions, Jie Jack Lie, 3rd Edn., Springer

16. Organic Electrochemistry, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

<b>Program: M.Sc. Organic Chemistry</b>				<b>Semester: III</b>	
<b>Course: Natural products and Spectroscopy</b>				<b>Course Code: PSMACHO303</b>	
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>	
<b>Lecture (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutori al (Hours)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks - 25)</b>	<b>Semester End Examinations (SEE) (Marks- 75 in Question Paper)</b>

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		<b>per week)</b>			
4	4	N/A	4 + 2	15 +10	75

**Learning Objectives:**

The objective of the course is to introduce students to importance of

1. Various natural products such carbohydrates, alkaloids etc. and synthesis of natural products.
2. Proton and <sup>13</sup>C-NMR spectroscopy and advanced 2D-NMR techniques used in the characterization of organic compounds.
3. In practical, student would be able to do the separation of a ternary mixture (S-S-S, S-S-L, S-L-L and L-L-L) of organic compounds using micro-scale technique.

**Course Outcomes:**

After completion of the course, learners would be able to:

- CO1:** Occurrence and classifications of carbohydrates, alkaloids, natural pigments and insect pheromones and their applications.
- CO2:** Multi-step synthesis of various natural products.
- CO3:** Introduction to Proton and C<sup>13</sup>NMR spectroscopy, how to solve spectral problems based on UV, IR, <sup>1</sup>HNMR and <sup>13</sup>CNMR and Mass spectrometry.
- CO4:** Other Advanced NMR techniques such as DEPT, NOE and 2D-NMR techniques like COSY, TOCSY, NOESY, ROESY, HMBC, HSQC and HMQC.

**Outline of Syllabus: (per session plan)**

Module	Description	No of Hours
1	Natural products-I	15 L
2	Natural products-II	15 L
3	Nuclear Magnetic Spectroscopy -I	15 L
4	Nuclear Magnetic Spectroscopy -II	15 L
	Natural products-I	15 L
<b>PRACTICALS</b>		

*To develop scientific temper and interest by exposure through industrial visits and study/educational tours is recommended in each semester*

### PRACTICAL III

Unit	Topic	No. of Hours/Credits
<b>Module 1</b>	<b>Natural products-I</b>	<b>15 L</b>
	<p>1.1 Carbohydrates: Recapitulation-Open chain and cyclic structures of monosaccharides, Determination of configuration and determination of ring size of carbohydrates. Introduction to naturally occurring sugars: Deoxysugars, aminosugars, branched sugars. Structure elucidation of lactose and D-glucosamine (synthesis not expected). Structural features and applications of inositol, starch, cellulose, chitin and heparin.</p> <p>1.2 Natural pigments: General structural features, occurrence, biological importance and applications of: carotenoids, anthocyanins, quinones, flavones, pterins and porphyrins (chlorophyll). Structure elucidation of <math>\beta</math>-carotene and Cyanin (with synthesis). Synthesis of ubiquinone.</p> <p>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.</p> <p>1.4 Alkaloids: Occurrence and physiological importance of morphine and atropine. Structure elucidation, spectral data and synthesis of coniine.</p>	
<b>Module 2</b>	<b>Natural products-II</b>	<b>15 L</b>
	<p>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:</p> <ol style="list-style-type: none"> <li>a) Woodward synthesis of Reserpine from benzoquinone</li> <li>b) Corey synthesis of Longifoline from resorcinol</li> <li>c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol</li> <li>d) Corey's Synthesis of Caryophyllene from 2-Cyclohexenone and Isobutylene</li> <li>e) Synthesis of Juvabione.</li> <li>f) Synthesis of Taxol.</li> </ol> <p>2.2 Prostaglandins: Classification, general structure and biological importance. Structure elucidation of PGE1.</p> <p>2.3 Lipids: Classification, role of lipids, Fatty acids and glycerol derived from oils and fats.</p> <p>2.4 Insect growth regulators: General idea, structures of JH2 and JH3.</p>	

	2.5 Plant growth regulators: Structural features and applications of arylacetic acids, gibberellic acids and triacontanol. Synthesis of triacontanol.	
<b>Module 3</b>	<b>Nuclear Magnetic Spectroscopy-I</b>	<b>15 L</b>
	<p>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).</p> <p>3.2 Coupling constant: Coupling in diastereotopic systems, Long range coupling-Allylic coupling, 'W' coupling and Coupling in aromatic and heteroaromatic systems. Temperature effects, Simplification of complex spectra, nuclear magnetic double resonance, chemical shift reagents.</p> <p>3.3 <sup>13</sup>C –NMR spectroscopy: 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.</p> <p>3.4 Spectral problems based on UV, IR, <sup>1</sup>H NMR and <sup>13</sup>C NMR and Mass spectrometry.</p>	
<b>Module 4</b>	<b>Nuclear Magnetic Spectroscopy-II</b>	<b>15 L</b>
	<p>4.1 Pulse Sequences, Pulse width, spins, magnetization vectors</p> <p>4.2 DEPT experiment, determining number of attached hydrogens (Methyl/methylene/methine and quaternary carbons), NOE</p> <p>4.3 2D-Homonuclear Spectroscopy Experiments: Correlation Spectroscopy (COSY) and advance COSY experiments, TOCSY, NOESY, ROESY</p> <p>4.4 2D-Heteronuclear Spectroscopy Experiments: HSQC and HMQC, HMBC</p>	

**Course code: PSMACHO3P3**

**Separation of a ternary mixture of organic compounds purification using micro-scale technique**

Separation of a ternary mixture (**S-S-S, S-S-L, S-L-L and L-L-L**) based upon differences in the physical and the chemical properties of the components.

(Minimum 8 experiments)

Ternary mixture separation + Identification (one compound) + **TLC (1 compounds)**

**Suggested Readings**

1. Natural products chemistry and applications, Sujata V. Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House, 2011.
2. Organic Chemistry Natural Products Volume-II, O. P. Agarwal, Krishna Prakashan, 2011.
3. Chemistry of Natural products, F. F. Bentley and F. R. Dollish, 1974
4. Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S. Ito Majori and S. Nozoo,

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- Academic Press, 1974.
5. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co. 2008.
  6. Heterocyclic chemistry, 3rd edition, Thomas L. Gilchrist, Pearson Education, 2007.
  7. Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, R. K. Bansal, Wiley Eastern Ltd., 1990.
  8. Heterocyclic Chemistry, J. A. Joule and G. F. Smith, ELBS, 2nd edition, 1982.
  9. The Conformational Analysis of Heterocyclic Compounds, F.G. Riddell, Academic Press, 1980.
  10. Principles of Modern Heterocyclic Chemistry, L.A. Paquette, W.B. Benjamin, Inc., 1978.
  11. An Introduction to the Chemistry of Heterocyclic Compounds, 2nd edition, B.M. Acheson, 1975.
  12. Natural Products: Chemistry and Biological Significance Interscience, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J. B. Harborne, Longman, Essex, 1994.
  13. Organic Chemistry, Vol 2, I.L. Finar, ELBS, 6th edition, Pearson.
  14. Stereoselective Synthesis: A Practical Approach, M. Nogradi, Wiley-VCH, 1995.
  15. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
  16. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
  17. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers, 1998.
  18. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers, 1998.
  19. Insecticides of Natural Origin, SukhDev, Harwood Academic Publishers.
  20. Total. Synthesis of Longifolene, J. Am. Chem. Soc., E. J. Corey, M. Ohno, R. B. Mitra, and P. A. Vatakencherry. 1964, 86, 478.
  21. Total. Synthesis of Longifolene, J. Am. Chem. Soc. 1961, 83, 1251.
  22. The structure and total synthesis of 5-Vetivone, J. A. Marshall and P. C. Johnson, J. Org. Chem., 35, 192 (1970).
  23. Total synthesis of spirovetivanes, J. Am. Chem. Soc. 1967, 89, 2750.
  24. The Total Synthesis of Reserpine, Woodward, R. B.; Bader, F. E.; Bickel, H., Frey, A. J.; Kierstead, R. W. Tetrahedron 1958, 2, 1-57.
  25. Total synthesis of Griseofulvin, Stork, G.; Tomasz, M. J. Am. Chem. Soc. 1962, 84, 310.
  26. Synthesis of ( $\pm$ )-4-demethoxydaunomycinone, A. V. Rama Rao, G. Venkatswamy, S. M. Javed M., V. H. Deshpande, B. Ramamohan Rao, J. Org. Chem., 1983, 48 (9), 1552.
  27. The Alkaloids, The fundamental Chemistry A biogenetic approach, Marcel Dekker Inc. New York, 1979.
  28. Comprehensive Organic Chemistry by Barton and Ollis, Pergamon Press, Oxford, 1979.
  29. Medicinal Natural Products, a Biosynthetic Approach, Derick Paul, John Wiley and Sons, 2002.
  30. Biosynthesis of Natural Products, Mannitto Paolo, Ellis Horwood Limited, 1981.
  31. Selected Organic synthesis, Ian Fleming, John Wiley and Sons, 1973.
  32. Total synthesis of Natural Products, J. Apsimon, John Wiley and Sons.
  33. The Logic of Chemical Synthesis, E. J. Corey and Xue-Min Cheng, Wiley Interscience.
  34. Classics in Total Synthesis, K. C. Nicolaou and E. J. Sorensen, Weinheim: VCH, 1996.
  35. Spectroscopy of Organic compounds, P.S. Kalsi, New Age International Pub. Ltd. And Wiley Eastern Ltd., Second edition, 1995.
  36. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India 1987.
  37. 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.



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38. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989.
39. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987.
40. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., .3122
41. Introduction to spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, 4th ed., 2009.
42. Organic spectroscopic structure determination: a problem-based learning approach Douglass F. Taber, Oxford University Press, 17Sep-2007.
43. Organic Spectroscopy: Principles and Applications, Jag Mohan, Alpha Science International Ltd., 30-Mar-2004 46.
44. Biotransformations in Organic Chemistry, 5thEdition, Kurt Faber, Springer
45. Structure Determination of Organic Compounds, EPretsch, P. Buhlmann, C.Affolter, Springer
46. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., .3122
47. Introduction to spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, 4th ed., 2009.

<b>Program: M.Sc. Organic Chemistry</b>				<b>Semester: III</b>	
<b>Course: Medicinal, Biogenesis and Green Chemistry</b>				<b>Course Code: PSMACHO304</b>	
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>	
<b>Lecture (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutori al (Hours)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks - 25)</b>	<b>Semester End Examinations (SEE) (Marks- 75 in Question Paper)</b>

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		<b>per week)</b>			
4	4	N/A	4 + 2	15 +10	75
<b>Learning Objectives:</b>					
The objective of the course is to introduce students to importance of,					
<ol style="list-style-type: none"> <li>1. Drug discovery design and development. Concept of lead compounds.</li> <li>2. Different terminology used in the medicinal chemistry.</li> <li>3. Biosynthesis of natural products</li> </ol>					
<b>Course Outcomes:</b>					
After completion of the course, learners would be able to:					
<b>CO1:</b> Important terms used in medicinal chemistry, procedures in drug design, drug discovery without lead.					
<b>CO2:</b> QSAR parameters, steric effects, The Taft and other equations.					
<b>CO3:</b> Concept of prodrugs and soft drugs.					
<b>CO4:</b> Primary and secondary metabolites and the building blocks, general pathway of amino acid biosynthesis.					
<b>CO5:</b> Basic principles of green chemistry, designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts					
<b>Outline of Syllabus: (per session plan)</b>					
<b>Module</b>	<b>Description</b>				<b>No of Hours</b>
<b>1</b>	<b>Drug discovery, design and development</b>				<b>15 L</b>
<b>2</b>	<b>Drug design, development and synthesis</b>				<b>15 L</b>
<b>3</b>	<b>Biogenesis and biosynthesis of natural products</b>				<b>15 L</b>
<b>4</b>	<b>Green chemistry</b>				<b>15 L</b>
	<b>Total</b>				<b>60 L</b>
<b>PRACTICALS</b>					

*To develop scientific temper and interest by exposure through industrial visits and study/educational tours is recommended in each semester*

### PRACTICAL IV

Course code: PSMACHO3P4

Unit	Topic	No. of Hours/Credits
<b>Module 1</b>	<b>Drug discovery, design and development</b>	<b>15L</b>
	<p>1.1 Introduction, important terms used in medicinal chemistry: receptor, therapeutic index, bioavailability, and 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.</p> <p>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).</p>	
<b>Module 2</b>	<b>Drug design, development and synthesis</b>	<b>15 L</b>
	<p>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.</p> <p>2.2 Introduction to modern methods of drug design and synthesis- drug design via enzyme inhibition (reversible and irreversible), bioinformatics and drug design.</p> <p>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.</p> <p>2.4 Synthesis and application of the following drugs: Fluoxetine, cetirizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate.</p>	
<b>Module 3</b>	<b>Biogenesis and biosynthesis of natural products</b>	<b>15L</b>
	<p>3.1 Primary and secondary metabolites and the building blocks, general pathway of amino acid biosynthesis.</p> <p>3.2 Acetate pathway: Biosynthesis of malonylCoA, saturated fatty acids, prostaglandins from arachidonic acid, aromatic polyketides.</p> <p>3.3 Shikimic Acid pathway: Biosynthesis of shikimic acid, aromatic aminoacids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, flavonoids and isoflavonoids.</p>	

	3.4 Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes, geranyl cation and its derivatives, sesquiterpenes – farnesylation and its derivatives and diterpenes.	
<b>Module 4</b>	<b>Green chemistry</b>	<b>15L</b>
	<p>4.1 Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts.</p> <p>4.2 Use of the following in green synthesis with suitable examples. Green reagents (dimethylcarbonate, polymer supported reagents), 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), Green solvents (water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide) , Solid state reactions (solid phase synthesis, solid supported synthesis ) Microwave assisted synthesis (reactions in water, reactions in organic solvents, solvent free reactions) , Ultrasound assisted reactions.</p> <p>4.3 Comparison of traditional processes versus green processes in the syntheses of ibuprofen, adipic acid, 4-aminodiphenylamine, p-bromotoluene and benzimidazole.</p> <p>4.4 Green Catalysts: Nanocatalyst, Types of nanocatalysts, Advantages and Disadvantages of Nanocatalysts, Idea of Magnetically separable nanocatalysts.</p>	

Research paper review of current topic/literature review along with report preparation.

### **Suggested Readings**

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. Stryer, Lubert; Biochemistry; W. H. Freeman publishers.
3. Voet, D. and J. G. Voet (2004) Biochemistry, 3<sup>rd</sup> Edition, John Wiley & sons, Inc. USA.
4. Zubay, Goffrey L; Biochemistry; Wm C. Brown publishers.
5. V. Polshettiwar, R. Luque, A. Fihri, H. Zhu, M. Bouhrara and J-M Basset, Chem. Rev. 2011, 111, 3036-3075;
6. R. B. NasirBaig and R. S. Varma, Chem. Comm., 2013, 49, 752-770; 7.M. B. Gawande, A. K. Rathi, P. S. Varma, Appl. Sci., 2013, 3, 656-674;
7. J. Govan and Y. K. Gun'ko, Nanomaterials, 2014, 4, 222-214.
8. K. Philippot and P. Serp, Nanomaterials in catalysis, First Edition. Edited by P. Serp and K. Philippot; 2013 Wiley –VCH Verlag GmbH & Co. KGaA
9. D. Astruc, Nanomaterials and Catalysis, Wiley-VCH Verlag GmbH & Co. KGaA, 2008, 1-48;
10. C. N. R. Roa, A. Muller and A. K. Cheetham, The chemistry of Nanomaterials, Wiley-VCH Verlag GmbH & Co. KGaA, 2005, 1-11;
11. Richard B. Silverman, The organic chemistry of drug design and drug action, 2nd edition, Academic Press
12. Medicinal chemistry, D. Sriram and P. Yogeeswari, 2nd edition, Pearson
13. An introduction to drug design-S. S. Pandeya and J. R. Dimmock (New age international)

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14. Burger's medicinal chemistry and drug discovery. by Manfred E. Wolf
15. Introduction to Medicinal chemistry. by Graham Patrick
16. Medicinal chemistry-William O. Foye
17. T. B. of Organic medicinal and pharmaceutical chemistry-Wilson and Gisvold's (Ed. Robert F. Dorge)
18. An introduction to medicinal chemistry-Graham L. Patrick, OUP Oxford, 2009.
19. Principles of medicinal chemistry (Vol. I and II)-S. S. Kadam, K. R.
  - a. Mahadik and K.G. Bothara ,Niraliprakashan.
20. Medicinal chemistry (Vol. I and II)-Burger
21. Strategies for organic drug synthesis and design - D. Lednicer Wiley
22. Pharmacological basis of therapeutics-Goodman and Gilman's (McGraw Hill)
23. Enzyme catalysis in organic synthesis, 3rd edition. Edited by KarlheinzDrauz, Harold Groger, and Oliver May, Wiley-VCH Verlag GmbH & Co KgaA, 2012.
24. Biochemistry, Dr U Satyanarayan and Dr U Chakrapani, Books and Allied (P) Ltd.
25. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
26. The Organic Chemistry of Enzyme-Catalysed Reactions, Academic Press, By Richard B. Silverman
27. Enzymes: Practical Introduction to structure, mechanism and data analysis, By Robert A. Copeland, Wiley-VCH, Inc.
28. The Organic Chemistry of Biological Pathways By John McMurry, Tadhg Begley by Robert and company publishers
29. Bioorganic Chemistry- A practical approach to Enzyme action, H. Dugas and C. Penny. Springer Verlag, 1931
30. Biochemistry: The chemical reactions in living cells, by E. Metzler. Academic Press.
31. Concepts in biotechnology by D. Balasubramanian& others
32. Principals of biochemistry by Horton & others.
33. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
34. Medicinal Natural Products: A Biosynthetic Approach by Paul M. Dewick. 3<sup>rd</sup> Edition, Wiley.
35. Natural product chemistry, A mechanistic, biosynthetic and ecological approach, Kurt B. G. Torssell, Apotekarsocieteten – Swedish pharmaceutical press.
36. Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House.
37. Natural Products Volume- 2, By O. P. Agarwal.
38. Chemistry of Natural Products, F. F. Bentley and F. R. Dollish, 1974.
39. Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S.ItoMajori and S. Nozoo, Academic Press, 1974.
40. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co.
41. Green Chemistry: An Introductory Text, 2nd Edition, Published by Royal Society of Chemistry, Authored by Mike Lancater.
42. Organic synthesis in water. By Paul A. Grieco, Blackie.
43. Green chemistry, Theory and Practical, Paul T. Anastas and John C. Warner.
44. New trends in green chemistry By V. K. Ahulwalia and M. Kidwai, 2nd edition, Anamaya Publishers, New Delhi.
45. An introduction to green chemistry, V. Kumar, Vishal Publishing Co.
46. Organic synthesis: Special techniques. V.K.Ahulwalia and RenuAggarwal





Shri Vile Parle Kelavani Mandal's  
**MITHIBAI COLLEGE OF ARTS, CHAUHAN INSTITUTE OF SCIENCE &  
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(AUTONOMOUS)

*NAAC Reaccredited 'A' grade, CGPA: 3.57 (February 2016),  
Granted under RUSA, FIST-DST & -Star College Scheme of DBT, Government of India  
Best College (2016-17), University of Mumbai*

Affiliated to the  
**UNIVERSITY OF MUMBAI**

**Program: M.Sc.**

**Course: Organic Chemistry**

**Semester IV**

**Choice Based Credit System (CBCS) with effect from the  
Academic year-2020-2021**

## **PROGRAMME SPECIFIC OUTCOMES (PSO'S)**

On completion of the **M.Sc.-Organic Chemistry**, the learners should be enriched with knowledge and be able to-

- PSO9:** gain complete knowledge about all fundamental aspects of all the elements of organic chemistry.
- PSO10:** develop analytical thinking and apply the same for the understanding of underlining principles, proposing mechanism, problem solving, identification of chemical species and arriving to logical conclusion.
- PSO11:** understands the background of organic reaction mechanisms, complex chemical structure, and molecular rearrangements.
- PSO12:** gain knowledge in classical laboratory techniques and be able to use modern instrumentation, so that they can perform new experiments, obtain experimental data and its spectral interpretation through theoretical principals.
- PSO13:** integrate knowledge learned in chemistry to various industry and pharmaceutical needs.
- PSO14:** learn about the potential uses of medicinal chemistry and green chemistry.
- PSO15:** carry out experiments in the area of organic analysis, estimation, separation, derivative process.
- PSO16:** access, search and use the chemical literature for research article review and research project work.

### **Preamble**

The purpose of post-graduate education in science is to create highly skilled manpower in specific areas, which will lead to generation of new knowledge and creation of wealth for the country. Chemistry is a fundamental science and has contributed immensely to the improvement of the life of human beings by providing many of human requirements and essentialities. The credit system has been adopted for all these courses, which would allow students to develop a strong foundation in the fundamentals and specialize in the disciplines of his/her liking and abilities. The courses are designed so that the students pursuing these courses will obtain fundamental knowledge about the subject in the respective specialization. The students are also expected to get corresponding experimental training during the practical courses.

### **Evaluation Pattern**



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The performance of the learner will be evaluated in two components. The first component will be a Continuous Assessment with a weightage of 25% of total marks per course. The second component will be a Semester end Examination with a weightage of 75% of the total marks per course. The allocation of marks for the Continuous Assessment and Semester end Examinations is as shown below:

**c) Details of Continuous Assessment (CA)**

25% of the total marks per course:

<b>Continuous Assessment</b>	<b>Details</b>	<b>Marks</b>
<b>Component 1 (CA-1)</b>	Test	15 marks
<b>Component 2 (CA-2)</b>	Assignment	10 marks

**d) Details of Semester End Examination**

75% of the total marks per course. Duration of examination will be two and half hours.

<b>Question Number</b>	<b>Description</b>	<b>Marks</b>	<b>Total Marks</b>
1	Attempt any Three out of Five	15 Marks	15 Marks
2	Attempt any Three out of Five	15 Marks	15 Marks
4	Attempt any Three out of Five	15 Marks	15 Marks
4	Attempt any Three out of Five	15 Marks	15 Marks
5	Attempt any Three out of Four	15 Marks	15 Marks
<b>Total Marks</b>			<b>75</b>

Signature

Signature

Signature

HOD

Approved by Vice –Principal

Approved by Principal

<b>Program- M.Sc. Organic Chemistry</b>	<b>Semester : IV</b>
<b>Course : Theoretical organic chemistry-II</b>	<b>Course Code: PSMACHO401</b>
<b>Teaching Scheme</b>	<b>Evaluation Scheme</b>

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Lecture (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks - 25)	Semester End Examinations (SEE) (Marks- 75 in Question Paper)
4	4	N/A	4 + 2	15 +10	75

**Learning Objectives:**

The objective of the course is to introduce students to importance of,

1. Physical organic chemistry and factor affecting the organic reactions.
2. Supramolecular chemistry and its applications.
3. Stereochemistry of chiral compounds.
4. Asymmetric synthesis and factor affecting.

**Course Outcomes:**

After completion of the course, learners would be able to:

**CO4:** Linear free energy relationship (LFER) in determination of organic reaction mechanism.

**CO5:** Hammett equation and its uses. The Taft model.

**CO6:** Synthesis, properties and uses of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins.

**CO7:** Racemisation and resolution of racemates.

**CO8:** Molecular dissymmetry and chiroptical properties.

**CO9:** Circular birefringence and circular dichroism.

**CO10:** Principles of asymmetric synthesis, Cram's rule, Felkin-Anh model, Sharplessenantioselectiveepoxidation.

**CO11:** Use of chiral BINOLs, BINAPs and chiral oxazolines and oxazolidines asymmetric transformations.

**Outline of Syllabus: (per session plan)**

Module	Description	No of Hours
1	Physical organic chemistry	15 L
2	Supramolecular Chemistry	15 L
3	Stereochemistry - II	15 L
4	Asymmetric Synthesis	15 L
	Total	60 L

**PRACTICALS**

*To develop scientific temper and interest by exposure through industrial visits and study/educational tours is recommended in each semester*

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Unit	Topic	No. of Hours/Credits
<b>Module 1</b>	<b>Physical organic chemistry</b>	<b>15L</b>
	<p><b>1.1. Structural effects and reactivity:</b> Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation, substituent constants, theories of substituent effects, interpretation of <math>\sigma</math>-values, reaction constants <math>\rho</math>, Yukawa-Tsuno equation.</p> <p><b>1.2.</b> Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants, The Taft model, <math>\sigma_I</math> and <math>\sigma_R</math> scales, steric parameters <math>E_s</math> and <math>\beta</math>. Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's <math>s_{ET}</math> parameter, Solvatochromism scale, Spectroscopic Correlations, Thermodynamic Implications.</p>	
<b>Module 2</b>	<b>Supramolecular Chemistry</b>	<b>15L</b>
	<p>2.1 Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes.</p> <p>2.2 Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.</p> <p>2.3 Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.</p> <p>2.4 Molecular recognition and catalysis, molecular self assembly. Supramolecular Polymers, Gels and Fibers.</p>	
<b>Module 3</b>	<b>Stereochemistry - II</b>	<b>15L</b>
	<p>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.</p> <p>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).</p>	

**PRACTICAL I**

	<p>3.3 Correlative method for configurational assignment: chemical Method without involving the chiral centre, optical rotation, and NMR spectroscopy.</p> <p>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 <math>\alpha</math>-haloketone rule with applications.</p>	
<b>Module 4</b>	<b>Asymmetric Synthesis</b>	<b>15L</b>
	<p>4.1 Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions.</p> <p>4.2 Synthesis of L-DOPA [Knowles's Mosanto process]. Asymmetric reactions with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharplessenantioselectiveepoxidation.</p> <p>4.3 Dihydroxylation/Sharpless Asymmetric Dihydroxylation, aminohydroxylation,</p> <p>4.4 Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.</p> <p>4.5 Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines and oxazolidines asymmetric transformations.</p>	

**Course code: PSMACHO4P1**

**Two steps preparations**

1. Acetophenone → Acetophenone phenyl hydrazine → 2-phenylindole.
2. 2-naphthol → 1-phenyl azo-2-naphthol → 1-amino-2-naphthol.
3. Cyclohexanone → cyclohexanoneoxime → Caprolactum.
4. Hydroquinone → hydroquinone diacetate → 2,5-dihydroxyacetophenone.
5. 4-nitrotoluene → 4-nitrobenzoic acid → 4-aminobenzoic acid.
6. *o*-nitroaniline → *o*-phenylenediamine → Benzimidazole.
7. Benzophenone → benzophenoneoxime → benzanilide.
8. *o*-chlorobenzoic acid → N-phenyl anthranilic acid → acridone.
9. Benzoin → benzil → benzilic acid.
10. Phthalic acid → phthalimide → anthranilic acid.
11. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-methyl-7-acetoxy coumarin.
12. Anthracene → anthraquinone → anthrone.

**(Minimum 8 experiments)**

**HPTLC(Demonstration)**

**Suggested Readings**

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 1969.
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. 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, 5<sup>th</sup>, 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. Modern methods of Organic Synthesis, 4 Organic chemistry, 8th edition, John McMurryth Edition W. Carruthers and Iain Coldham, Cambridge University Press 2004.
20. Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books, 2006
21. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.
22. Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd
23. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India.
24. Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
25. Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005.

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26. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers.
27. Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
28. Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
29. Large ring compounds, J.A. Semlyen, Wiley-VCH, 1997.
30. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley- Eastern.
31. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
32. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
33. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
34. Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
35. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
36. Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A John Wiley and Sons, Ltd., Publication).

<b>Program: M.Sc. Organic Chemistry</b>				<b>Semester : IV</b>	
<b>Course : Synthetic Organic Chemistry-II</b>				<b>Course Code: PSMACHO402</b>	
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>	
<b>Lecture (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks - 25)</b>	<b>Semester End Examinations (SEE) (Marks- 75 in Question Paper)</b>
4	4	N/A	4 + 2	15 +10	75
<b>Learning Objectives:</b> The objective of the course is to introduce students to importance of,					

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1. Protection and deprotection in organic synthesis.
2. Concept of reversal of polarity and design of organic synthesis.
3. Organic Electrochemistry
4. 18 electron rule's and Application of rare earth metals such as Pd, Pt, Ni, Co and Cr etc.

**Course Outcomes:**

After completion of the course, learners would be able to:

**CO1:** Protection and deprotection of functional groups and approaches in retrosynthesis.

**CO2:** Concept of umpolung (reversal of polarity)

**CO3:** Basic electro-organic chemistry and selected methods of organic synthesis.

**CO4:** 18 electron rule, Chemistry of Palladium in organic reaction.

**CO5:** Application of rare earth metals such as Pd, Pt, Ni, Co and Cr etc.

**CO6:** Application of samarium iodide and Ce (IV) based compounds in organic synthesis.

**Outline of Syllabus: (per session plan)**

<b>Module</b>	<b>Description</b>	<b>No of Hours</b>
<b>1</b>	<b>Designing Organic Synthesis-I</b>	<b>15 L</b>
<b>2</b>	<b>Designing Organic Synthesis-II</b>	<b>15 L</b>
<b>3</b>	<b>Electro-organic chemistry and Selected methods of Organic synthesis</b>	<b>15 L</b>
<b>4</b>	<b>Transition and rare earth metals in organic synthesis</b>	<b>15 L</b>
	<b>Total</b>	<b>60L</b>
<b>PRACTICALS</b>		

*To develop scientific temper and interest by exposure through industrial visits and study/educational tours is recommended in each semester*

**PRACTICAL II**

**Course code: PSMACHO4P2**

**Two steps preparations (Continued from Paper I)**

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After the preparation of organic compounds in paper-I practical, student will do the purification of prepared compound by techniques such as Steam distillation/Vacuum distillation or Column

<b>Unit</b>	<b>Topic</b>	<b>No. of Hours/Credits</b>
<b>Module 1</b>	<b>Designing Organic Synthesis- I</b>	<b>15L</b>
	<p>1.1 Protecting groups in Organic Synthesis: Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications.</p> <p>1.2 Concept of umpolung (Reversal of polarity): Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethylsulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.</p> <p>1.3 Selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity</p> <p>1.4 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)</p> <p>1.5 Aromatic substitutions and importance of order of events in organic synthesis</p>	
<b>Module 2</b>	<b>Designing Organic Synthesis-II</b>	<b>15L</b>
	<p>2.1 General strategy: choosing a disconnection-simplification, symmetry, high yielding steps, and recognisable starting material.</p> <p>2.2 One group Disconnections (C-C and C-X): Alcohols (including stereoselectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis, control in carbonyl condensations, amine synthesis, reactions of epoxide.</p> <p>2.3 Two group C-C Disconnections: Diels-Alder reactions, <math>\alpha</math>, <math>\beta</math>-unsaturated compounds, Michael addition and Robinson annulation.</p> <p>2.4 Retrosynthetic analysis of 1,2- 1,3- 1,4- 1,5- and 1,6-difunctionalized compounds.</p>	
<b>Module 3</b>	<b>Electro-organic chemistry and Selected methods of Organic synthesis</b>	<b>15L</b>
	<p>3.1 Electro-organic chemistry:</p> <p>3.1.1 Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes.</p> <p>3.1.2 Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitro compounds, olefins, arenes, electro-dimerization.</p>	



	<p>3.1.3 Anodic oxidation: Oxidation of alkylbenzene, Kolbe reaction, Non Kolbe oxidation, Shono oxidation.</p> <p>3.2 Selected Methods of Organic synthesis Applications of the following in organic synthesis:</p> <p>3.2.1 Crown ethers, cryptands, micelles, cyclodextrins, catenanes.</p> <p>3.2.2 Organocatalysts: Proline, Imidazolidinone.</p> <p>3.2.3 Pd-catalysed cycloaddition reactions: Stille reaction, Saegusa-Ito oxidation to enones, Negishi coupling.</p> <p>3.2.4 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 and its role as a de-protecting agent.</p>	
<b>Module 4</b>	<b>Transition and rare earth metals in organic synthesis</b>	<b>15L</b>
	<p>4.1 Introduction to basic concepts: 18 electron rule, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion.</p> <p>4.2 Palladium in organic synthesis: <math>\pi</math>-bonding of Pd with olefins, applications in C-C bond formation, carbonylation, alkene isomerisation, cross-coupling of organometallics and halides. Representative examples: Heck reaction, Suzuki-Miyaura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N, S, or P atoms.</p> <p>4.3 Olefin metathesis using Grubb's catalyst.</p> <p>4.4 Application of Ni, Co, Fe, Rh, and Cr carbonyls in organic synthesis.</p> <p>4.5 Application of samarium iodide including reduction of organic halides, aldehydes and ketones, <math>\alpha</math>-functionalised carbonyl and nitro compounds.</p> <p>4.6 Application of Ce(IV) in synthesis of heterocyclic quinoxaline derivatives.</p>	

chromatography and check its purity with TLC and physical constant in Paper-II practical (Minimum 8 experiments).

**Note:**

- 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.
- 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.

**Suggested Readings**

- Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5<sup>th</sup> Edition, Springer Verlag

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2. Modern Methods of Organic Synthesis, 4<sup>th</sup> Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
3. Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam.
4. Organic Chemistry, ClaydenGreeves Warren and Wothers, Oxford Press (2001).
5. Moder Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).
6. Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002).
7. Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3<sup>rd</sup>Edn., Nelson Thornes
8. Organic Chemistry, 7<sup>th</sup>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, 2<sup>nd</sup>Edn., B. Miller & R. Prasad, Pearson
11. Organic reactions and their mechanisms, 3<sup>rd</sup>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<sup>nd</sup>Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
14. 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

<b>Program:M.Sc. Organic Chemistry</b>				<b>Semester : IV</b>	
<b>Course : Natural products and Heterocyclic chemistry</b>				<b>Course Code: PSMACHO403</b>	
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>	
<b>Lecture (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks - 25)</b>	<b>Semester End Examinations (SEE) (Marks- 75 in Question Paper)</b>
4	4	N/A	4 + 2	15 +10	75

**Learning Objectives:**

The objective of the course is to introduce students to

1. Importance of natural product such as Vitamins, Steroids, Terpenes etc.
2. Chemistry of a number of heterocyclic compounds and their applications.

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<b>Course Outcomes:</b> After completion of the course, learners would be able to: <b>CO1:</b> General structure, classification. Occurrence, biological role, important structural and stereochemical features of steroids. <b>CO2:</b> Chemistry of Vitamins, Terpenes and Antibiotics. <b>CO3:</b> Reactivity, synthesis and applications of heterocycles.		
<b>Outline of Syllabus: (per session plan)</b>		
<b>Module</b>	<b>Description</b>	<b>No of Hours</b>
1	Natural products-III	15 L
2	Natural products-IV	15 L
3	Heterocyclic compounds-I	15 L
4	Heterocyclic compounds-II	15 L
	Total	60 L
<b>PRACTICALS</b>		

*To develop scientific temper and interest by exposure through industrial visits and study/educational tours is recommended in each semester*

### PRACTICAL III

**Course code: PSMACHO4P3**  
**2D NMR interpretation (Minimum 8)**

**COSY, TOCSY, INADIQUATE, NOSEY, ROSEY, HMQC, HSQC, and HMBS**

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Unit	Topic	No. of Hours/Credits
<b>Module 1</b>	<b>Natural products-III</b>	<b>15L</b>
	<p>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.</p> <p>1.2 Synthesis of 16-DPA from cholesterol and plant saponin.</p> <p>1.3 Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone.</p> <p>1.4 Synthesis of cinerolone, jasmolone, exaltone and muscone.</p>	
<b>Module 2</b>	<b>Natural products-IV</b>	<b>15L</b>
	<p>2.1 Vitamins: Classification, sources and biological importance of vitamin B<sub>1</sub>, B<sub>2</sub>, B<sub>6</sub>, folic acid, B<sub>12</sub>, C, D<sub>1</sub>, E (<math>\alpha</math>-tocopherol), K<sub>1</sub>, K<sub>2</sub>, H (<math>\beta</math>- biotin).            Synthesis of the following:            Vitamin A from <math>\beta</math>-ionone and bromoester moiety.            Vitamin B<sub>1</sub> including synthesis of pyrimidine and thiazole moieties            Vitamin B<sub>2</sub> from 3, 4-dimethylaniline and D (-) ribose            Vitamin B<sub>6</sub> from: 1) ethoxyacetylacetone and cyanoacetamide, 2) ethyl ester of N-formyl-DL-alanine (Harris synthesis)            Vitamin E (<math>\alpha</math>-tocopherol) from trimethylquinol and phetyl bromide            Vitamin K<sub>1</sub> from 2-methyl-1, 4-naphthaquinone and phytol.</p> <p>2.2 Antibiotics: Classification on the basis of activity. Structure elucidation, spectral data of penicillin-G, cephalosporin-C and chloramphenicol. Synthesis of chloramphenicol (from benzaldehyde and <math>\beta</math>-nitroethanol) penicillin-G and phenoxymethylpenicillin from D-penicillamine and t-butyl phthalimide malonaldehyde (synthesis of D-penicillamine and t-butyl phthalimide malonaldehyde expected)</p> <p>2.3 Naturally occurring insecticides: Sources, structure and biological properties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis of pyrethrin I.</p> <p>2.4 Terpenoids: General classification of terpenoids; Occurrence, stereochemistry, spectral data and synthesis of zingiberene and structure elucidation of zingiberene, <math>\alpha</math>-Pinene and Camphor            General chemistry of the following compounds- Artemisinin, Azadirachtin.</p>	

<b>Module 3</b>	<b>Heterocyclic Chemistry – I</b>	<b>15 L</b>
	<p>3.1 Recapitulation: Basic heterocycles (Furan, Thiophene, Pyrrole, Pyridine).</p> <p>3.2 Nomenclature of heterocyclic compounds Common, systematic (Hantzsch-Widman) and replacement nomenclature of (i) 3 – 6 membered monocyclic compounds (ii) 5 – 6 membered bicyclic / tricyclic fused heterocycles (up to three atoms).</p> <p>3.3 Monocyclic heterocyclic compounds with one heteroatom in ring <i>2 – Pyrone and 4 – Pyrone</i> Reactions: With electrophilic agents (Nitration, Bromination); With nucleophilic agents (aqueous alkali, Grignard, amines); Cycloaddition reactions. Synthesis: From 1, 3 – and 1, 3, 5 – di / tricarbonyl compounds.</p> <p>3.4 Benzanellated heterocyclic compounds with one heteroatom in ring 3.4.1 <i>Quinoline and Isoquinoline</i> Reactions: With electrophilic agents (Protonation, Nitration, Sulphonation, Halogenation); With nucleophilic agents (alkylation, arylation, amination, hydroxylation); With reducing agents (H<sub>2</sub> / Pt, NaBH<sub>4</sub>); Metallation and metal halogen exchange reaction. Synthesis: Skraup synthesis, Doebner Miller synthesis, Bischler Napileranshi synthesis, Pictet – Spengler synthesis. 3.4.2 <i>Coumarin and Chromone</i> Reactions: With electrophilic agents (Protonation, Bromination, Nitration Mannich reaction); With nucleophilic reagents (Hydroxide, amines, Grignard, lithiation); With reducing agents (LiAlH<sub>4</sub>); With oxidizing agents (epoxidation); Cycloaddition reactions. Synthesis: Pechmann synthesis, Fromo–hydroxy aldehydes, suitably substituted aromatic carbonyl compounds (Chromones). 3.4.3 <i>Indole, Benzothiophene, Benzofuran</i> Reactions: With electrophilic reagents (Protonation, nitration, sulphonation, halogenation, formylation, acylation, alkylation, conjugate addition); With bases; With reducing agents: Metal / NH<sub>3</sub>, catalytic reduction, sodium cynoborohydride; Metallation, metal halogen exchange reaction. Synthesis: Fischer synthesis, Reissert synthesis, Madelung synthesis, Bischler synthesis, Bartoli synthesis, suitably substituted aldehydes, keones or acids (benzothiophene, benzofuran).</p>	
<b>Module 4</b>	<b>Heterocyclic Chemistry – II</b>	<b>15 L</b>

**Suggested Readings**

	<p>4.1 Monocyclic heterocyclic compounds with two heteroatoms in ring</p> <p>4.1.1 <i>Pyridazine, Pyrimidine, Pyrazine</i>  Reactions: With electrophilic reagents (Protonation, alkylation, halogenation); With nucleophilic reagents (Hydrazine, alkyl / aryl lithium, amines); Metallation and metal halogen exchange reaction.  Synthesis: From 1,2-, 1,3-, 1,4 – dicarbonyl compounds; from 2 – amino ketones</p> <p>4.1.2 <i>Imidazole, Thiazole, Oxazole</i>  Reactions: With electrophilic reagents (Protonation, alkylation, acylation, nitration, sulphonation, halogenation); With nucleophilic reagents (Halogen replacement); With bases; C – Metallation and metal halogen exchange reactions  Synthesis: From <math>\alpha</math> – halo carbonyl compounds; from 1,2 – diketones; from <math>\alpha</math> – acylamino carbonyl compounds.</p> <p>4.1.3 <i>Pyrazole, Isothiazole, Isoxazole</i>  Reactions: With electrophilic reagents (Protonation, alkylation, acylation, nitration, halogenation); With bases; C – Metallation and metal halogen exchange reactions  Synthesis: From 1,3 – dicarbonyl compounds, by dipolar cycloaddition reaction.</p> <p>4.2 Benzannellated heterocyclic compounds with two heteroatoms in heterocyclic ring  <i>Benzimidazole, benzoxazole, benzothiazole</i>  Reactions: With electrophilic reagents (Protonation, alkylation, nitration, bromination); With nucleophilic reagents (Thiourea, amines); Ring metalation reactions.  Synthesis: From ortho – heteroatom substituted arenes, ortho – haloaryl ketone oxime.</p> <p>4.3 Overview of applications of heterocycles  In plastics and polymers, fungicides and herbicides, Dyes and pigments, Medicines, Biochemistry.</p>	
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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., 1990.
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.

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12. An Introduction to the Chemistry of Heterocyclic Compounds, 2nd 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. Rama Rao, 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, 1979.
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, 1987.
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, 1989.
41. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987.
42. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4<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.

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44. Organic spectroscopic structure determination: a problem-based learning approach Douglass F. Taber, Oxford University Press, 17Sep-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, EPretsch, P. Buhlmann, C.Affolter, Springer.

<b>Program: M. Sc. Organic Chemistry</b>				<b>Semester : IV</b>	
<b>Course :Research Methodology</b>				<b>Course Code: PSMACHO404</b>	
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>	
<b>Lecture (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Lecture (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Lecture (Hours per week)</b>	<b>Practical (Hours per week)</b>
4	4	4	4	4	4
<b>Learning Objectives:</b> The objective of the course is to introduce students to importance of, <ol style="list-style-type: none"> <li>1. Research journals and webs.</li> <li>2. Data Analysis.</li> <li>3. Various methods scientific research</li> <li>4. Chemical safety &amp; ethical handling of chemicals.</li> </ol>					
<b>Course Outcomes:</b> After completion of the course, learners would be able to: <p><b>CO1:</b> Various sources of information like print and digital sources, importance of chemical abstract.</p> <p><b>CO2:</b> Data analysis and its different method.</p> <p><b>CO3:</b> How to do referencing and to write a scientific research paper.</p> <p><b>CO4:</b> Chemical safety and handling of chemicals.</p>					



Outline of Syllabus: (per session plan)		
Module	Description	No of Hours
1	Print: Primary, Secondary and Tertiary sources.	15 L
2	Data Analysis	15 L
3	Methods of Scientific Research and Writing Scientific Papers	15 L
4	Chemical Safety & Ethical Handling of Chemicals	15 L
	Total	60 L
<b>PRACTICALS</b>		

*To develop scientific temper and interest by exposure through industrial visits and study/educational tours is recommended in each semester*

## PRACTICAL IV

**Course code: PSMACHO4P4**  
**Research Project Evaluation**

### Suggested Readings

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), Practical skills in Chemistry, 2<sup>nd</sup> Ed., Prentice Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) Data Analysis for Chemistry Oxford University Press.
3. Topping, J., (1984) Errors of Observation and their Treatment 4<sup>th</sup> Ed., Chapman Hill, London.
4. Harris, D. C. (2007) Quantative Chemical Analysis 6<sup>th</sup> Ed., Freeman Chapters 3-5
5. Levie, R. De. (2001) How to use Excel in Analytical Chemistry and in general scientific data analysis Cambridge Universty Press.

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6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

<b>Unit</b>	<b>Topic</b>	<b>No. of Hours/Credits</b>
<b>Module 1</b>	<b>Print: Primary, Secondary and Tertiary sources</b>	<b>15 L</b>
	<p>Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, textbooks, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.</p> <p>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.</p> <p>Information Technology and Library Resources: The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.</p>	
<b>Module 2</b>	<b>DATA ANALYSIS</b>	<b>15 L</b>
	<p>The Investigative Approach: Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.</p> <p>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.</p>	
<b>Module 3</b>	<b>METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS</b>	<b>15 L</b>
	<p>Reporting practical and project work, writing literature surveys and reviews, organizing a poster display, giving an oral presentation.</p> <p>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.</p>	
<b>Module 4</b>	<b>CHEMICAL SAFETY &amp; ETHICAL HANDLING OF CHEMICALS</b>	<b>15 L</b>

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	<p>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.</p>	
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