GAYATRI VIDYA PARISHAD
COLLEGE FOR DEGREE AND PG COURSES (AUTONOMOUS)
Affiliated to Andhra University || Accredited by NAAC and NBA
VISAKHAPATNAM

DEPARTMENT OF ORGANIC CHEMISTRY

SEMESTER-IV, PAPER-I -MODERN SYNTHETIC METHODOLOGY IN ORGANIC CHEMISTRY

(Effective from the admitted batch of 2024-2025)

Credits: 4	Paper/Course Code-4591	Theory: 4 Hours
Max Marks: 100	External: 60	Internal: 40

Course Objectives (COs):

CO 1: Create new methods using the knowledge of modern synthetic methods.
CO 2: Create new reactions using multicomponent reactions.
CO 3: Apply the concept of click chemistry and biorthogonal chemistry in modern synthesis.
CO 4: Apply the knowledge and understanding the reactions of unactivated C-H bonds.
CO 5: Analyze and evaluate new methods in modern organic synthesis.

Course Learning Outcomes (LOs):

Upon completion of the course the students should be able to:

LO 1: Explain and apply modern synthetic methods in preparing new molecules
LO 2: Analyze various multicomponent reactions
LO 3: Apply the new concept of click chemistry in organic synthesis and biological system
LO 4: Explain and apply the knowledge and understanding the reactions of unactivated C-H bonds,
LO 5: Solve and analyze new green chemistry methods in organic synthesis.
LO 6: Compare various modern synthetic methods, multicomponent reactions, oxidation, reduction and green chemistry related reactions

UNIT – I: Modern Synthetic Methods [12 Hours]

Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction. Brook rearrangement; Nozaki-Hiyama, Ullmann coupling reaction.

UNIT-II: Multi component Reactions: [12 Hours]

Ugi reaction, Buchwald-Hartwig Passerini reaction, Biginelli reaction, Hantzsch reaction and Mannich reaction. Tebbeolefination, Metathesis: Grubb's 1st generation and 2nd generation catalyst, Olefin Cross coupling Metathesis (OCM), Ring Closing Metathesis (RCM), Ring Opening Metathesis (ROM) and applications.

UNIT-III: Click Chemistry: [12 Hours]

Introduction to click chemistry Copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC), Strain-promoted azide-alkyne cycloaddition (SPAAC), Strain-promoted alkyne-nitrone cycloaddition (SPANC)

Reactions of strained alkenes: Alkene and azide [3+2] cycloaddition, Alkene and tetrazine inverse-demand Diels-Alder, Biorthogonal Chemistry:

UNIT-IV: Reactions of un-activated carbon-hydrogen bonds: [12 Hours]Un-activated carbon-hydrogen bonds: Definition, mechanism and synthetic applications- TheHoffmann-Loeffler-Freytag reaction (HLF reaction)-Cyclisation reactions of Nitrenes-the Barton Reaction-Photolysis of organic hypohalites, hypochlorites, hypobromites and hypoiodites,

UNIT-V: Newer methods in Organic Synthesis: [12 Hours]
Green Chemistry: Introduction, principles, atom economy and scope (illustrate with two examples) **Microwave induced reactions:** Principle conditions, advantages over conventional heating methods-applications **Ionic liquids:** Introduction and applications in organic synthesis (illustrate with two examples). **Nanomaterials:** Introduction, methods of preparation, applications in organic synthesis **Phase-transfer catalysis:** solid-solid, solid-liquid systems-mechanism of catalytic action, type of catalysts, application in few important reactions

Text Books:

1. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge
   University Press, Cambridge, 1988.
2. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
3. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
4. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley& Sons, 2003.
5. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
6. Introduction: Click Chemistry by Neal K. Devaraj&M. G. Finn
7. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis Elsevier Academic Press, 2005.
8. Green chemistry, Theory and Practical, Paul T.Anastas and John C.Warner.
9. New trends in green chemistry By V.K.Ahulwalia and M.Kidwai.
10. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Agarwal

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DEPARTMENT OF ORGANIC CHEMISTRY

SEMESTER-IV, PAPER-II-ORGANIC SPECTROSCOPYAND PRINCIPLES OFINSTRUMENTATION
(Effective from the admitted batch of 2024-2025)

Credits: 4	Paper/Course Code-4592	Theory: 4 Hours
Max Marks: 100	External: 60	Internal: 40

Course Objectives (COs):

CO 1: Apply the knowledge of ^{13}C NMR Spectroscopy in evaluating the organic molecules.
CO 2: Analyze the complex structures using 2D NMR, FT NMR, COSY and HETCOR.
CO 3: Analyze the optical isomer structures using ORD and CD spectroscopy.
CO 4: Solve the structures of natural products using 2D NMR, COSY, HETCOR, ORD and CD spectroscopy.
CO 5: Analyze the organic moleculesusing various chromatographic separation techniques like GC, HPLC and XRD.

Course Learning Outcomes (LOs):

Upon completion of the course the students should be able to:
LO 1: Explain theory and values of ^{13}C NMR Spectroscopy
LO 2: Analyze and apply the concept of 2D NMR and Instrumentation, learn FT NMR spectroscopy, 2D-NMR, COSY and HETCOR in molecular structure determination
LO 3: Apply the concept of ORD and CD spectroscopy and structural determination of natural products by spectroscopy
LO 4: Interpret, Analyze and solve the structure of organic compounds using ^{13}C NMR, HNMR, 2D NMR, COSY and HETCOR.
LO 5: Explain various chromatographic separation techniques. Principle and instrumentation of GC, HPLC and XRD

UNIT-I: ^{13}C NMR spectroscopy [12 Hours]

Introduction, ^{13}C-chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and aromatic compounds. Types of ^{13}C NMR spectra: Proton-coupled, proton-decoupled and OFF-resonance decoupled (ORD) spectra, DEPT. ^{13}C-NMR solvents:

UNIT-II: NMR Instrumentation, 2D-NMR techniques [12 Hours]

NMR Instrumentation: Types of NMR Spectrometers-Continuous Wave (CW)-NMR, Fourier Transform (FT)-NMR, NMR solvents, sample preparation.

2D-NMR techniques: Principles of 2D NMR, Correlation spectroscopy (COSY) HOMO COSY (^1H-^1H COSY), Hetero COSY (^1H,^{13}C COSY, HMQC), long range ^1H,^{13}C COSY (HMBC), NOESY and 2D-INADEQUATE experiments and their applications.

UNIT-III: Optical Rotatory Dispersion (ORD) and CD Spectroscopy: [12 Hours]

Optical rotation, circular birefringence, and circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Application of the rules to the study of absolute configuration and conformations of organic molecules.

UNIT-IV: Structure Determination of Natural Products by Spectral Methods [12 Hours]

Sructure elucidation - Spectroscopic techniques IR, UV, ^{1}H-NMR, ^{13}C-NMR, COSY, HETEROCOSY, and MS- natural products - Examples, flavones - Apigenin, flavanones-Hesperetin, isoflavones - Genistein, coumarins-7-hydroxycoumarin, alkaloids - morphine, quinine, terpenoids - (-)-Menthol, Steroids - stigmasterol, Glycosides - salicin (Alcoholic β-glucoside)

UNIT-V: Heteronuclear NMR spectroscopy and Principles of Instrumentation techniques [12 Hours]

Heteronuclear couplings: ^{13}C-^{1}H, ^{13}C-D, ^{13}C-^{19}F, ^{13}C-^{31}P.^{1}H-D, ^{1}H-^{19}F, ^{1}H-^{31}P,
Instrumentation – Gas Chromatography - High Performance LiquidChromatography - X – Ray Diffraction (XRD).

Text books:

1. Spectroscopy, fourth edition, D. L Pavia, G. M Lampman CENGAGE Learning, 2012
2. Spectroscopic Methods in Organic Chemistry. Fourth Edition D.M. Williams and I. Fleming Tata - McGraw Hill, New Delhi, 1990. For all spectral methods except ORD and CD and ESR.
3. Organic Spectroscopy, Second Edition, W.Kemp, ELBS Macmillan, 1987 for ORD and CD and ESR.
4. Chemistry of natural products, S. V. Bhat, Narosa Publishing House, 6th reprint 2010(For IV th unit)
5. Applications of absorption spectroscopy of Organic Compounds J.R.Dyer, Prentice Hall of India, New Delhi, 1984.
6. Spectrometric identification of Organic Compounds, Fourth Edition, R.M. Silverstein: G.C.Vassiellr and T.C. Merill, Johne Willey, Singapore, 1981.
7. For ORD and CD "Applications of Optical rotation and Circular Dichroism", G.C. Barret, in "Elucidation of Organic structures by Physical and Chemical Methods" Part I (Eds)
8. K.W. Bentley and G.W.Kirty John Wiley, 1972, Chapter VIII (only those aspects mentioned in the syllabus).

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DEPARTMENT OF ORGANIC CHEMISTRY

SEMESTER-IV, PAPER-III-DESIGNING ORGANICSYNTHESIS ANDSYNTHETIC APPLICATIONS OF ORGANO-BORANES AND SILANES
(Effective from the admitted batch of 2024-2025)

Credits: 4	Paper/Course Code-4593	Theory: 4 Hours
Max Marks: 100	External: 60	Internal: 40

Course Objectives (COs):

CO 1: Apply the knowledge of principles of disconnection approach in organic synthesis.
CO 2: Analyze various synthetic strategies using one group disconnection.
CO 3: Analyze various synthetic strategies usingtwo group disconnection.
CO 4: Evaluate the synthetic strategies using various organoboranes.
CO 5: Evaluate the synthetic strategies using various organosilanes.

Course Learning Outcomes (LOs):

Upon completion of the course the students should be able to:
LO 1: Apply principles of disconnection approach.
LO 2: Apply in analyzing molecules using various synthetic strategies for one group disconnection.
LO 3: Analyze molecules using various synthetic strategies for one group disconnection.
LO 4: Apply different organoborane reagents in organic synthesis.
LO 5: Apply different organosilanes reagents in organic synthesis.

UNIT-I: Disconnection Approach – Principles [12 Hours]

Introduction, Terminology: Retrosynthesis, Target Molecule (TM), synthon, synthetic equivalent, functional group interconversion (FGI). Linear and convergent synthesis. Criteria for selection of target. Order of events in retrosynthesis with reference to Salbutamol, Proparcaine and Dopamine. Chemoselectivity, Regioselectivity, reversal of polarity and cyclizations. Protecting groups- Principles of protection of alcohols, amine, carbonyl and carboxyl groups

UNIT-II: Synthetic Strategies - One group Disconnections [12 Hours]

Introduction to one group disconnections: C-C disconnection-alcohols and carbonyl compounds; C-X disconnections- alcohols and carbonyl compounds and sulphides two group C-C and C-X Disconnections.

UNIT-III: Synthetic Strategies - Two group Disconnections [12Hours]

Introduction to Two group C-C disconnections; Diels-Alder reaction, 1,5-difunctionalized compounds, Michael addition and Robinson annulation. Two group C-X disconnections; 1, 1-difunctionalised, 1, 2-difunctionalised and 1, 3-difunctionalised compounds. Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid.

UNIT –IV: Organoboranes **[12 Hours]**

Hydroboration- Preparation of Organoboranes. Reagents – dicylohexyl borane, disiamyl borane, thexyl borane, 9-BBN and mono-, di-isopinocamphenyl borane. Functional group transformations of Organoboranes-Oxidation, protonolysis and rearrangements. Formation of carbon-carbon-bonds viz organoboranes-carbonylation, cyanoboration.

UNIT –V: Organosilanes **[12 Hours]**

Preparation and synthetic applications of trimethylsilyl chloride, dimethyl-t-butylsilylchloride, trimethylsilylcyanide, trimethylsilyliodide and trimethylsilyltriflate. Protection of functional groups - Trimethylsilylethers, Silylenolethers. Synthetic applications of α-silylcarbanions, β-silylcarbonium ions. Peterson's olefination.

Text Books:

1. Organic syntheses via boranes / Herbert C. Brown; with techniques by Gary W. Kramer,
2. Alan B. Levy, M. Mark Midland. New York: Wiley, 1975
3. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
4. Organic Synthesis: The disconnection approach, S. Warrant John Wiley & sons, New York, 1984.
5. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benzamine Inc. Menio Park, California, 1972.
6. Principle of Organic Synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
7. Organic Synthesis: Special techniques. V.K. Ahulwalia and Renu Aggarwal.
8. Organic Synthesis by C Willis and M Willis
9. Problems on organic synthesis by Stuart Warren

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DEPARTMENT OF ORGANIC CHEMISTRY

SEMESTER-IV, PAPER-IV-DRUG DESIGN AND DRUG CHEMISTRY
(Effective from the admitted batch of 2024-2025)

Credits: 4	Paper/Course Code-4594	Theory: 4 Hours
Max Marks: 100	External: 60	Internal: 40

Course Objectives (COs):

CO 1: Acquire the knowledge on basics of drug design.
CO 2: Apply the knowledge on drug targets for designing new drugs.
CO 3: Evaluate the structure activity relationship (SAR) and quantitative structure activity relationships (QSAR) for drug designing.
CO 4: Create new drugs using the knowledge of the synthesis, mode of action, properties, uses and dosage of antineoplastic agents.
CO 5: Create new drugs using the knowledge of the synthesis, mode of action, properties, uses and dosage of cardiovascular drugs.

Course Learning Outcomes (LOs):

Upon completion of the course the students should be able to:

LO 1: Explain basics of drugs, their classification, drug metabolism and drug development, Structure Activity Relationship in drugs.
LO 2: Apply the knowledge of drug targets in drug discovery.
LO 3: Apply the knowledge of SAR & QSAR in drug discovery.
LO 4: Apply the knowledge on mechanism of action, synthesis of antineoplastic agents.
LO 5: Apply the knowledge on mechanism of action, synthesis of cardiovascular drugs.

UNIT I: Introduction to Drugs **[12 Hours]**

General Classification, nomenclature, Development of drugs: Procedure followed in drug design, concepts of lead compound and lead modification, Intermolecular bonding forces: Electrostatic or ionic bonds, Hydrogen bonds, Van der Waals interactions and Dipole–dipole and ion–dipole interactions. High-throughput screening, Lipinski rule of 5, Introduction to drug Absorption, Distribution, Metabolism, Elimination and Toxicity (ADMET). Understanding of the biological activity parameters such as Ki, Kd, LD50, EC50, IC50.

UNIT-II: Drug Targets **[12 Hours]**

Primary, secondary, tertiary and quaternary structures of Protein, Binding/active site, Drug target understanding: Enzymes as drug targets: The active site of an enzyme: Reversible inhibitors, Irreversible inhibitors and inhibitors acting at allosteric binding sites. Receptors as drug targets: Types of receptors, Agonist, Antagonist with examples, G-protein-coupled receptors and Kinase-linked receptors, Nucleic acids as drug targets Intercalating drugs acting on DNA.

UNIT III: Drug Activity: **[12 Hours]**

Structure Activity Relationship (SAR)- binding role of functional groups, isosterism, bio-isosterism, concept of prodrugs, Extension of the structure, Simplification of the structure, spatial considerations, Quantitative Structure

Activity Relationships (QSAR)-Concepts of drug receptors. Types of molecular descriptors, Elementary treatment of. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, Concept of stereochemistry in terms of biological response with examples.

UNIT IV: Antineoplastic Agents: **[12 Hours]**

Introduction, classification-alkylating agents- mechanism and mode of action, nitrogen mustards-synthesis, properties, uses and dosage - Chlorambucil and melphalan. Antimetobolites- synthesis, properties, uses and dosage-pyrimidine analogues-5-flurouracil, purine analogues-6-mercaptopurine, folic acid analogues-Methotrexate. Antibiotics-structure, properties and dosage-Doxorubicin.

UNIT V: Cardiovascular Drugs: **[12 Hours]**

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol.

Text Books:

1. Text book of medicinal chemistry, Volume 1 & II, Third edition by V Alagarsamy, CBS-publishers
2. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH.
3. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge.
4. An Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International.
5. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter.-9 and Ch-14), Ed. M. E. Wolff, John Wiley.
6. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
7. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.
8. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

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SEMESTER-IV, PAPER-V-Practical-I
(Effective from the admitted batch of 2024-2025)

Credits: 4	Paper/Course Code-4595	Lab: 9 Hours
Max Marks: 100	External: 50	Internal: 50

PRACTICAL-I SYLLABUS

1. Analysis of four organic mixtures containing two components.

SEMESTER-IV, PAPER-VI-Practical-II
(Effective from the admitted batch of 2024-2025)

Credits: 4	Paper/Course Code -4596	Lab: 6 Hours
Max Marks: 100	External: 50	Internal: 50

PRACTICAL-IISYLLABUS

Computational Chemistry and Spectroscopy

1. Marvin sketch: Drawing the structures of simple aliphatic, aromatic, heterocyclic compounds with different substituents. Identification of IUPAC name, calculating properties of molecules, saving in different formats.
2. How to find protein structure in Protein Data Bank, saving protein in PDB format.
3. How to find ligands in different data base
4. Identification of simple organic molecules by ^{1}HNMR, ^{13}CNMR and MASS

Text Books:

1. Vogel's Practical Organic Chemistry,A.R. Tatchell, B.S. Furnis, A.J. Hannaford and P.W.G. Smith, 5th Edition, Pearson,New Delhi, 2017.
2. Vogel's Text book of Quantitative Inorganic Analysis,
3. J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th Edition,
4. Pearson Education, New Delhi, 2008.
5. Chemistry of Natural Products: A Laboratory Handbook, N.R. Krishnaswamy,
6. Universities Press, Hyderabad, 2013.
7. A Laboratory Manual of Organic Chemistry, R.K. Bansal,New Age International Publishers, New Delhi, 2008.
8. Practical Organic Chemistry, F.G. Mann & B.C. Saunders, Pearson, New Delhi, 2001.

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SEMESTER-IV, PAPER-VII-PROJECT WORK

(Effective from the admitted batch of 2024-2025)

Credits: 4	Paper/Course Code-4597	Lab: 3 Hours

Course Learning Outcomes:

Upon completion of the course the students should be able to:

LO 1:	Apply the knowledge of synthesis of organic molecules in the Contract Research Organization (CRO)
LO 2:	Apply the skills of analysis of organic molecules in the pharmaceutical industries.
LO 3:	Can emerge into an entrepreneur in the field of chemical and pharmaceutical sectors.

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VALUE ADDED COURSE
SEMESTER-IV, PAPER-VIII -RESEARCH METHODOLOGY
(Effective from the admitted batch of 2024-2025)

Credits: 2	Paper/Course Code - VA-4598	Theory: 2 Hours
Max Marks: 50	External: --	Internal: 50

Course Objectives (COs):

CO 1: To illustrate effective literature studies and familiarize with research problem characteristics.

CO 2: Students will acquire the skills to prepare research papers for journals, seminars, and conferences using appropriate templates, understand journal metrics.

CO 3: Acquire the knowledge on ethical issues andreproduction of published material, plagiarism, citation and acknowledgement.

Course Learning Outcomes (LOs):

Upon completion of the course the students should be able to:

LO 1: Can design research objectives and investigate the problems involved.

LO 2: Students can prepare project proposals to apply for various funding agencies.

LO 3: Students can apply the ethics in writing a good research paper/ manuscript for publication.

Unit 1–Science and Research [10 hours]

Definition – History – Evolution of Scientific Inquiry, Scientific Research: Definition, Characteristics, types, need of research. Identification of the problem, assessing the status of the problem, formulating the objectives, preparing design Actual investigation.

Unit 2-Introduction to Research Methodology [10 hours]

Meaning and importance of Research – Types of Research – Selection and formulation of Research Problem Research Design –. Analysis of Literature Review – Primary and Secondary Sources, Web sources –critical Literature Review Hypothesis –Preparing Research papers for journals, Seminars and Conferences – Design of paper using template, Impact factor of a journal, citation Index, ISBN & ISSN. Preparation of Project Proposal - Title, Abstract, Introduction – Rationale, Objectives, Methodology – Time frame and work plan – Budget and Justification

Unit 3–Ethics and Documentation [10 hours]

Ethical Issues –Bibliography Ethical Committees Reproduction of published material – Plagiarism – Citation and Acknowledgement – Reproducibility and accountability, Documentation and scientific writing Results and Conclusions, Preparation of manuscript for Publication of Research paper, Presenting a paper in scientific seminar, Thesis writing. Structure and Components of Research Report, Types of Report: research papers, thesis, Pictures and Graphs, citation styles, writing a review of paper.

BOOKS:

1. Garg.B.L., Karadia, R., Agarwal, F. and Agarwal, U.K., 2002. An introduction to Research Methodology, RBSA Publishers.
2. Kothari, C.R. (2008). Research Methodology: Methods and Techniques. Second Edition. New Age International Publishers, New Delhi.
3. Sinha, S.C. and Dhiman, A.K., 2002. Research Methodology, Ess Publications. 2 volumes.