Frameworks for VII and VIII semesters

B.Sc. (H) Applied Life Sciences with Agrochemicals and Pest Management

Semester	DSC Credits 4	DSE Credits 4
VII	DSC 07 (3T+1P)	DSE I (2T + 2P) DSE II (2T + 2P) DSE III (2T + 2P)
VIII	DSC 08 (3T+1P)	DSE IV (2T + 2P) DSE V (2T + 2P) DSE VI (2T + 2P)

	➤ DSC 07: Agrochemicals for Insect and Mite Control
	➤DSE I: Research Methodology in Agrochemistry
VII	➤DSE II: Physical Principles in Agrochemicals
	➤ DSE III: Analytical Techniques in Pesticide Analysis

✓DSC 08: Agrochemical for Fungi, Nematodes, and Weeds

✓DSE IV: Environmental health and Agrochemicals

✓DSE V Introduction to Natural Pesticides: Biopesticides and Plant Toxins

✓DSE VI: Pesticide Formulation and Application Equipment

SEMESTER -VII

BSc. (Hons)Applied Life Sciences with Agrochemicals and Pest Management

Swami Shraddhanand College

DISCIPLINE SPECIFIC CORE COURSE – 01

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course Lecture Tutorial Practical/ Practice			Eligibility criteria	Pre- requisite of the course (if any)
Agrochemicals for Insect and Mite Control: DSC 07	4	3	0	1	-	NIL

Course objectives

The Learning Objectives of this course are as follows:

- to familiarize students to different types of classification of pesticides.
- to familiarize with factors that make the organic compound to be considered as pesticide.
- Develop a solid knowledge base regarding the chemistry, classification, and synthesis of agrochemicals—including insecticides and acaricides (pesticides used against mites).
- This entails learning about key chemical classes (such as organophosphates, pyrethroids, carbamates) and their modes of action and effective chemical control strategies

Learning outcomes

The Learning Outcomes of this course are as follows:

- To analyze important aspects attributing pesticidal activity to organic molecules.
- To explain the strategies involved in synthesis of different pesticides.
- To handle pesticides safely in view of human health and environment.
- To help the students to gain an in-depth understanding of both the theoretical and practical aspects of using agrochemicals for pest management

SYLLABUS OF DSC-07

THEORY COMPONENT-

UNIT 1: (17 Hours)

A Structure, properties, uses, structure-activity relationship (QSAR) and toxicity with reference to selective examples each from class of selected examples of pesticides:

Discussion on stereochemical aspects of pesticides insecticides, where ever required.

- a) Organochlorines
- b) Organophosphorus
- c) Carbamates
- **B** Structure, uses and toxicity examples each from:Pyrethrins,Pyrethroids and Neonicotinoids. Discussion on stereochemical aspects of pesticides insecticides, where ever required.
 - a) Pyrethrins
 - b) Synthetic Pyrethroids
 - c) Neonicotinoids pesticides

UNIT 2:(10Hours)

Introduction to Insecticide synergists:Concept, Significance, andimportance,role in resistance management,mode of action,Common insecticide synergists-piperonylbutoxide and MGK-264 (n-octylbicycloheptanedicarboximide), Synergists Work Efficacy, Resistance Management, Reduced Insecticide Use

UNIT3: (10 Hours)

Introduction to Synthetic IGRs:Synthetic IGRs- Concept, Significance, and importance, Use of Synthetic IGRs- Mimicking Hormones, Disrupting Chitin Synthesis, targeting Specific Life Stages,

Advantages of Synthetic IGRs - Reduced Environmental Impact, Reduced Resistance Development, Compatibility with Integrated Pest Management (IPM),

Examples of Synthetic IGRs: Methoprene, Diflubenzuron, teflubenzuronChlorfluazuron ,Fenoxycarb

UNIT4: (8 Hours)

Fumigants and other chemicals for post-harvest storage of agricultural commodities

Synthesis of pesticides /analogues/intermediates

- 1. Preparation of carbamate derivative from phenylisocynate and alcohol/phenol.
- 2. Preparation of DDT from chlorobenzene and chloral
- 3. Preparation of other chlorinated hydrocarbons DDE, and Methoxychlor
- 4. Preparation of organophosphorus Insecticide-Part A –phosphorodichloridite, and Part B -phosphonate
- 5. Preparation and characterization of oxime ether, Preparation of DDVP.
- 6. Preparation of acyl phenyl hydrazine
- 7. Preparation of of 3,5-dimethylpyrazole
- 8. Preparation of mosquito repellent Diethyl phthalate in two steps:
 - Step-1: Preparation of phthalic anhydride
 - Step-2: preparation of Diethyl phthalate
- 9. Writing the assigned an in-depth analysis of at least three insecticides to be allotted by instructor fromorganochlorines, organophosphorus, carbamates, pyrethroids, and neonicotinoids. It must cover the detailed aspects of: Chemical Structure, Uses, Mode of Action, Toxicity and GHS labelling, Human Health Implications

ESSENTIAL/RECOMMENDED READINGS

- 1. G.T. (1976). Chlorinated Insecticides (Vols. I–II). CRC Press.
- 2. Buchel, K. H. (Ed.). (1992). Chemistry of Pesticides. John Wiley & Sons.
- 3. Cremlyn, R. J. (1990). Pesticides: Preparation and Mode of Action. Wiley.
- 4. Eto, M. (1979). Organophosphorus Pesticides: Organic and Biological Chemistry. CRC Press. (Note: Corrected to insert a space between "Biological" and "Chemistry".)
- 5. Kuhr, R. J., &Dorough, H. W. (1979). Carbamate Insecticide Chemistry and Biochemistry. CRC Press.
- 6. Leahey, J. P. (1985). The Pyrethroid Insecticides. Taylor & Francis.
- 7. Metlosky, G., Nadasy, M., & Andriska, V. (1988). Pesticide Chemistry. Elsevier.
- 8. Perry, U. K., Yamamoto, A. S., Ishaaya, I., & Perry, R. (1998). *Insecticides in Agriculture and Environment: Retrospects and Prospects*. Narosa.

KEYWORDS: QSAR, Stereochemical activity of Pesticides, Insecticide synergists, Synthetic synergists, Fumigants, Pesticide activity

DISCIPLINE SPECIFIC ELECTIVE COURSE – 01

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit Lecture	distribution course Tutorial	Eligibility criteria	Pre- requisite of the course (if any)	
Research Methodology inAgrochemistry	4	2	0	2	-	NIL

Course objectives

The Learning Objectives of this course are as follows:

- Understand Fundamental Concepts of research.
- Develop researchable questions and hypotheses related to pesticide application, efficacy, environmental impact, or health effects.
- Design Appropriate Research Methodologies and Distinguish between qualitative, quantitative, and mixed-method approaches in pesticide research.
- Use statistical tools to analyze pesticide research data. Address Ethical and Regulatory Considerations Describe relevant national and international pesticide regulations.
- Learning computational toxicology
- Develop Scientific Communication Skills. Write research proposals, reports, and scientific papers on pesticide-related topics.

Learning outcomes

The Learning Outcomes of this course are as follows:

- Recall and identify key concepts and terminology related to research methodology.
- Analyze the strengths and weaknesses of different research methodologies in relation to specific research contexts or objectives.
- Apply the principles of a specific research methodology to design a research study or experiment.
- Computer in pesticide development.

SYLLABUS OF DSE-01

THEORY COMPONENT-

UNIT 1: (8Hours)

Introduction of Research and Writing scientific report:

Meaning and objectives of research, criteria of good research, research methods vs research methodology, selection of research problem, literature review, types of hypotheses. Maintaining a laboratory record; On-line literature searching, Database, Sci-finder, Scopus, Citation Index, Impact Factor.

Planning, preparation, draft, revision and refining; writing project proposal to funding agency, Paper writing for Journals, Conference presentation, preparation of effective slides and presentation. Numbers, units, abbreviations and nomenclature used in scientific writing. Writing references. Scientific writing and ethics, Introduction to copyright-academic misconduct/plagiarism, Acknowledgement,Fellowships/Research Grants, Introduction to guidelines, Insecticides Act 1968 and Insecticides rules 1971

UNIT 2: (8Hours)

Computational tools used in chemical structure designing:

AutoDock, PyMOL, or ChemSketch, Marvin (Chem Axon), Determination of some selected physiochemical properties

UNIT 3: (10Hours)

Computational toxicology

A. Introduction to Toxicity prediction and hazard identification

Applicability domain (AD) of a QSAR mode, brief discussion on the models available for predicting toxicological endpoints, Physicochemical properties associated with toxicity, QSAR approaches and the definition of structural similarity a key aspect of silico prediction.

- **B.** Software and expert systems in relation to the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) initiative and Organization for Economic Cooperation and Development (OECD) principles.
- **C.** Computational models for toxicology,their Limitations of chemical similarity and Readacross for regulatory purposes.
- **D.** Freely available Software for Toxicity prediction:

OECD QSAR Toolbox, EPA's Toxicity Estimation Software Tool (TEST), OPERA, VEGA, ProTox 3.0,SwissADME (Several other available software as per requirement may be used)

UNIT 4: (4 Hours)

Data exploration for the pesticide molecules:

Manually curated database sites for pesticides like ChEMBL, ChEBI, Agrochemical Database @ USDA, chemspider, BRENDA (enzyme data and metabolic information), UniProt (Enzyme database) PubChem etc. to be introduced.

PRACTICAL COMPONENT

(60Hours)

For review and data analysis to be carried out for the given pesticides

- 1 **Utilization of Academic Search Engines and Databases.** Practice using platforms like Google Scholar, Scopus, and PubMed to locate and retrieve relevant research and review articles.
- 2 Conduct systematic reviews. Choose a topic (e.g., pesticide resistance in insects). Use online databases to find 5–10 relevant papers. Analyze them for research gaps, methods used, and key findings
- Practice data entry and statistical analysis. Provide sample data (e.g., pesticide residue levels in water). Clean and organize data in Excel or R. Perform correlation or regression analysis. Interpret results.
- 4 Collection of data, interpretation, and presentation of data through writing short research or review papers
- Develop skills to write concise and informative titles and abstracts for research manuscripts.
- 6 Use reference management tools (Zotero, Mendeley, EndNote) to format citations and bibliographies according to various journal styles.
- Learn how to check for plagiarism using software tools (Turnitin, Grammarly, etc.) and maintain academic integrity.
- 8 Explore the basics of computational tools used in pesticide design (such as AutoDock, PyMOL, or ChemSketch).
- 9. Writing the assigned an in-depth analysis of at least three pesticides to be allotted by instructor for their computational study for physicochemical data and toxicity prediction.

ESSENTIAL/RECOMMENDED READINGS

- 1. G.R.Chatwal, Instrumental method of chemical analysis.
- 2. A text of inorganic quantitative analysis by Shree Ramulu.
- 3. Instrumental methods of chemicals analysis by Willard, Meritt
- 4. Rastogi S.C. Mendecutta, N.Bioinformatics Methods and application
- 5. Sharma B.K. Instrumental Methods of chemical analysis
- 6. Chopra &Kanvar, Analytical agriculture chemistry
- 7. Robert Brown, Introduction to instrumental Analysis
- 8. Peter Atkins, Physical chemistry
- 9. Sivasankari, Bioseparation Principles and Techniques.
- 10. Practical Research Methods, Catherine Dawson, UBS Publishers Distribution, New Delhi 2002.
- 11. Research Methodology Methods and Techniques, C. R. Kothari, Wiley Easter Ltd, New Delhi 1985.
- 12. Research Methodology A Step by step Guide for Beginners 2 ndedn. Kumar Ranjit, Pearson Education, Singapore, 2005.
- 13. Introduction to Research and Research Methodology M. S. Sridhar.
- 14. The Information Specialist's Guide to Searching & Researching on the Internate& the World Wide Web by Ernest Ackermann, Karen Hartman, Fitrzroy Dearborn Publishers, London.
- 15. Learning to Use the World Wide Web, Ernest Ackermann, BPB Publications development and formulation development. Use of computer-based equipment for pesticide analysis.

KEYWORDS:

Research methodology, Citation Index, Computational tools, QSAR approaches, Silico prediction, REACH, OECD, Computational models for toxicology, Toxicological endpoints, Agrochemical Database, Plagiarism

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

DISCIPLINE SPECIFIC ELECTIVE COURSE – 02

Course title & Code	Credits	Credit Lecture	distribution course Tutorial	Eligibility criteria	Pre- requisite of the course	
Physical Principles in Agrochemicals	4	2	0	2	-	(if any) NIL

Course objectives

The Learning Objectives of this course are as follows:

- explain the laws of thermodynamics and their applications in agrochemical formulation and stability.
- Compute and interpret enthalpy, entropy, and Gibbs free energy changes in agrochemical reactions.
- Principles of catalysis and enzyme kinetics, particularly in the context of bio-pesticide action.
- Role of surfactants and micelles in pesticide formulations and critical micelle concentration (CMC).
- Analyze how pKa and pH affect the ionization and solubility of pesticides in different environmental conditions.
- Correlate lipophilicity with pesticide bioavailability, uptake, and systemic activity in target organisms

Learning outcomes

The Learning Outcomes of this course are as follows:

- Define key physicochemical properties of pesticides (e.g., solubility, volatility, vapor pressure, partition coefficient, and degradation rates).
- Describe the fundamental principles of enzyme kinetics

- Define photochemical transformation and its relevance in the environmental fate of pesticides.
- Explain the mechanisms of direct and indirect photolysis of pesticides under natural and artificial light sources

SYLLABUS OF DSE-02

THEORY COMPONENT-

UNIT 1: (7Hours)

Physicochemical Properties of Pesticides: Physicochemical properties (solubility, octanol-water partition coefficient, vapor pressure, soil adsorption coefficient, emulsion stability, half-life, shelf-life etc.) and their testing, Formulation-toxicant interactions. Distribution coefficient of pesticide-its mobility, persistence, and potential to contaminate environment. Significance of studying the physiochemical properties.

UNIT 2: (7Hours)

Photochemical transformation of pesticides:Introduction to photochemistry, direct and indirect photolysis, photosensitizers, quenchers, light filters, quantum yield. Photo transformation pesticides and their significance. An overview of broken-down Pesticide and health risk of altered transformed products photochemically.

UNIT 3: (10 Hours)

Enzyme Kinetics and Application in Agrochemical Degradation: Factors affecting the enzyme activity- Concentration, pH and temperature. Kinetics of a single-substrate enzyme catalysed reaction, Michealis-Menten Equation, Km, Vmax, L.B Plot, Turnover number, Kcat. Enzyme specificity. Active site, Principles of activation energy, transition state. Interaction between enzyme and substrate- Lock and Key Theory. Kinetics of Enzyme Inhibition- irreversible and reversible, types of reversible inhibitions- competitive and noncompetitive. Feedback inhibition.

UNIT 4: (6Hours)

Surface and Colloid Chemistry in Agrochemicals:Critical micelle concentration (CMC), Emulsions, suspensions, and colloidal stability. Adsorption isotherms (Langmuir and Freundlich): application in soil-pesticide interaction. Wettability, contact angle, and spreadability on leaf surfaces.

PRACTICAL COMPONENT

(60Hours)

- 1. To measure the solubility of a pesticide in water at room temperature.
- 2. To evaluate the lipophilicity of a pesticide by calculating log P using 1-Octanol/Water System.
- 3. To determine the dissociation constant (pKa) of an agrochemical using UV-Visible Spectroscopy.
- 4. To study how solubility varies with pH due to ionization of pesticide.
- 5. Determination of surface tension and contact angle of formulations.
- 6. Study of adsorption of pesticide on soil using isotherms.
- 7. Kinetics of pesticide degradation under various pH conditions.
- 8. To determine the distribution coefficient of a pesticide by studying its adsorption onto soil from an aqueous solution.
- 9. Writing the assigned an in-depth analysis of at least three pesticides to be allotted by instructor for evaluation of Physical principles by surveying the data from literature.

ESSENTIAL/RECOMMENDED READINGS

- 1. "Physical Chemistry" P.W. Atkins
- 2. "Pesticide Formulation and Adjuvant Technology" Chester L. Foy
- 3. "Agrochemical Discovery: Insect, Weed and Fungal Control" John J. Beck
- 4. Journal Articles from Pest Management Science, Journal of Agricultural and Food Chemistry
- 5. K.H. Buchel "Chemistry of Pesticides" Classic text explaining the chemistry, mode of action, and environmental aspects.
- 6. K.S. Birdi- "Surface Chemistry"
- 7. B.D. Khosla -Practical Physical Chemistry
- 8. S.S. Balpande- Laboratory Manual for Soil and Agrochemical Analysis
- 9. Fundamentals of Enzymology: Nicholas Price & Lewis Stevens

KEYWORDS: Physicochemical Properties of Pesticides, Formulation-toxicant

interactions, Photochemical transformation of pesticides, Kinetics of

Enzyme, Kinetics of Enzyme

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

DISCIPLINE SPECIFIC ELECTIVE COURSE – 03

Course title & Code	Credits	Credit distribution of the course Lecture Tutorial Practical/ Practice			Eligibility criteria	Pre- requisite of the course (if any)
Analytical Techniques in Pesticide analysis	4	2	0	2	-	NIL

Course objectives

The Learning Objectives of this course are as follows:

- To understand the principles behind preparing standard solutions, analytical reagents, qualitative reagents, and indicators.
- To Learn to construct standard curves essential for titrimetric and analytical applications.
- To learn the fundamentals and practical applications of separation methods including solvent extraction, thin layer chromatography (TLC), paper chromatography, and column chromatography.
- To gain insight into the applications of instrumental techniques like Ultravioletvisible (UV-Vis) spectroscopy, infrared (IR) spectroscopy, atomic absorption spectroscopy (AAS), and mass spectrometry (MS)
- To understand how these methods are applied in pesticide formulation analysis and quality control.

Learning outcomes

The Learning Outcomes of this course are as follows:

- Learn chromatography (TLC, paper, and column methods) to effectively isolate and identify agrochemical compounds from environmental and food samples.
- Critically Evaluate Analytical Methods
- Independently prepare reliable standard solutions and reagents required for a variety of analytical and titrimetric analyses in pesticide assessment.
- Analyze complex data sets, making informed decisions about method suitability and analytical outcomes.

SYLLABUS OF DSE-03

THEORY COMPONENT-

UNIT 1: (6Hours)

Preparation of Solutions for Analytical and Titrimetric Applications:

Preparation of solutions for standard curves, analytical reagents, qualitative reagents, indicators and standard solutions for acid-base, oxidation- reduction and complexometric titration.

UNIT 2: (8 Hours)

Chemical analysis in Pesticide formulation: Titrimetric Methods: Acid-base,non-aqueous, iodimetric titration, oxidation-reduction (redox), precipitation and complexometric titrations

UNIT 3: (6 Hours)

General methods of characterization, separation and purification: Agrochemical compounds from soil, food stuff etc, Solvent extraction, Thin layer chromatography, paper chromatography and column chromatography

UNIT 4: (10Hours)

Instrumental analysis in Agro-chemistry: Applications of gas chromatography and liquid chromatography. Applications of Ultraviolet-visible spectroscopy, infrared spectroscopy, Atomic absorption spectroscopy, Mass spectrometry.

PRACTICAL COMPONENT

(60Hours)

- 1. Extraction of pesticides from water samples using immiscible organic solvents.
- 2. Extract pesticide residues from soil using a solvent mixture.
- 3. Extraction from Leafy Vegetables (Spinach/Cabbage)
- 4. Extract Cleanup using Solid Phase Extraction (SPE)
- 5. To identify and compare multiple pesticides by determining their $\mathbf{R_f}$ values using \mathbf{TLC} with suitable mobile phases and visualization methods. (e.g., Malathion, Carbaryl, Atrazine,
 - 2,4-D, Endosulfan)
- 6. Quantitative analysis of Pesticides using UV-Vis spectroscopy
- 7. To verify Beer-Lambert's law and prepare a calibration curve for a pesticide that absorbs in the UV-visible range (e.g., malathion, carbaryl, 2,4-D, or glyphosate).

- 8. To identify the functional groups, present in pesticide samples using Fourier Transform Infrared (FTIR) spectroscopy by analyzing their characteristic absorption bands.
- 9. To identify the structure of a pesticide for which mass spectra data is provided.

ESSENTIAL/RECOMMENDED READINGS

- 1. R.J Cremlyn, Agrochemicals: Preparation and mode of Action, 2nd Edition, Wiley Blackwell publishers, New Jersey (1991).
- 2. S.M Khopkar, Concepts in Analytical Chemistry, 3rd Edition, New Academic Science, New York (2008).
- 3. Willard, Merittee and Dean, Instrumental methods of Analysis, 5th Edition, Van Nostrand Publishers, Newyork (1974).

KEYWORDS: Analytical Applications, Titrimetric Applications, Chemical analysis in Pesticide formulation, Separation and purification techniques, Instrumental analysis in Agro-chemistry

SEMESTER -VIII

BSc. (Hons)Applied Life Sciences with Agrochemicals and Pest Management

Swami Shraddhanand College

DISCIPLINE SPECIFIC CORE COURSE – 02

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre- requisite
		Lecture	Tutorial	Practical/ Practice		of the course (if any)
Agrochemical for Fungi, Nematodes, and Weeds: DSC 08	4	3	0	1	-	NIL

Course objectives

The Learning Objectives of this course are as follows:

- Learners will gain knowledge about agrochemicals used for the control of fungi, nematodes and weeds.
- To study interactions of fungi, nematodes, and weed species in agricultural systems.
- To understand how these organisms, affect crop health and yield.
- Understand the biochemical and physiological mechanisms by which these chemicals control pest populations.

Learning outcomes

The Learning Outcomes of this course are as follows:

- Articulate the modes of action for various agrochemical agents and explain how these mechanisms disrupt the life processes of pests.
- Develop strategies for minimizing adverse effects through careful selection, timing, and application of agrochemicals.
- Learners will explain, compare, and critically assess the major classes of agrochemicals (fungicides, nematicides, and herbicides) and their specific modes of action.

SYLLABUS OF DSC-08

THEORY COMPONENT-

A. FUNGICIDES

UNIT 1: (16Hours)

Preparation, properties, uses, structure-activity relationship and mode of action of selected fungicides: Organophosphorus compounds and dithiocarbamatesPolyhalogenalkanes, sulfenyl compounds, phenols, quinones, carboxamides, carboximides.

Preparation, properties, uses, structure-activity relationship and mode of action of Azoles and other heterocyclics compounds as fungicides.

UNIT 2: (8 Hours)

A comprehensive view, with reference to two suitable examples of fungicides, for each of the followingMode of action

- a) Membrane sterol biosynthesis
- b) Lipid synthesis, transport, or membrane function
- c) Respiration inhibitor
- d) Nucleic acid metabolism

B. NEMATICIDES

UNIT 3:(6 Hours)

Preparation, properties, usesand mode of action of selected Nematicides: halocarbons, organophosphorus compounds, carbamates.

C. HERBICIDES

UNIT 4: (15Hours)

Properties, uses, structure-activity relationship and mode of action of phenoxyalkanoic acids, carbamates and substituted phenylureas, sulfonylureas

Properties, uses, structure-activity relationship and mode of action of triazines, pyridinium compounds,imidazolinones and dinitroanilines.,

Herbicide safeners and Synthetic plant growth regulators

A comprehensive view, with reference to suitable examples of herbicides, for each of the followingMode of action

- a) Inhibition of Photosynthesis at PS II and PSI
- b) Inhibition of Cellulose Synthesis
- c) Inhibition of Microtubule Assembly

PRACTICAL COMPONENT

(30Hours)

Synthesis of pesticides /analogues/intermediates

- 1. Preparation of 2,4-dichlorophenoxy acetic acid herbicide or its synthetic analogues (any one of the following)
 - a) 4-chlorophenoxy acetic acid
 - b) 4-methylphenoxy acetic acid
 - c) 2-methylphenoxy acetic acid
- 2. Preparation of ethyl ester or butyl ester of any one of phenoxy acetic acid mentioned in experiment-1.
- 3. Preparation of 2-naphthoxyacetic acid (BNOA or β-naphthoxyacetic acid)
- 4. Preparation of Dithiocarbamate fungicide analogous from aromatic/aliphatic amine and separated as sodium /zinc/ manganese salt.
- 5. Preparation of Zineb (Z)
- 6. Preparation of urea derivative from phenylisocynate and aniline.
- 7. Preparation of thiourea derivative from phenylisothiocynate and aniline.
- 8. Preparation of benzimidazole/2-benzylimidazole/2-Methylbenzimidazole
- 9. Preparation of Maleic anhydride -an intermediate for agrochemicals
- 10. Writing the assigned an in-depth analysis of at least three fungicides /Nematicide/Herbicides to be allotted by the instructor. It must cover the detailed aspects of: Chemical Structure, Uses, Mode of Action, Toxicity and GHS labelling, Human Health Implications.

ESSENTIAL/RECOMMENDED READINGS

- 1. Audus, L.J. (1964), The Physiology and Biochemistry of Herbicides, Academic Press.
- 2.Bell, C.V. and Alford, D.V. (2000), _Pest and Disease Management Handbook, British Crop Protection Council; Wiley-Blackwell
- 3.Buchel, K.H. (Ed.) (1992), Chemistry of Pesticides, John Wiley & Sons
- 4. Copping, L.G., Hewitt, H.G. and Leonard, G.C. (1998), Chemistry and Mode of Action of Crop Protection Agents, Royal Society of Chemistry.

- 5. Cremlyn, R.J. (1990), Pesticides: Preparation and Mode of Action, John Wiley & Sons, U.K
- 6. Kearnay, P.C. and Kaufman, D.D. (1975), Herbicides: Chemistry, Degradation and Mode of Action_ (Vols. I, II), Marcel Dekker.
- 7. Kramer, W.K. and Ulrich, S. (2007), Modern Crop Protection Compounds, Wiley-VCH Verlag GmbH
- 8. Metlosky, G., Nadasy, M. and Andriska, V. (1988), Pesticide Chemistry, Elsevier
- 9. Nene, Y.L. and Thapliyal, P.N. (1989), Fungicides in Plant Disease Control, India Book House
- 10. Roy, N.K. (2002), Chemistry of Pesticides, CBS Publishers, New Delhi.
- 11. Unger, T.A. (1996), Pesticide Synthesis Hand Book, William Andrew.
- 12. Vyas, S.C. (1984), Handbook of Systemic Fungicides, Tata McGraw Hill.

KEYWORDS: Fungicides, mode of action of fungicides, Nematicides, mode of action of herbicides, Herbicide safeners, Synthetic plant growth regulators

DISCIPLINE SPECIFIC ELECTIVE COURSE – 04

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre- requisite
		Lecture	Tutorial	Practical/ Practice		of the course (if any)
Environmental health and Agrochemicals	4	2	0	2	-	NIL

Course objectives

The Learning Objectives of this course are as follows:

- Understand the mechanisms of pesticide entry and dispersion in environmental compartments.
- Explore the interactions between pesticide residues and soil/water/microbial systems.
- Assess the toxicological and ecological implications of pesticide residues.
- Implications of pesticide persistence on human health.
- Impact of Pesticide Residues on Human Health and Society

Learning outcomes

The Learning Outcomes of this course are as follows:

- Describe the environmental pathways of pesticide residues in air, water, and soil.
- Analyze the physicochemical and biological processes governing pesticide degradation and transport.
- Evaluate the impact of pesticide residues on ecosystems, food safety, and public health.
- Persistence of pesticides in environment.
- Propose sustainable practices and policy interventions to mitigate agrochemical pollution.

SYLLABUS OF DSE- 04

THEORY COMPONENT-

UNIT 1: (6Hours)

Residues of Agrochemicals in the Atmosphere:

Entry pathways of pesticides into the atmosphere, Fate of Pesticides in the atmosphere, Transport of vapors, Precipitation, Impact of airborne residues, air quality and climate, effect of residues on human health

UNIT 2: (6 Hours)

Residues of Agrochemicals in Water system:

Nature and origin of pollution of aquatic systems, Point and Non-Point pollution. Runoff, leaching, and effluent discharge into water bodies, Physicochemical properties influencing aquatic fate (solubility, hydrolysis, photolysis). Dynamics of pesticides in aquatic environment. Toxicological effects on aquatic flora and fauna

UNIT 3: (6 Hours)

Pesticides residues in the Soil:

Absorption, Retention, Transport and Degradation of pesticides in the soil, persistence and half-life of various pesticide classes in soil. Effect on microorganisms and Consequent effect on the soil condition, Fertility, nutrient cycle and crop productivity. Interactions between pesticides and soil organic/inorganic matter

UNIT 4: (12Hours)

A Persistence of Pesticides in the Environment:

Low, moderate and high persistent pesticides, Persistent organic pollutants, Physical, chemical, biochemical and environmental factors affecting pesticide of persistence in the environment.

B Pesticide Dissipation and Fate in The Environment:

Various dissipation processes, Role of drift, volatilization, adsorption, desorption, runoff etc.in pesticide dissipation, Leaching and risk of groundwater pollution, Dissipation time (Half-life-DT50, DT90), Rate kinetics (1st order, 2nd order), Behavior and fate of pesticides in soil and crops.

C Impact of Pesticide Residues on Human Health and Society:

Direct and indirect exposure pathways in humans (food, water, air, occupational). Acute and chronic health effects (carcinogenicity, neurotoxicity, endocrine disruption, genotoxicity, skin sensitization, reproductive and developmental toxicity).

PRACTICAL COMPONENT

(60Hours)

- 1. To study degradation of airborne pesticides when exposed to UV radiation.
- 2. To observe chemical degradation (hydrolysis and photolysis) of pesticides in water
- 3. To measure how different soils, retain pesticides through adsorption.
- 4. To determine the degradation rate and persistence of a pesticide in soil.
- 5. To analyze enzyme activity or nutrient availability in pesticide-treated soil.
- 6. To study whether washing, peeling, or boiling reduces pesticide residues and protects food quality.
- 7. Writing the assigned an in-depth analysis of at least three pesticides to be allotted by instructor. It must cover the detailed aspects of: Chemical Structure, Impact on environment and its persistence, Toxicity, Human Health Implications and GHS labelling

ESSENTIAL/RECOMMENDED READINGS

- 1. Ogwu, M. C., &Izah, S. C. (Eds.). (2023). One health implications of agrochemicals and their sustainable alternatives (Vol. 34). Springer Nature.
 - 2. WHO (World Health Organ.), FAO (U. N. Food Agric. Organ.). (2019). Global situation of pesticide management in agriculture and public health: report of a 2018 WHO-FAO survey WHO, Geneva.

https://apps.who.int/iris/handle/10665/329971] (https://apps.who.int/iris/handle/10665/329971) (https://apps.who.int/iris/handle/iris/ha

- 3. Vaz Jr, S. (2019). Sustainable agrochemistry. Springer International Publishing, New York, US.
- 4. Naeem, M., Juan Francisco Jimenez Bremont, Abid Ali Ansari, &Sarvajeet Singh Gill. Agrochemicals in Soil and Environment.
- 5. Devi, P. I., Manjula, M., &Bhavani, R. V. (2022). Agrochemicals, environment, and human health. Annual Review of Environment and Resources, 47(1), 399-421.

- 6. Dowdall, C. M., & Klotz, R. J. (2016). Pesticides and global health: understanding agrochemical dependence and investing in sustainable solutions. Routledge. [https://doi.org/10.4324/9781315422695] (https://doi.org/10.4324/9781315422695)
- 7. Yassi, A. (2001). Basic environmental health. Oxford University Press.
- 8. Akpan, G. E., Ndukwu, M. C., Etim, P. J., Ekop, I. E., &Udoh, I. E. (2023). Food Safety and Agrochemicals: Risk Assessment and Food Security Implications. In One Health Implications of Agrochemicals and their Sustainable Alternatives (pp. 301-333). Springer Nature Singapore.
- 9. Frumkin, H. (Ed.). (2016). Environmental health: from global to local. John Wiley & Sons.
- 10. Nriagu, J. O. (2019). Encyclopedia of environmental health. Elsevier.
- 11. Pretty, J. (Ed.). (2012). The pesticide detox: towards a more sustainable agriculture. Routledge.
- 12. Hamilton, D., & Crossley, S. (Eds.). (2004). *Pesticide residues in food and drinking water: human exposure and risks*. John Wiley & Sons.
- 13. Horrigan, L., Lawrence, R. S., & Walker, P. (2002). How sustainable agriculture can address the environmental and human health harms of industrial agriculture. Environmental Health Perspectives, 110(5), 445-456.
- 14. Schnoor, J. L. (Ed.). (1992). Fate of Pesticides and Chemicals in the Environment. John Wiley & Sons.
- 15. Shahamat U Khan. 1980. Pesticides in the Soil Environment (Editor: R. J. Wakeman) Elsevier.

KEYWORDS: Residues of Agrochemicals, Fate of Pesticides in the atmosphere,
Toxicological effects, Transport and Degradation of pesticides,
Persistence of Pesticides, Pesticide Dissipation in environmental

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

DISCIPLINE SPECIFIC ELECTIVE COURSE – 05

Course title & Code	Credits	Credit	distribution course	Eligibility criteria	Pre- requisite	
		Lecture	Tutorial	Practical/ Practice		of the course (if any)
Introduction to Natural Pesticides: Biopesticides and Plant Toxins	4	2	0	2	-	NIL

Course objectives

The Learning Objectives of this course are as follows:

- Define natural pesticide, including biopesticides and plant toxins.
- Differentiate between biopesticides and synthetic chemical pesticides.
- Identify common examples of biopesticides and plant-derived toxins. Analyze the advantages and limitations of using natural pesticides.
- Discuss the environmental and health benefits of biopesticides over synthetic pesticides.
- Evaluate real-world applications and case studies of natural pesticides in modern agriculture.

Learning outcomes

The Learning Outcomes of this course are as follows:

- Demonstrate an understanding of biopesticides and plant toxins in pest control.
- Apply knowledge of natural pesticides to sustainable farming practices.
- Assess the role of biopesticides in reducing chemical pesticide dependency.
- Critically evaluate different biopesticide strategies for pest management.

SYLLABUS OF DSE-05

THEORY COMPONENT-

UNIT 1: (9Hours)

Isolation, characterization, properties and mode of action of important groups of naturally occurring insecticides (pyrethroids, nicotinoids, rotenoids, limonoids, microbial macrolides). Sources of bio pesticides and extraction (ASE, SFE /solvent extraction)

UNIT 2: (5 Hours)

A Bacillus thuringiensis and nuclear polyhedrosis virus based insecticides and other biopesticides.

B Semi chemicals, insect hormones, insect growth regulators, feeding deterrents and repellents etc

UNIT 3 (4Hours)

Natural nematicides, fungicides, mollusicides and rodenticides

UNIT 4 (12Hours)

- A Introduction to Plant Toxins Based on Plant Family
- B Classification Plant Toxins Based on Chemical Structure
- C Biological Activity and Mode of Action of Plant Toxins

PRACTICAL COMPONENT

(60Hours)

- 1. Extraction by hydrodistillation, isolation of pure compounds, their characterization,
- 2. Extraction of tobacco leaves
- 3. isolation of nicotine and its identification,
- 4. Extraction of neem seed kernels, enrichment of azadirachtin, analysis of azadirachtin and its analysis.
- 5. To extract azadirachtin, a bio-pesticidal compound, from neem seeds using organic solvents.
- 6. To extract caffeine from tea leaves by solvent extraction method using dichloromethane.
- 7. To extract and estimate the amount of **allicin**, a bioactive compound, from fresh garlic using spectrophotometry.
- 8. Writing the assigned an in-depth analysis of at least three biopesticides to be allotted by instructor from different sources from theory portion. It must cover the detailed aspects of: Source, Chemical Structure, extraction /isolation from natural source, Uses, Advantages and disadvantages with respect to synthetic pesticides, Toxicity, Human Health Implications (if any), GHS labelling.

ESSENTIAL/RECOMMENDED READINGS

1. Alexander, M. (1999). Biodegradation and Bioremediation (2nd ed.). Academic Press.

- 2. Copping, L.G. (1996). Crop Protection Agents from Nature: Natural Products and Analogues. Royal Soc. Chem., London, 136.
- 3. Dev, S. & Koul, O. (1997). Insecticides of Natural Origin. Harwood Acad. Publishers.
- 4. Godfrey, C.R.A. (1995). Agrochemicals from Natural Products Marcel Dekker.
- Hall, J.C., Hoagland, R.E. &Zablotowicz, R.M (2001). Pesticide Biotransformation in Plants and Microorganisms: Similarities and Divergences. ACS Symposium Series, 777. Washington, DC.
- 6. Hassal, K.A.(1990). The Biochemistry. Plenum Press.
- 7. Jacobson, M. (1965). Insect Sex Attractants. John Wiley & Sons.
- 8. Jacobson, M. (1970). Naturally Occurring Insecticides. John Wiley & Sons.
- 9. Khan, S.U. (1980). Pesticides in the Soil Environment. Elsevier.
- 10. Leahey, J.P. (1985). The Pyrethroid Insecticides. Taylor & Francis.
- 11. Matsumura, F. (1975). Toxicology of Insecticides. Plenum Press.
- 12. Menzie, C.M (1980). Metabolism of Pesticides. Update III US Fish and Wildlife Service Special Scientific Report.
- 13. Parmar, B.S. &Devakumar, C (1990). In: Botanical and Biopesticides. Westvill Publ. House.
- 14. Racke, K.D., Skidmore, M.W., Hamilton, D.J., Unsworth, J.B., Miyamoto, J. & Cohen, S.Z. (1997). Pesticide Fate in Tropical SoilsPure and Appl. Chem., 69(6), 1349–1371.
- 15. Mtewa, A. G., Egbuna, C., & Rao, G. M. N. (Eds.). (2021). Poisonous plants and phytochemicals in drug discovery / edited by Andrew G. Mtewa, (First edition.). John Wiley & Sons
- 16. Osman, A. M. G., Chittiboyina, A. G., & Khan, I. A. (2013). Plant toxins. In *Foodborne infections and intoxications* (pp. 435-451). Academic Press.
- 17. Keeler, R. F., &Tu, A. T. (Eds.). (1991). *Toxicology of plant and fungal compounds*. M. Dekker.
- 18. Dauncey, E. A., & Larsson, S. (2018). *Plants that kill: A natural history of the world's most poisonous plants*. Princeton University Press.

KEYWORDS: Bio pesticides, Bacillus thuringiensis, Nuclear polyhedrosis virus, Semi chemicals, Insect growth regulators, Natural nematicides, mollusicides and rodenticides

DISCIPLINE SPECIFIC ELECTIVE COURSE – 06

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit	distribution course	Eligibility criteria	Pre- requisite	
		Lecture	Tutorial	Practical/ Practice		of the course (if any)
Pesticide Formulation and Application Equipment	4	2	0	2	-	NIL

Course objectives

The Learning Objectives of this course are as follows:

- Identify various types of pesticide formulations (e.g., emulsifiable concentrates, wettable powders, granules, suspension concentrates) and discuss their specific characteristics, advantages, and limitations.
- Analyze the chemical and physical properties that affect the formulation's stability, efficacy, and compatibility.
- Importance of pesticide Labelling
- Analyze how the choice of formulation impacts the selection and performance of application equipment.
- Describe the function and importance of key components in application equipment, such as nozzles, pumps, and pressure mechanisms.

Learning outcomes

The Learning Outcomes of this course are as follows:

- Classify different pesticide formulations with an explanation of their components and respective functions
- Demonstrate Knowledge of Pesticide Formulation and labelling

- Select suitable pesticide application equipment based on specific crop requirements, target pest types, and environmental conditions.
- Ensure Safety and Compliance assurance requirements.

SYLLABUS OF DSE-06

THEORY COMPONENT-

UNIT 1: (7 Hours)

Introduction and Types of Pesticide formulations:

A Definition, purpose of formulations, Important formulation terms: Active Ingredient, Inert Ingredient, Phytotoxicity, Adjuvant, Carrier, surfactants, emulsifiers, stabilizers, wetting agents, Spray Mix Terminology: solution, suspension, emulsion

B International codes for the formulation type. Wettable powders, soluble powder, solutions, emulsifiable concentrates, aerosols, dusts and granules. Controlled Release Pesticides, Bait. Advantages and disadvantages of individual pesticide formulation

UNIT 2: (12 Hours)

Key aspects for creating a formulation and Conventional formulation:

A Type of surface, Training and equipment, Runoff or drift, Safety to people, animals, and the environment, Habits of the pest, Consideration of mixed pesticides for their capabilities and incompatibilities

B Dusting, Powders/ Dust Formulations (DP), Granules (GR), Water Dispersible Powders/Wettable powders (WDP/WP), Soluble Concentrates (SC), Emulsifiable concentrates (EC), Ultra Low volume (ULV) with respect to their ingredients, advantages and disadvantages.

UNIT 3: (4 Hours)

Introduction to pesticide Application Equipment:

Overview of pesticide application equipment (with few selected examples), each tailored to type of the formulation.

- 1. Dusters: Manually and Power Operated Dusters
- 2. Sprayers: Knapsack Sprayers, Hydraulic Sprayers, Aerial Sprayers (Aircraft or drones)

- 3. Modern trends in pesticide application with Precision Application Equipment: Technological advancement with GPS-guided sprayers and drone-based application systems
- 4. Types of nozzles: Function of nozzles with different size and hole diameter available as an attachment with these sprayers.

UNIT 4: (7 Hours)

Understanding pesticide Label and Labeling:

Definition, purpose of Label and Labeling, Common Terms Used in Pesticides Labels, Precautionary Statements, Direction for Use Environmental Hazards, Color coding Information on the label Symbols, Toxicity information/statements, Pictograms, Labels (GHS) warning statements, Information about type of formulation, Name of pesticide, active and inert material, Name of manufacturer, Quantity

PRACTICAL COMPONENT

(60Hours)

- 1. Preparation of Emulsifiable concentrate (EC) formulation of given organic compound as oil in water emulsion(O/W).
- 2. Preparation of EC formulation: Emulsifiable concentrate of neem oil.
- 3. Preparation of standard hard water.
- 4. To determine the emulsion stability of given EC formulation.
- 5. Determination of bulk density of pesticidal wettable powder (WP).
- 6. Preparation of WP formulation.
- 7. Volumetric determination of acidity/ alkalinity of WP.
- 8. Preparation of Suspension Concentrate (SC) formulation.
- 9. Determination of wettability of pesticidal WP / Dust/SP.
- 10. To draw pictograms and indicate:
 - a. Advice, Warning and their meaning
 - b. Colour Codes and their meaning
- 11. Write the colour identification band and warning symbol as per toxicity Data (LD₅₀) following Government of India Recommendations (*see*reference -2)
- 12. Each student to be assigned project for designing the label manually for any five pesticides. It must cover the detailed aspects of: Pesticide formulation,
 Manufacturers name, Quantity of Active and inert ingredient, Pictograms/GHS labelling/Toxicity statement(s), Handling instruction, Any other information required for label

13. Student to be demonstrate / visit to the manufacturing unit for pesticide Application Equipment

ESSENTIAL/RECOMMENDED READINGS

- 1. Agrochemicals-Pesticide formulations | IUPAC https://agrochemicals.iupac.org
- 2. Report of the committee on manner of labelling of pesticides as per toxicity Dated 09 August,20I9 Ministry of Agriculture & Farmers Welfare Government of India No. 24-01/2019-CIR.Ihttps://ppqs.gov.in/sites/default/files/public_notice_0.pdf
- 3. Cardarelli, N.F. (2018). Controlled Release Pesticides Formulations.CRC Press.
- 4. Foy, C.L., & Pritchard, D.W. (1996). Pesticide Formulation and Adjuvant Technology. CRC Press.
- 5. Hall, F.R., Berger, P.D., & Collins, H.M. (1995). Pesticide Formulations and Application Systems (Vol. 14).
- Knowles, D.A. (1998). Chemistry and Technology of Agrochemical Formulations.
 Springer.
- 7. Parmar, B.S., &Tomar, S.S. (2004). Pesticide Formulation Theory and Practice. CBS Publishers & Distributors.
- 8. Wade, R. (1973). Pesticide Formulation. Dekker, Inc.
- 9. Wade, V.V., Sugavanam, B., &Khetan, S.K. (1998). Pesticide Formulation. New Age International Publishers.
- 10. Ware, G.W. (1994). The Pesticide Book (4th ed.). W.H. Freeman: Fresno, CA.

KEYWORDS: Pesticide formulations, Conventional formulation, pesticide application equipment, Pesticide Label and Labeling, Suspension Concentrate formulation

SKILL ENHANCEMENT COURSE (SEC-1): Advanced Software Utilities for Chemists

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre- requisite of the
		Lecture	Tutorial	Practical/		course
				Practice		(if any)
Advanced	2	1	0	1	12 th class	NIL
Software Utilities					with science	
for Chemists						
SEC-1						

Course objectives

Course Objectives:

- To develop basic understanding of important software utilities *Gnuplot* and using this tool for presentation of data in graphical form for research purpose.
- To develop basic understanding of software utilities for designing and formatting chemical structures.
- To develop a basic understanding of functioning of a Large Language Model utility; *ChemCrow* for Chemists.

Learning outcomes

After completing the course, the students will be able to:

- Develop standard research quality graphs and analyze the graph for understanding acquired data.
- Use software utilities for designing chemical structures in varied representations for example, in research articles and presentations.
- Use Large Language Model utility; *ChemCrow* for applying molecule tool, safety tool, and chemical reaction tool for analyzing chemical reaction and scientific data for literature survey.

THEORY

UNIT 1: Software Utilities for Chemists

(15 Hours)

Gnuplot Software Utility

Graphical analysis and visualization of computational data. Need and limitations of Graphical analysis. Introduction to *Gnuplot* plotting tool, a command-driven interactive function and data plotting program.

Basic *Gnuplot* commands: simple plots, plotting data from a file, saving and exporting, multiple data sets per file. Locations on a graph, Editing and Styling plots (plot ranges, line styles, colours, fonts, terminal types). Use of multiple axes and multiple plots in a single page.

Basics of three-dimensional plots, generating surface and contour plots, plotting data from a file. Understanding colour spaces, defining palettes, creating coloured graphs with palettes. Advanced plotting concepts; Multiplot, Higher math and special occasions, Mathematical Functions and curve fitting. Exporting graphs to file.

Software Utilities for drawing Chemical Structure and ROSHAMBO Utility

Introduction to software utilities for designing molecules species and representation of chemical reaction and ROSHAMBO utility for molecular alignment and 3D similarity scoring.

Large Language Model utility: ChemCrow

Introduction to *ChemCrow*; *General tool*, *Molecule tool*, *Safety tool NameRXN*, *RXNPredict*, *RXNPlanner* tool for using the software for designing chemical structure, literature survey, exploring safety of materials and prediction and planning reactions.

Practicals: Credits: 01

(Laboratory periods: 15 classes of 2 hours each)

- 1. Plotting graphs using Gnuplot
 - (i) Installing Gnuplot and plotting simple 2-D plots: linear, sine, cosine, exponential
 - (ii) Ideal gas isotherms
 - (iii) Pressure-volume curves of van der Waals gas (van der Waals isotherms)
 - (iv) Planck's distribution law
 - (v) Radial distribution curves for hydrogen like orbitals
 - (vi) Maxwell-Boltzmann distribution curves as function of temperature and molecular weight
 - (vii) Data from phase equilibria studies.
 - (viii) Graphical solution of equations.
 - (ix) Simulation of pH metric titration curves.
 - (x) Simple 3D functions such as sin(x)*cos(y)
 - (xi) Parametric plots in spherical polar coordinates
 - (xii) Probability density surface as a function of angle for Hydrogen atom

- 2. Drawing chemical structures of various compounds (aliphatic, aromatic, heterocyclic with different functional groups, using Free, Open Source, Proprietary and Online software utilities i.e. ACD Chemsketch and 3-D viewer, ChemDraw, ChemDraw online & ROSHAMBO utility.
- 3. Exploring organic name reactions in ChemCrow

Essential/recommended readings

Theory:

- 1. Janert P. K., (2010) Gnuplot in Action, Manning Publications Co., Greenwich, CT.
- 2. Phillips L., (2012) Gnuplot Cookbook, Packt Publishing, Birmingham U.K.
- 3. Moore B.G., Orbital Plots Using Gnuplot, J. Chem. Edu., 77 (6), (2000) 785-789.
- 4. Atwi R., Wang Y., Sciabola S., and Antoszewski A., ROSHAMBO: Open-Source Molecular Alignment and 3D Similarity Scoring, J. Chem. Inf. Model., 64, (2024) 8098–8104.
- 5. https://fitzkee.chemistry.msstate.edu/sites/default/files/ch8613/ibm-gnuplot.pdf
- 6. https://fitzkee.chemistry.msstate.edu/sites/default/files/bootcamp/2022/session-08 gnuplot-tutorial.pdf
- 7. https://emleddin.github.io/comp-chem-website/Analysisguide-gnuplot.html
- 8. https://www.acdlabs.com/resources/free-chemistry-software-apps/chemsketch-freeware/
- 9. https://chemaxon.com/marvin
- 10. https://www.insilicochemistry.io/tutorials/foundations/gpt-4-for-chemistry#h.kfv6wyq239nc

Practical:

- 1. Janert P. K., (2010) Gnuplot in Action, Manning Publications Co., Greenwich, CT.
- 2. Phillips L., (2012) Gnuplot Cookbook, Packt Publishing, Birmingham U.K.
- 3. Moore B.G., Orbital Plots Using Gnuplot, J. Chem. Edu., 77 (6), (2000) 785-789.
- 4. Atwi R., Wang Y., Sciabola S., and Antoszewski A., ROSHAMBO: Open-Source Molecular Alignment and 3D Similarity Scoring, J. Chem. Inf. Model., 64, (2024) 8098–8104.
- 5. https://fitzkee.chemistry.msstate.edu/sites/default/files/ch8613/ibm-gnuplot.pdf
- 6. https://fitzkee.chemistry.msstate.edu/sites/default/files/bootcamp/2022/session-08 gnuplot-tutorial.pdf

- 7. https://emleddin.github.io/comp-chem-website/Analysisguide-gnuplot.html
- 8. https://www.acdlabs.com/resources/free-chemistry-software-apps/chemsketch-freeware/
- 9. https://chemaxon.com/marvin
- 10. https://www.insilicochemistry.io/tutorials/foundations/gpt-4-for-chemistry#h.kfv6wyq239nc

Assessment Methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SKILL ENHANCEMENT COURSE (SEC-2): Lab-Based Learning: Analytical Instruments

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre- requisite of the
		Lecture	Tutorial	Practical/		course
				Practice		(if any)
Lab-Based	2	1	0	1	12 th class	NIL
Learning:					with science	
Analytical						
Instruments						
SEC-2						

Course objectives

Course Objectives:

- To learn about the fundamentals of separation techniques employed in organic synthesis and the purification of organic compounds.
- To understand instrumentation (hardware/software) employed in the analysis and identification of organic compounds.
- Hands-on training on spectroscopic instruments and separation techniques employed in organic synthesis.

Learning outcomes

After completing the course, the students will:

- gain experience in various separation techniques typically employed for monitoring reaction progress and the purification of pure compounds from a mixture.
- work independently on sophisticated equipment used in organic synthesis, correlating with the principle and the instrumentation part.

THEORY

UNIT 1: Separation and Analytical Instruments

(15 Hours)

Thin Layer Chromatography

Principle of using TLC in monitoring organic reactions, Polarity of Solvents, Retention factor, Principle and application of HP TLC.

Column Chromatography

Theory of Column Chromatography, Gradient Solvent Systems, Application of Column Chromatography in purification of mixtures.

UV-VIS Spectroscopy

Basics and applications of UV-vis spectroscopy, Instrumentation of UV-vis spectroscopy, Applications of UV-vis spectroscopy.

Optical Rotation

Importance of optical activity, Instrumentation of Polarimeter, Sample preparation, Recording Optical rotation of organic compounds.

Practicals: Credits: 01

(Laboratory periods: 15 classes of 2 hours each)

- 1. To determine the number of organic compounds present in the given mixture by TLC, and calculate their respective R_f values.
- 2. To determine the relative polarities of a set of given organic compounds by comparing their R_f on TLC.
- 3. To separate a mixture of two or more non-polar organic compounds by column chromatography using a gradient solvent system (Hexanes/EtOAc).
- 4. To separate a mixture of two or more medium/high polarity organic compounds by column chromatography using a gradient solvent system (MeOH/DCM).
- 5. Hands-on training on running a UV-vis spectroscopy and sample preparation.
- 6. To verify the linear relationship between absorbance and concentration using a coloured organic compound.
- 7. To investigate the effect of solvent polarity on the keto-enol equilibrium of acetylacetone by analyzing UV-Visible absorption spectra.
- 8. To study the effect of pH on the UV-Vis spectrum of an indicator (e.g., methyl orange).
- 9. Hands-on training on running a polarimeter and sample preparation.
- 10. To measure the optical rotation of a pair of enantiomers.

Essential/recommended readings

Theory:

- 1. Furniss B. S., Hannford A. J., Smith, P. W. G., Tatcheli, A. R., "Vogel's Textbook of Practical Organic Chemistry" 5th ed., Longman Scientific & Technical
- 2. Kemp W., 'Organic Spectroscopy', 3rd ed., Palgrave, New York (1991).

- 3. Willard H. H., Merritt Jr. L. L., Dean J. A., Settle F. A. S., "Instrumental Methods of Analysis", 7th Ed., Wadsworth, 2009, Cengage Learning India Pvt. Ltd. Fifth Indian reprint by CBS Publishers & Distributors Pvt. Ltd.
- 4. Silverstein R. M., and Webster F. X., "Spectrometric Identification of Organic Compounds", 6th ed., John Wiley & Sons, New York (1998).
- **5.** Skoog D. A., Holler F. J., and Crouch S. R., "Principles of Instrumental Analysis", 6th ed., Thomson Brooks/Cole, Cengage Learning, New Delhi (2007).

Practical:

- 1. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy.
- 2. Donald A. McQuarrie and John D. Simon, Physical Chemistry: A Molecular Approach.
- 3. J. Michael Hollas, Modern Spectroscopy.
- 4. Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis.
- 5. Donald L. Pavia, Gary M. Lampman, George S. Kriz, Introduction to Spectroscopy.
- 6. Vogel, A. I. (2012), Quantitative Organic Analysis, Part 3, Pearson Education.
- 7. Mann, F. G., Saunders, B.C. (2009), Practical Organic Chemistry, Pearson Education.
- 8. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (2012), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
- 9. Ahluwalia, V.K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.

Assessment Methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.