DISCIPLINE SPECIFIC ELECTIVE COURSE – 01

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

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
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 Co-operation and Development (OECD) principles.

C. Computational models for toxicology,their Limitations of chemical similarity and Read-across 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

3 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

5 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.

7 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 ofat 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

Note: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.