



## Ph.D. Course Work Common Syllabus

<b>Paper Name: Research Methodology</b>	<b>Paper Code: PHD-101/RM</b>	<b>Credits: 4 (4-0-0)</b>
<b>Evaluation (Maximum Marks = 100)</b>	<b>Internal = 30</b>	<b>External = 70</b>
<b>Course Objectives</b>		
1. To introduce the fundamental concepts, methods, and ethics of scientific research. 2. To develop skills in research design, data collection, analysis, and interpretation. 3. To enable students to formulate research problems and communicate findings effectively.		

<b>Unit</b>	<b>Contents</b>	<b>Lectures</b>
<b>I</b>	Foundations of Research: Meaning, Objectives, Motivation, Utility. Concept of theory, empiricism, deductive and inductive theory. Characteristics of scientific method – Understanding the language of research – Concept, Construct, Definition, Variable. Research Process. Problem Identification & Formulation – Research Question – Investigation Question – Measurement Issues – Hypothesis – Qualities of a good Hypothesis – Null Hypothesis & Alternative Hypothesis. Hypothesis Testing – Logic & Importance.	<b>10</b>
<b>II</b>	Research Design: Concept and Importance in Research – Features of a good research design – Exploratory Research Design – concept, types and uses, Descriptive Research Designs – concept, types and uses. Experimental Design: Concept of Independent & Dependent variables. Qualitative and Quantitative Research: Qualitative research – Quantitative research – Concept of measurement, causality, generalization, replication. Merging the two approaches.	<b>10</b>
<b>III</b>	Sampling: Concepts of Statistical approach, Sample, Sampling Frame, Sampling Error, Sample Size. Characteristics of a good sample. Probability Sample – Simple Random Sample, Systematic Sample, Stratified Random Sample & Multi-stage sampling. Determining size of the sample – Practical considerations in sampling and sample size. Data Analysis: Data Preparation – Univariate analysis (frequency tables, bar charts, pie charts, percentages), Bivariate analysis – Cross tabulations and Chi-square test including testing hypothesis of association.	<b>15</b>
<b>IV</b>	Measurement: Concept of measurement – what is measured? Problems in measurement in research – Validity and Reliability. Techniques of Scientific Measurement. Interpretation of Data and Paper Writing – Layout of a Research Paper, Journals in Computer Science, Impact factor of Journals, When and where to publish? Ethical issues related to publishing, Plagiarism and Self-Plagiarism. Use of Encyclopedias, The art of Scientific Communication.	<b>12</b>

<b>V</b>	Use of tools/techniques for Research: methods to search required information effectively, Reference Management Software like Endnote/Zotero/Mendeley, Software for paper formatting like LaTeX/MS Office, Software for detection of Plagiarism. Presentation in Seminars and Conferences, Sponsored Research-basics, Major funding bodies for research, National- DST, UGC, CSIR, ICMR, DBT, SERB, ISRO, and DRDO, International- NSF, NIH, Horizon Europe and UNESCO.	<b>13</b>
	<b>Total</b>	<b>60</b>

### Suggested Readings

1. Kothari, C. R., and Gaurav Garg. Research Methodology: Methods and Techniques. 4th ed., New Age International Publishers, 2019.
2. Creswell, John W., and J. David Creswell. Research Design: Qualitative, Quantitative, and Mixed Methods Approaches. 5th ed., SAGE Publications, 2018. <https://us.sagepub.com/en-us/nam/research-design/book255675>
3. Saunders, Mark, Philip Lewis, and Adrian Thornhill. Research Methods for Business Students. 8th ed., Pearson Education, 2019.
4. Bryman, Alan. Social Research Methods. 5th ed., Oxford University Press, 2016. <https://global.oup.com/ukhe/product/social-research-methods-9780199689453>
5. Flick, Uwe. An Introduction to Qualitative Research. 6th ed., SAGE Publications, 2018.
6. Walliman, Nicholas. Research Methods: The Basics. 2nd ed., Routledge, 2017. <https://www.routledge.com/Research-Methods-The-Basics/Walliman/p/book/9781138693981>
7. Kumar, Ranjit. Research Methodology: A Step-by-Step Guide for Beginners. 5th ed., SAGE Publications, 2022.
8. Neuman, W. Lawrence. Social Research Methods: Qualitative and Quantitative Approaches. 8th ed., Pearson, 2014.
9. Research Methods in Psychology. <https://www.saylor.org/courses/psych301/>
10. [https://onlinecourses.nptel.ac.in/noc23\\_ge36/preview](https://onlinecourses.nptel.ac.in/noc23_ge36/preview)
11. [https://onlinecourses.nptel.ac.in/noc22\\_ge08/preview](https://onlinecourses.nptel.ac.in/noc22_ge08/preview)



## Ph.D. Course Work Common Syllabus

<b>Paper Name: Research and Publication Ethics</b>	<b>Paper Code: PHD-102/RPE</b>	<b>Credits: 2 (2-0-0)</b>
<b>Evaluation (Maximum Marks = 100)</b>	Active participation, group discussion and quizzes (25%); Practical: 40%; and End Semester written examination: 35 %	

### Introduction:

This course is designed to create awareness among doctoral students about research and publication ethics and different types of unethical practices and misconduct in publications. This course has total 6 units focusing on basics of philosophy of science and ethics, research integrity, publication ethics. Hands-on-sessions are designed to identify research misconduct and predatory publications. Indexing and citation databases, Open Access publications, research metrics (citations, h-index, Impact Factor, etc.) and Plagiarism tools will be introduced in this course.

### Course Structure

The course comprises of six modules listed in table below. Each module has 4-5 units.

<b>Modules</b>	<b>Unit title</b>	<b>Teaching hours</b>
<b>Theory</b>		
RPE 01	Philosophy and Ethics	4
RPE 02	Scientific Conduct	4
RPE 03	Publication Ethics	7
<b>Practice</b>		
RPE 04	Open Access Publishing	4
RPE05	Publications Misconduct	4
RPE 06	Databases and Research Metrics	7
	<b>Total</b>	<b>30</b>

## THEORY

### **RPE 01: PHILOSOPHY AND ETHICS (3 hrs.)**

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgements and reactions

### **RPE 02: SCIENTIFIC CONDUCT (5hrs.)**

1. Ethics with respect to science and research.
2. Intellectual honesty and research integrity.
3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentations of data.

### **RPE 03: PUBLICATION ETHICS (7 hrs.)**

1. Publication ethics: definition, introduction and importance
2. Best practices/standards setting initiatives and guidelines: CARE, COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
5. Violation of publication ethics, authorship and contributorship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

## PRACTICE

### **RPE 04: OPEN ACCESS PUBLISHING (4 hrs.)**

1. Open Access Publications and Initiatives
2. SHERPA/RoMEO online resource to check publisher copyright & self- archiving policies
3. Software Tools to Identify Predatory Publications
4. Journal Finder/Journal Suggestion Tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

## RPE 05: PUBLICATION MISCONDUCT (4 hrs.)

### **A. Group Discussions (2 hrs.)**

1. Subject specific ethical issues, falsification, fabrication, and plagiarism (FFP), authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad

### **B. Software tools (2hrs.)**

- Use of plagiarism software, like, Turnitin, Urkund and open-source software tools.

## RPE 06: DATABASES AND RESEARCH METRICS (7 hrs.)

### **A. Databases (4 hrs.)**

1. Indexing Databases
2. Citation Databases: Web of Science, Scopus, etc.

### **B. Research Metrics (3hrs.)**

- 1 Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPR, Cite Score
- 2 Metrics: h-index, g-index, i10 index, altmetrics

## Essential Readings

- Suber, P. (2012). [Open Access](#). Cambridge, MA, USA: MIT Press.
- Resnik, D.B. (2011). [What Is Ethics in Research & Why Is it Important](#). National Institute of Environmental Health Sciences, I-10.
- National Academy of Sciences, National academy of Engineering and Institute of Medicine (2009). [On Being a Scientist: A Guide of Responsible Conduct in Research](#): Third Edition, National Academies Press.
- Madalli, D.P. (2015). [Concepts of Openness and Open Access](#). UNESCO Curriculum for Researchers, Module 2. Paris: UNESCO.
- MacIntyre, Alasdair (1967). A Short History of Ethics. London.
- Kanjilal, U. & Das, A.K. (2015). [Introduction to Open Access](#). UNESCO Curriculum for Library Schools, Module 1. Paris: UNESCO.
- INSA (2019). [Ethics in Science Education, Research and Governance](#), Edited by K. Muralidhar, A. Ghosh, & A.K. Singhvi. New Delhi: Indian National Science Academy. ISBN: 9788193948217.
- Das, A.K. (2015). [Research Evaluation Metrics](#). UNESCO Curriculum for Researchers, Module 4. Paris: UNESCO.

- Das, A.K. & Mishra, S. (2014). [Genesis of Altmetrics or Article-level Metrics for Measuring Efficacy of Scholarly Communications: Current Perspectives](#). *Journal of Scientometric Research*, 3(2): 82-92.
- Chaudhari, N. & Baliga, V. (2015). [Intellectual Property Rights](#). UNESCO Curriculum for Researchers, Module 3. Paris: UNESCO.
- Chaddah, P. (2018). [Ethics in Competitive Research: Do Not Get Scooped; To Not Plagiarized](#). ISBN: 9789387480865
- Bird, A. (2006). [Philosophy of Science](#). Routledge.

### Supplementary Readings

- ICMR (2017). [National Ethical Guidelines for Biomedical and Health Research Involving Human Participants](#). New Delhi: Indian Council of Medical Research.
- Indian Sociological Society (2020). [ISS Code of Ethics](#). New Delhi: Indian Sociological Society.
- PSA (2019). [Draft National Policy on Academic Ethics](#). New Delhi: Principal Scientific Adviser (PSA) to the Government of India.
- The InterAcademy Partnership (2022). [Report: Combatting Predatory Academic Journals and Conferences](#). Trieste: The InterAcademy Partnership.
- UGC (2019). [Consortium for Academic Research and Ethics \(CARE\)](#). New Delhi: University Grants Commission.
- UGC (2020). [Good Academic Research Practices](#). New Delhi: University Grants Commission.
- UNESCO (2021). [UNESCO Recommendation on Open Science](#). Paris: UNESCO.
- Das, A.K. (2008). [Open Access to Knowledge and Information: Scholarly Literature and Digital Library Initiatives - the South Asian Scenario](#). New Delhi: UNESCO, ISBN 9788189218218.
- Das, A.K. (2015). [Scholarly Communications](#). UNESCO Curriculum for Researchers, Module 1. Paris: UNESCO.
- Das, A.K. (2019). [Research Integrity in the Context of Responsible Research and Innovation Framework](#). *DESIDOC Journal of Library & Information Technology*, 39(2): 82-86.
- Das, A.K. (2020). [UNESCO Recommendation on Open Science: An Upcoming Milestone in Global Science](#). *Science Diplomacy Review*, 2(3): 39- 43.
- Mishra, S. & Das, A.K. (2015). [Sharing your Work in Open Access](#). UNESCO Curriculum for Researchers, Module 5. Paris: UNESCO.

- Nisha, F., Das, A.K. & Tripathi, M. (2020). [Stemming the Rising Tide of Predatory Journals and Conferences: A Selective Review of Literature](#). *Annals of Library and Information Studies*, 67(3): 173-182.
- Smith, I. (2015). [Open Access Infrastructure](#). UNESCO Curriculum for Library Schools, Module 2. Paris: UNESCO.
- Bealt, J. (2012). [Predatory Publishers Are Corrupting Open Access](#). *Nature*, 489(7415),179-179.



## Ph.D. Course Work Common Syllabus

<b>Paper Name: Computer Application</b>	<b>Paper Code: PHD-103/CA</b>	<b>Credits: 4 (4-0-0)</b>
<b>Evaluation (Maximum Marks = 100)</b>	<b>Internal = 30</b>	<b>External = 70</b>
<b>Course Objectives</b> <ol style="list-style-type: none"><li>1. To introduce the fundamental concepts, architecture, and classifications of computers along with operating systems like Windows and Linux.</li><li>2. To develop proficiency in using Microsoft Office tools (Word, Excel, PowerPoint) for document preparation, data analysis, and presentations.</li><li>3. To familiarize students with internet usage, email communication, and basic networking concepts for effective digital connectivity and communication.</li></ol>		

<b>Unit</b>	<b>Contents</b>	<b>Lectures</b>
<b>I</b>	Definition and Characteristics of systems-Hardware & Software, Windows and Linux (Latest Version) Microsoft Tools- Definition and Characteristics of Computers: Classification of Computers; Application of Computers; Hardware; Software; Functional Units of a Computer System; Computer Architecture; Bit, Nibble and Byte. Windows: Introduction to Windows Operating System; Windows Features; Starting Windows; Parts of Windows Screen; Shortcuts in Windows; Windows Applets; Windows : My Computer; Working with files and Folders; what is MS-DOS? Booting Process; The DOS Directory Structure; Referencing Group of files; Command Syntax; Types of Commands; Microsoft Word (Latest Version): Introduction to Microsoft Tools; Starting Word; Mail Merge.	<b>15</b>
<b>II</b>	Microsoft Excel; (Latest Version) Excel Features; Entering data into a Cell; Entering Numbers; Spreadsheets Operations; Freezing Window Panes; Excel Offers Several Methods for Selecting Cells; Erasing the Content of A Cell; Formatting Cells from the Home Tab; The Format Painter; Formulas and Functions; Using Logical Functions; Date and Time Functions; Math and Trigonometric Functions; Statistical Functions; Copying Formulas; Charts; Creating a New Embedded Chart; Type of Charts; Formatting Chart Elements from the Format tab.	<b>15</b>
<b>III</b>	Microsoft PowerPoint (Latest Version) What is Presentation? Introduction to PowerPoint; Starting PowerPoint; PowerPoint Views; Save a Presentation; Exiting PowerPoint; Working with Slides.	<b>10</b>
<b>IV</b>	Introduction to Internet and E-Mail Hardware requirement; to connect to the Internet; Types of Connections; Internet Service Providers; Internet Addressing; Resource Addressing; The World Wide Web; E-Mail.	<b>10</b>
<b>V</b>	Networking Concepts What is a Networks?; Uses of Computer Networks; Network Topologies; Network Hardware and Software.	<b>10</b>

	<b>Total</b>	<b>60</b>
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## **Suggested Readings**

1. Rajaraman, V. Fundamentals of Computers. 6th ed., PHI Learning, 2018.
2. Sinha, P. K., and Priti Sinha. Computer Fundamentals. BPB Publications, 2010.
3. Balagurusamy, E. Programming in ANSI C. 8th ed., McGraw Hill Education, 2019.
4. Forouzan, Behrouz A. Data Communications and Networking. 5th ed., McGraw Hill Education, 2017.
5. Tanenbaum, Andrew S., and Herbert Bos. Modern Operating Systems. 4th ed., Pearson, 2014.
6. Stallings, William. Computer Organization and Architecture: Designing for Performance. 10th ed., Pearson, 2016.
7. Riley, David, and Kenny Hunt. Computational Thinking for the Modern Problem Solver. CRC Press, 2014.
8. Rouse, Margaret Z. Information Technology for Management. Wiley, 2020.
9. Evans, Alan, Kendall Martin, and Mary Anne Poatsy. Technology in Action: Introductory. 15th ed., Pearson, 2019.
10. NPTEL. Computer Science and Engineering, <https://nptel.ac.in/course.html>
11. GeeksforGeeks. Computer Science Portal for Geeks, <https://www.geeksforgeeks.org/>
12. Coursera. Computer Science Courses, <https://www.coursera.org/browse/computer-science>
13. TutorialsPoint. Computer Programming and IT Tutorials, <https://www.tutorialspoint.com/index.htm>
14. <https://nptel.ac.in/courses/106106092>



## Glocal School of Science

### Ph.D. Course Work Chemistry- Elective

<b>Paper Name: Advanced Organic Chemistry</b>	<b>Paper Code: PHD-104/CH (I)</b>	<b>Credits: 4 (4-0-0)</b>
<b>Evaluation (Maximum Marks = 100)</b>	<b>Internal = 30</b>	<b>External = 70</b>
<b>Course Objectives</b>		
<ol style="list-style-type: none"><li>1. To acquaints students with stereochemistry of ring system.</li><li>2. To make students understand the principles of asymmetric catalysis and retrosynthesis.</li><li>3. To understand the concept of rearrangement reactions and reagents.</li><li>4. To learn the basic principles of green chemistry.</li></ol>		

<b>Unit</b>	<b>Contents</b>	<b>Lectures</b>
<b>I</b>	Stereochemistry and Stereo-isomeric Synthesis: Stereochemistry of ring system: Stereochemistry of allenes, spiranes, biphenyls, and bridged biphenyls. Conformational analysis: Conformations and stability of cyclohexanes and some substituted cyclohexanes, cyclohexenes, cyclohexanones, decalins. Stereospecific and stereoselective synthesis (elementary examples), asymmetric synthesis based on Cram's rule. acyclic diastereoselective in cyclic systems. Enantioselective synthesis: Enantioselective hydroboration, hydrogenation, epoxidation, enantioselective synthesis via hydrazones. Role of enzymes in chiral synthesis.	<b>20</b>
<b>II</b>	Asymmetric catalysis: Organocatalysis. Iminium and enamine catalysis. N-heterocyclic carbenes (NHC). Enzyme catalysis and biocatalysis. Light mediated reactions.	<b>10</b>
<b>III</b>	Retrosynthesis: Retrosynthetic analysis of functionalised aliphatic, aromatic and simple heterocyclic compounds involving single and multiple C-C and C-X disconnections. Concept of synthons, Synthetic equivalents, FGI, Functional group interconversions of aromatic and mono and biheterocyclic compounds involving oxidation, reduction, substitution, addition, elimination and rearrangement reactions.	<b>10</b>
<b>IV</b>	Reactions and reagents: Favorskii reaction; Stork enamine reactions; Sharpless asymmetric epoxidation; Ene reaction; Barton reaction; Hofmann- Loffler-Freytag reaction; Shapiro reaction; Baeyer villager reaction; Chichibabin reaction, Newer reagents: NBS, DCC, Fermy's salt, LDA, DDQ, Wilkinson catalyst, Gillmann reagent, 1,3 dithiane.	<b>10</b>
<b>V</b>	Green Chemistry: Basic principles of green chemistry, Application of non-conventional techniques in organic synthesis (ultrasonic, microwave, and grinding). Solid-state synthesis and synthesis under solvent-free conditions. Use of ionic liquids.	<b>10</b>
	<b>Total</b>	<b>60</b>

## Suggested Readings

1. J. Clayden, N. Geeves, S. Warren, Organic Chemistry, 2nd Edition. Oxford University Press, 2012. M. B. Smith, Organic Synthesis, Academic Press, 2009.
2. I.L.Finar, Organic Chemistry. Vol.2, 6<sup>th</sup> edition, PearsonIndia, New Delhi, 2002.
3. Peter Sykes, A Guidebook to Mechanisms in Organic Chemistry, 6<sup>th</sup> edition, PearsonIndia, New Delhi, 2009.
4. E. J. Corey and X.-M. Cheng, The logic of Chemical Synthesis, Wiley, 2005.
5. P .S. Kalsi, Stereochemistry – Conformation and Mechanism, 6<sup>th</sup> edition, New Age International Ltd., India, 2005.
6. <https://www.youtube.com/watch?v=T6xDcGWOEro&list=PLkYdyF4D1TZ97faC41ctHFpF7WX4cPZF0>
7. <https://www.youtube.com/watch?v=T6xDcGWOEro&list=PLkYdyF4D1TZ97faC41ctHFpF7WX4cPZF0>
8. <https://www.youtube.com/watch?v=iaj0YISzWzU&list=PLnvaVenEZ6Q5gB6DOL0jT5IH4si7W6d0K>
9. [https://onlinecourses.swayam2.ac.in/ugc19\\_ch01/preview](https://onlinecourses.swayam2.ac.in/ugc19_ch01/preview)



## Glocal School of Science Ph.D. Course Work Chemistry- Elective

<b>Paper Name: Trends in Natural Products Chemistry</b>	<b>Paper Code: PHD-104/CH(II)</b>	<b>Credits: 4 (3-1-0)</b>
<b>Evaluation (Maximum Marks = 100)</b>	<b>Internal = 30</b>	<b>External = 70</b>
<b>Course Objectives</b> This course will deal with the classical and advanced concepts and theories of isolation and structure elucidation of biologically important pure molecules from natural products. It will be based on leading text books of the domain as well as references to current literature.		

<b>Unit</b>	<b>Contents</b>	<b>Lectures</b>
<b>I</b>	Introduction: Sources (plant, animal, microbial, marine) and classes of natural products.	<b>8</b>
<b>II</b>	Extraction Methods: Conventional and modern extraction methods including maceration, percolation, Soxhlet extraction, batch extraction, continuous extraction, counter current extraction, accelerated solvent extraction and super critical fluid extraction. Concepts of extraction with respect to activity guided fractionation.	<b>12</b>
<b>III</b>	Analytical Techniques: Introduction to high performance thin layer chromatography (HPTLC), high performance liquid chromatography (HPLC), gas chromatography (GC), chiral chromatography and reverse phase chromatography. Application of these techniques in identification of markers/biomarkers.	<b>20</b>
<b>IV</b>	Structure Elucidation and Synthesis: Structure elucidation of well-known bioactive molecules of natural origin by IR, UV, 1H, 13C, 2D-NMR and mass spectra and their synthesis.	<b>20</b>
	<b>Total</b>	<b>60</b>

### **Suggested Readings**

1. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., Spectrometric Identification of Organic Compounds, 8th Ed., Wiley India: New Delhi, 2015.
2. Patrick, G. L., An Introduction to Medicinal Chemistry. 5th Ed.; Oxford University Press, New Delhi (2013).
3. Nicolaou, K. C.; Sorensen, E. J. Classics in Total Synthesis: Targets, Strategies, Methods; Wiley-VCH: New York, 1996.
4. Mann, J.; Davidson, R. S.; Hobbs, J. B.; Banthrope, D. V.; Harborne, J. B. Natural Products, Their Chemistry and Biological Significance; Longman: Essex, 1994.
5. Lemke, T. L.; Zito, S. W.; Roche, V. F.; Williams, D. A. Essentials of Foye's Principles of Medicinal Chemistry; Wolters Kluwer India: New Delhi, 2016.
6. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Edition. Oxford University Press, 2012.  
M. B. Smith, Organic Synthesis, Academic Press, 2009.
7. I.L.Finar, Organic Chemistry. Vol.2, 6th edition, Pearson India, New Delhi, 2002.



## Glocal School of Science Ph.D. Course Work Chemistry- Elective

<b>Paper Name: Techniques in Molecular Modeling</b>	<b>Paper Code: PHD-104/CH(III)</b>	<b>Credits: 4 (3-1-0)</b>
<b>Evaluation (Maximum Marks = 100)</b>	<b>Internal = 30</b>	<b>External = 70</b>
<b>Course Objectives</b>		
1. To provide understanding of concepts in computational methods used in molecular modeling. 2. Applying quantum and classical modeling techniques for solving chemical problems. 3. Apply and analyses the molecular data using software/ tools relevant to their research areas.		

<b>Unit</b>	<b>Contents</b>	<b>Lectures</b>
<b>I</b>	Overview of modeling techniques: Quantum vs Classical viewpoint, Potential energy surfaces (PES), Born-Oppenheimer approximation, Coordinate systems (Cartesian, internal), Force fields and parameterization basics.	<b>10</b>
<b>II</b>	<b>Quantum Mechanical Methods</b> Ab initio methods: Hartree-Fock, post-HF methods (MP2, CI, CCSD), Semi-empirical methods (AM1, PM3, MNDO), Density Functional Theory (DFT) basics.	<b>10</b>
<b>III</b>	<b>Molecular mechanics:</b> principles and energy components, Common force fields (AMBER, CHARMM, OPLS, GROMOS).	<b>15</b>
<b>IV</b>	<b>Models</b> Molecular Dynamics (MD) and Monte Carlo (MC) Simulations Basics of MD: equations of motion, integrators, thermostats, Free energy calculations.	<b>10</b>
<b>V</b>	<b>Applications and Software</b> Modeling of small molecules, proteins, and materials, Docking, QSAR, and drug design applications, Introduction to Software tools: Gaussian, ORCA, GAMESS, VASP, GROMACS, NAMD, AutoDock Vina. Energy minimization, property prediction.	<b>15</b>
	<b>Total</b>	<b>60</b>

### Suggested Readings

1. Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, Gerd Folkers. Molecular Modeling: Basic Principles and Applications, 3rd Edition, 2008.
2. <https://nptel.ac.in/courses/104101095>
3. <https://www.nature.com/articles/s41598-023-40160-2>
4. <https://link.springer.com/article/10.1007/s00706-023-03076-1>



## Glocal School of Science

### Ph.D. Course Work Chemistry- Elective

<b>Paper Name: Advanced Instrumentation Techniques</b>	<b>Paper Code: PHD-104/CH(IV)</b>	<b>Credits: 4 (3-1-0)</b>
<b>Evaluation (Maximum Marks = 100)</b>	<b>Internal = 30</b>	<b>External = 70</b>
<b>Course Objectives</b>		
<ol style="list-style-type: none"><li>1. To introduce the students about the concept of microscopy</li><li>2. To give an insight into the basics of various characterization Technique</li><li>3. To learn about the different physical characterization technique to identify the characteristics of materials</li><li>4. To acquaints students with various separation techniques used for analysis.</li></ol>		

<b>Unit</b>	<b>Contents</b>	<b>Lectures</b>
<b>I</b>	Spectroscopy: Ultra-Violet Spectroscopy: Absorption of dienes, polyenes, carbonyl compounds and $\alpha,\beta$ -unsaturated carbonyl compounds. Woodward rule and its application. Aromatic compounds. Infrared Spectroscopy: Vibration modes and bond stretching. Absorption of common functional groups, electrical and steric effects, effects of Hydrogen bonding. Fingerprint region and interpretation of IR spectra. NMR Spectroscopy: Interpretation of spectra, chemical shift, shielding mechanism and anisotropic effects. Spin-spin interactions, naming spin systems, magnitude of coupling constant: geminal, vicinal and long range couplings.	<b>20</b>
<b>II</b>	Microscopy techniques: Optical microscopy, transmission electron microscopy (TEM), scanning electron microscopy (SEM).	<b>10</b>
<b>III</b>	Thermal analysis technique: Differential thermal analysis (DTA), Differential Scanning Calorimetry (DSC), Thermogravimetric analysis (TGA); Electrical characterization techniques: Electrical resistivity, Hall effect, Magnetoresistance.	<b>15</b>
<b>IV</b>	Chromatography: Classification of chromatographic techniques and their principles, Theory of chromatography, band broadening, rate and plate theory factors responsible for separation. Column chromatography, TLC, Paper chromatography. Liquid Chromatography, HPLC & Gas Chromatography: Principle, Instrumentation and applications.	<b>15</b>
	<b>Total</b>	<b>60</b>

#### **Suggested Readings**

1. Electron microscopy and Analysis: P. J. Goodhew, J. Humphreys, R. Beanland, 3rd Edition, Taylor & Francis 2001.

2. Scanning Electron Microscopy and X-Ray Microanalysis: Joseph I. Goldstein, Dale E. Newbury, Joseph R. Michael, Nicholas W.M. Ritchie, John Henry J. Scott, David C. Joy, 4th Edition, Springer 2017.
3. Transmission Electron Microscopy: A Textbook for Materials Science: David B. Williams, C. Barry Carter, Springer 2008.
4. Elements of X-ray diffraction: B.D. Cullity, Pearson Education 2014.
5. [https://onlinecourses.nptel.ac.in/noc23\\_mm26/preview](https://onlinecourses.nptel.ac.in/noc23_mm26/preview)
6. <https://nptel.ac.in/courses/113107081>