



SHARDA
UNIVERSITY
Beyond Boundaries



**SHARDA SCHOOL OF
BASIC SCIENCES
& RESEARCH**

Department of Chemistry and Biochemistry



COURSE

**Software in
Chemistry**
(VAS303)

**VALUE ADDED
COURSE BROCHURE
2024-25**

SHARDA UNIVERSITY

Sharda University envisions to serve the society by being a global University of higher learning in pursuit of academic excellence, innovation and nurturing entrepreneurship. It has 13,000+ students from 95+ countries, 29 states, and Union Territories, providing cultural diversity and global exposure to students. It has 26000+ alumni who are today leaders in their realms. Sharda University is NAAC A+ University with Overall NIRF Rank of 87. Teaching Learning Center at Sharda University is to equip the faculty members with the expertise, skills and knowledge they need for capacity building of students. Teaching as a profession requires highly specialized skills and knowledge to impact significantly on student learning and therefore teachers must refine their conceptual and pedagogical skills.

ABOUT THE SCHOOL

Sharda School of Basic Sciences and Research (SSBSR) boasts of providing an interdisciplinary approach, exposure to different disciplines in science including Chemistry, Bio-Chemistry, Physics, Mathematics, Life Sciences, and Environmental Sciences. The Sharda School of Basic Sciences and Research is unique from other institutions of higher learning as it is committed to imparting knowledge in pure and applied sciences, which not only forms the foundation for further academic pursuits in science and technology but also acts as the foundation for students to pursue a career in multi facet directions. The academic programs are designed to meet the requirement of the latest technological developments and envisages to become a state-of-the-art department that cater the students at Graduate, Post- Graduate and Research level along with providing high- quality education and cutting-edge interdisciplinary research in sciences. SSBSR has well-equipped laboratories for Physics, MATLAB, Microbiology, Molecular Biology, Cell Culture, Virology, Biochemistry, Physical, Organic and Inorganic chemistry for Graduate and Post-Graduate Programs. In addition, there are Central Instrumentation Facility (CIF) and other advance research labs to promote research culture.

DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY

The Department of Chemistry & Biochemistry endeavors to be nationally recognized model for nurturing students who can contribute to the ever changing technology of 21st century. The Department is committed to provide an excellent teaching & learning atmosphere for Undergraduate as well as post graduate students.

Dr. Ashish Kumar Chalana

Dr. Ashish Kumar Chalana obtained his integrated BS-MS degree (2009-2014) from IISERTVM, Kerala, India. He held an inspire scholarship for his BS-MS degree. He did his PhD degree (2014-2019) from Shiv Nadar University, Greater Noida, U.P. on the topic of detoxification of heavy metals (Cu, Hg) using chalcogen based small molecules and nanomaterials under the supervision of Dr. Gouriprasanna Roy, Shiv Nadar University (SNU), U.P., India. He has published 9 research articles (Scopus/SCI index) in international journals (ACS, RSC, and Wiley etc.), one international patent, and one book chapter during his PhD tenure. He did his postdoctoral fellowship (2020-2021) from IIT Delhi under the supervision of Prof. Jayashree Bijwe Professor, CART IIT Delhi, India on the topic of development of novel adhesives and composites based on epoxy and nanoparticles. He has cleared national exams UGC-NET, IIT-JEE. His research interest includes synthesis of novel small molecules, nanoparticles which has application towards heavy metal detoxification, detection of various metal ions, antioxidant activities, developments of various adhesives and composites etc.

Schedule

Week 1	15 July - 21 July	2 lectures
Week 2	22 July - 28 July	2 lectures
Week 3	29 July - 04 August	2 lectures
Week 4	05 August - 11 August	2 lectures
Week 5	12 August - 18 August	2 lectures
Week 6	19 August - 25 August	2 lectures
Week 7	26 August - 01 September	2 lectures
Week 8	02 September - 08 September	2 lectures
Week 9	09 September - 15 September	2 lectures
Week 10	16 September - 22 September	2 lectures
Week 11	30 September - 06 October	2 lectures
Week 12	07 October - 13 October	2 lectures
Week 13	14 October - 20 October	2 lectures
Week 14	21 October - 27 October	2 lectures
Week 15	28 October - 03 November	2 lectures
Week 16	04 November - 10 November	2 lectures
Week 17	11 November - 17 November	2 lectures
Week 18	18 November - 24 November	2 lectures

MODULE

School: SSBSR		Batch : 2024-27
Program: B.Sc.		Current Academic Year: 2024-25
Branch: Chemistry/Biochemistry		Semester: Odd (Sem III)
1. Course Code	VAS303	
2. Course Title	Software in Chemistry	
3. Credits	0	
4. LTPC	2-0-0-0	
Course Type	Value added course	
5. Course Objective	<p>Students will gain knowledge and skills on the various important software tools used in chemistry. They will learn how to plot a graph in Microsoft Excel, origin, draw, and visualize the chemical structure in ChemDraw, origin, CCDC, etc. Students will also develop presentation skills in this course.</p> <p>Students will know of:</p> <ul style="list-style-type: none"> • Drawing the graph in Microsoft Excel, Origin • Drawing and visualizing the chemical structure in ChemDraw, origin, CCDC • Students will also develop presentation skills in this course. 	
6. Course Outcomes	<p>CO1: The student will be able to understand the basis of Microsoft Excel and the tool used in the plotting of graphs and calculations.</p> <p>CO2: The student will be able to learn how to draw structures in chem draw and chem craft.</p> <p>CO3: The student will be able to learn the basis of origin and plotting of graph in origin</p> <p>CO4: The student will be able to learn how to visualize and draw any chemical structure using CCDC and mercury</p> <p>CO5: The student will be able to gain knowledge of the importance of citation in a research article</p> <p>CO6: The student will be able to gain knowledge of the important software used in chemistry</p>	
7. Course Description	This course introduces the most frequent and important software and tools in chemistry for making and analyzing the structure and basics of Microsoft Excel, and PowerPoint. Students will be capable of utilizing this software knowledge during their research and higher studies.	
8. Outline syllabus		CO Mapping
Unit 1	Introduction to Microsoft Excel	
A	Download Microsoft Office 365, and Excel Program and view the basics of Excel, and Excel spreadsheets for data entry, and create simple formulas in an Excel spreadsheet to analyze data.	CO1/CO6
B	Introduction to Excel Charting, Chart and Graph Editing, Formatting Chart elements, Handling Graph in Chart	CO1/CO6
C	Application of Excel in chemistry with a few examples	CO1/CO6
Unit 2	ChemDraw and ChemSketch	
A	Introduction of ChemDraw, chemical name to structure conversion, chemical structure to name conversion	CO2/CO6
B	NMR spectrum simulation, structure clean up, 3D chemical structure.	CO2/CO6
C	Introduction to ChemSketch, creating and modifying images of chemical structures, writing and performing chemical equations and diagrams.	CO2/CO6
Unit 3	Originlab: Origin and OriginPro Masterclass	
A	Downloading and installing the origin software, Learning the basic interface of Origin & OriginPro.	CO3/CO6
B	Scatter plot, Line plot, customizing graphs to presentation quality levels, How to plot columns, bar, and stacked plots.	CO3/CO6
C	Functional plots Statistics like cross-tabulation, chi-square analysis, etc. Mathematics on Data Linear and non-linear fitting with built-in models	CO3/CO6
Unit 4	Software to Visualize the Structure	
A	Mercury 4.0: from visualization to analysis, design, and prediction, Three-dimensional visualization of X-ray crystal structure.	CO4/CO6
B	ORTEP: Three-dimensional visualization of the X-ray crystal structure of organic and inorganic compounds	CO4/CO6
C	CSD(CCDC): Deposition method of Three-dimensional of X-ray crystal structure of organic and inorganic compounds	CO4/CO6
Unit 5	Software to Manage references/citation	
A	Introduction to Reference/citation	CO5/CO6
B	Various methods and formats of Reference/citation in a research article	CO5/CO6
C	Mendeley: Managing references and citations.	CO5/CO6
Mode of examination	Assignments, Quizzes & Viva	