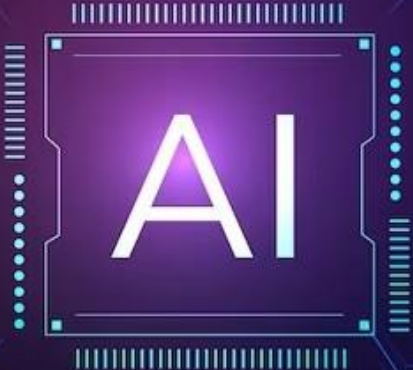




SHARDA
UNIVERSITY
Beyond Boundaries



SHARDA SCHOOL OF ENGINEERING & SCIENCE

A graphic of a computer chip with the letters 'AI' in the center, surrounded by circuit lines and dots.

COURSE **Fundamentals of** **Computer Applications** **in Chemistry**

VALUE ADDED COURSE
BROCHURE
2026-27

ABOUT THE UNIVERSITY

Sharda University is a private university located in Knowledge Park III, Greater Noida, Uttar Pradesh, India. The school is part of the Sharda Group of Institutions, which was founded by P. K. Gupta in 1996. The group has campuses in Agra, Mathura, and Greater Noida. The university takes pride in providing multidisciplinary education options to our international students by providing them a platform where knowledge meets achievement; history meets future and ambitions meet inspiration. Every year we welcome students from more than 95+ countries to our Greater Noida campus. Sharda University is not just a university but a community that values cultural diversity, and respect for religion, age, gender, and socio-economic status. The university continuously upgrades its academic offerings and services to meet the evolving demands of the global work force and ensure that the industry standards are met. All the programs offered by the university undergo constant review by accrediting bodies and are enhanced by the valuable insights from industrial partnerships and memberships with local and global organisations.

SHARDA SCHOOL OF ENGINEERING & SCIENCE

Sharda School of Engineering & Science acts as a platform where the intellectual and creative attributes of future scientists are developed and enhanced. The school emphasizes upon overall development of students so as to enable them to become effective leaders of tomorrow.

DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY

The Department of Chemistry & Biochemistry endeavors to be a nationally recognized model for nurturing students who can contribute to the everchanging technology of 21st century. The Department is committed to provide an excellent teaching & learning atmosphere for undergraduate as well as postgraduate students.

PROFILES

Resource Person: Dr. Priya Das

Dr. Priya Das is currently serving as an Assistant Professor in the Department of Chemistry & Biochemistry at Sharda University. She obtained her Bachelor's degree from Presidency University, Kolkata and completed her master's degree at IIT Guwahati with a specialization in physical chemistry. She pursued her doctoral studies at IIT Guwahati in the fascinating field of materials science. Throughout her doctoral journey, she accomplished a significant achievement in angular stacking of two-dimensional crystalline nanosheets. Her research focuses on the synthesis & characterization of novel materials. Her work aims to contribute to the development of advanced materials with diverse applications in various fields.



Fundamentals of Computer Applications in Chemistry

School	Sharda School of Engineering & Science (SSES)	
Department	Chemistry & Biochemistry	
Programme Code	SBR0102 & SBR0103	
Programme Name	Bachelor of Science (Chemistry/Biochemistry)	
Batch: 2025-2029	Semester: III	
Course Code	NV33121	
Course Name	Fundamentals of Computer Applications in Chemistry	
Credits	-	
Contact Hours (L-T-P)	30 hours	
Course Type	Value-added course	
Course Objective	1. To introduce students to basic computer tools and software used in chemistry. 2. To develop skills in data handling, graph plotting, and analysis using digital tools. 3. To enable students to draw and visualize chemical structures using appropriate software. 4. To enhance students' ability to prepare scientific reports and presentations. 1. To provide foundational knowledge of ICT tools for applications in chemistry and research.	
Course Outcomes	CO1: Describe basic Microsoft tools (Word, Excel, PowerPoint) and chemical software used in chemistry. CO2: Explain methods for chemical structure drawing, data visualization, and molecular visualization using appropriate software. CO3: Apply software tools to draw chemical structures, plot graphs, and visualize molecules in 3D. CO4: Analyze graphical data, molecular geometry, and experimental results for better interpretation. CO5: Evaluate scientific reports and presentations with respect to accuracy, formatting, and academic integrity (plagiarism and referencing). CO6: Design well-structured reports and presentations using digital tools and proper referencing techniques.	
Course Description	This course introduces undergraduate students to basic computer applications and digital tools used in chemistry. It focuses on developing essential skills in data handling, graph plotting, and chemical structure drawing using software such as Microsoft Excel, ChemDraw, and Avogadro. Students will also learn to visualize molecular structures, prepare scientific reports, and create effective presentations using Microsoft Word and Microsoft PowerPoint. Additionally, the course provides a basic introduction to reference management using Mendeley.	
Outline syllabus		CO mapping
Unit 1	Microsoft Tools in Chemistry	
A	Introduction and Basics of Word	CO1, CO6
B	Introduction and Basics of Excel	CO1, CO6
C	Introduction and Basics of Microsoft PowerPoint	CO1, CO6
Unit 2	Chemical Structure Drawing	
A	Introduction to ChemDraw/ChemSketch, Understanding the interface and toolbars, File creation, saving, and export options	CO2, CO6

B	Drawing basic organic molecules (alkanes, alkenes, alkynes), drawing functional groups (alcohols, acids, amines, etc.), Converting IUPAC names into structures, drawing simple chemical reactions (e.g., esterification, substitution), Clean-up structure tool, adjusting bond lengths and angles, Alignment and formatting of structures, adding charges, lone pairs, and radicals, Inserting text, labels, and reaction conditions	CO2, CO6
C	Practical Assignments: Draw at least 10 organic molecules (alkanes, alcohols, acids), convert given names into structures, and draw a simple reaction mechanism (e.g., esterification)	CO2, CO6
Unit 3	Data and Molecular Visualization	
A	Introduction to Origin (basic use), Plotting and formatting graphs, Basic linear fitting	CO3, CO4, CO6
B	Introduction to Avogadro/Mercury, 3D structure visualization: Bond angles and geometry	CO3, CO4, CO6
C	Practical Assignments: Plot a scatter graph and apply linear fitting; compare two datasets using graphs; export a graph for report use; and visualize 5 molecules in 3D. Measure bond angles and bond lengths, identify geometry (tetrahedral, trigonal planar, etc.)	CO3, CO4, CO6
Unit 4	Plagiarism & Writing Tools	
A	Basics of scientific writing and report structure, Components of a lab report (Title, Abstract, Introduction, Methodology, Results, Conclusion), Common errors in scientific writing, Importance of clarity, accuracy, and proper formatting	CO4, CO6
B	Meaning and types of plagiarism (copying, paraphrasing, self-plagiarism), Importance of academic integrity, Introduction to plagiarism detection tools like Turnitin, Basics of citation and referencing styles (APA, MLA), Introduction to Mendeley for managing references	CO4, CO6
C	Use of Microsoft Word for report writing (formatting, tables, figures), preparing presentations using Microsoft PowerPoint, Introduction to writing improvement tools like Grammarly, exporting documents, and maintaining proper file formats	CO4, CO6
Unit 5	Scientific Documentation & Presentation	
A	Preparation of a formatted lab report using Microsoft Word, structuring the report (Title, Introduction, Methodology, Results, Conclusion), formatting text, inserting tables, figures, and graphs	CO1, CO2, CO3, CO4, CO5, CO6
B	Creation of a 5–7 slide presentation using Microsoft PowerPoint, Presentation of chemical data using charts, images, and diagrams, and organizing content for clear and effective communication	CO1, CO2, CO3, CO4, CO5, CO6
C	Adding references in the lab report using Mendeley using basic citation styles (APA/MLA), preparing bibliography and maintaining proper referencing format	CO1, CO2, CO3, CO4, CO5, CO6
Mode of Examination	Assignments, Quizzes & Viva	
Text book/s*	1. Eklas Hossain , <i>Excel Crash Course for Engineers</i> , Springer (Basic Excel concepts and applications) 2. Zhenjiang Li et al. , <i>Review of Chemical Drawing Software: ChemDraw, ChemWindow, ISIS/Draw, ChemSketch</i> , Journal of Chemical Information and Computer Sciences Clare F. Macrae et al. , <i>Mercury 4.0: From Visualization to Analysis</i> , Journal of Applied Crystallography (basic visualization concepts)	
Other References	1. Curtis D. Frye , <i>Microsoft Excel Step by Step</i> , Microsoft Press (Comprehensive guide for Excel basics and data handling) Andrew R. Leach , <i>Molecular Modelling: Principles and Applications</i> , Pearson (Introductory concepts of molecular visualization and modeling)	

Schedule NV33121

Week 1	15 July to 21 July 2026	2 lectures
Week 2	22 July to 28 July 2026	2 lectures
Week 3	29 July to 4 August 2026	2 lectures
Week 4	5 August to 11 August 2026	2 lectures
Week 5	12 August to 18 August 2026	2 lectures
Week 6	19 August to 25 February 2026	2 lectures
Week 7	26 August to 1 September 2026	2 lectures
Week 8	2 September to 8 September 2026	2 lectures
Week 9	9 September to 15 September 2026	2 lectures
Week 10	16 September to 22 September 2026	2 lectures
Week 11	23 September to 29 September 2026	2 lectures
Week 12	30 September to 6 October 2026	2 lectures
Week 13	7 October to 13 October 2026	1 lecture
Week 14	14 October to 20 October 2026	1 lecture
Week 15	21 October to 27 October 2026	2 lectures
Week 16	28 October to 3 November 2026	2 lectures
Week 17	4 November to 11 November 2026	2 lectures