St. Xavier's College (Autonomous), Ahmedabad

Syllabus of Semester – III of the following departments under Faculty of Science based on Under Graduate Curriculum Framework - 2023 to be implemented from the Academic Year 2025-26.

FACULTY OF SCIENCE

DEPARTMENT OF CHEMISTRY

BSc. (Hons.) Chemistry
Category – III

Skill Enhancement Course: Computer for Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course Title & Code	Credit Distribution of The Course			Eligibility Criteria	Prequisite(s) of the Course (if any)
	Lecture	Tutorial	Practical / Practice		
Computer for Chemistry CHSE331C	1	0	2	10 + 2 from a recognized board in any stream	Basics Computer practices for Chemistry

LEARNING OBJECTIVES (LO)	
LO-1	To provide basic understanding and demonstrate the use of Excel, Using software for data analysis and visualization (e.g., Excel, Origin, GraphPad), Performing statistical analysis of chemical data, creating graphs and charts to present chemical data.
LO-2	To apply their understanding of Excel to solve problems in analytical chemistry, Students will learn about error analysis and its application in chemical calculations and experiments.
COURSE OUTCOMES (CO)	
On Completion of this course, the student will be able to	
CO-1	Basics in Computer for Chemistry" aims to equip students with fundamental computer skills learn to use common software applications like Microsoft Office (Word, PowerPoint, Excel) for tasks like report writing, data analysis, and presentations. and knowledge relevant to chemistry, enabling them to use

	computers for tasks like data analysis, simulations, and research.
CO-2	Students will understand the use of image creating software for fine tuning their scientific presentation or write up
CO-3	Students will learn how to analyze and visualize data, drawing structures, chemical reactions, nomenclature of compounds using software tools.

Unit-1	(15L)
A	Introduction to Microsoft word, Excel and PowerPoint. i Microsoft Office Word Create a file with at least 2-3 pages having Text, Image ii Excel - creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs and Links. iii Create Microsoft Power Point Presentation file with at least 8-10 slides having Text, Image, Graph, Video and Link, Google slides.
B	Introduction to Paint/Paint 3D/ any image-creating software i Prepare JPG, JPEG, PNG and Tiff image (two images each). Ii Simulation of pH metric titration curves, Potentiometric titration curve Excel functions LINEST and Least Squares. Numerical curve fitting, linear regression (rate constants from concentration time data, molar extinction coefficients from absorbance data), Graphical solution of equations.
Unit-2	(15L)
	Introduction to Chemistry software. Draw a chemical structure and predict the properties of organic/inorganic compounds/reaction

Suggestive Reading:

1. Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5
2. F. James Holler, Stanley R. Crouch Applications of Microsoft Excel in Analytical Chemistry Cengage Learning (2013)
3. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001) 487 pages.
4. Noggle, J. H. Physical chemistry on a Microcomputer. Little Brown & Co. (1985