Course Title: Chemistry Elective: Computer Applications in Chemistry *w.e.f. the session 2022-23 and onwards*	
Class: M.Sc. Pt.-I / Semester-I	**Course code: MCH-E104**
Lectures: 60	Credits : 04
MM: 70	Exam Hours: 03

NOTE: The question paper shall consist of Two sections (Sec.-A and Sec.-B). Sec.-A shall contain 10 short answer (about 150 words) type questions of SIX marks each and student shall be required to attempt any five questions. Sec.-B shall contain 08 descriptive type questions of TEN marks each and student shall be required to attempt any four questions. Both sections shall have questions from the entire syllabus. The previous year paper/model paper can be used as a guideline and the following syllabus should be strictly followed while setting the question paper.

COURSE CONTENTS:

Unit - I

Introduction to Computers: Block diagram of computers; Input and output devices-key board, mouse, scanner, VDU, plotter, Types of printers; Primary & secondary memory - RAM, ROM, Secondary Memory devices-Hard Disk, CD, Flash Drive and Memory card; Volatile and non-volatile memory; CPU - ALU and control unit; Hardware & software, Software - system software and application software.

Unit – II

Programming Languages, Number System and Operating System: Introduction to Algorithms and Flow charts, Programming languages - Machine, Assembly and high level language. Number System: Bits and Bytes, Decimal, binary and octal number system and their arithmetic. Operating system and its functions: Microsoft windows. Applications of Microsoft Office, Google classroom and Google meet.

Unit - III

C Programming: Introduction; Style of C language; Character set; keywords, data types, variables and constants in C; Operators-Arithmetic, Relational, Logical, Bitwise, Ternary, Cast and Sizeof operators in C; Input and output statements in C language; Control and conditional statement in C; break and continue statement in loop. Storage classes in C; Functions (built in and user defined): Introduction to arrays.

Unit - IV

Computer applications in Physical and Analytical Chemistry: Listing the C- program for the following: Determination of rate constant of first order reactions, determination of rate constant for second order reactions, study of rate constant with variation of ionic strength, obtaining the heat of reaction using Hess's law of constant heat summation, obtaining the heat of reaction at different temperatures using Kirchoff's equation. Determination of Normality, Molarity and Molality of solutions, Determination of concentration using Beer- Lambert's law.

Unit - V

Computer applications in Inorganic and Organic Chemistry:

Listing the C-program for the following: Determination of electronegativity of an atom from bond energy data using Pauling relation, determination of half life and average life of a radioactive nucleus. Determination of empirical formula of hydrocarbons and other organic compounds, Determination of molecular weights of organic compounds, Determination of molecular weights of organic compounds by Cryoscopic and ebullioscopic method. Determination of isoelectric point of amino acids.

Chemdraw software and its applications.

Suggested Readings:

1. Fundamentals of computer by V. Rajaraman
2. Programming in C (Schaum series outline) by Gotterfried.
3. "Computers in Chemistry" by K.V. Raman
4 Computer fundamentals and programming in C by Reema Thareja (2nd Edition)

COURSE OBJECTIVE:

The present course shall enable the students to gain knowledge about:

1. The computers, number system, operating systems.
2. The programming languages especially C-Language
3. The applications of computers in chemistry.
4. Working/operation of modern software based instruments.

COURSE OUTCOMES:

On completion of this course, student shall be able to:
CO 1: Understand the fundamentals and working of computer system.
CO 2: Enable to develop the simple programming in 'C' language.
CO 3: Apply the programming of 'C 'language in Physical, organic, inorganic and analytical Chemistry.
CO 4: Knowledge of software systems and application in software based modern instruments.
Mapping of Course outcomes (Cos) with Programme outcomes (POs)

Course outcomes/ Programme outcomes	1	2	3	4	5	6	7	8
CO 1				X				X
CO 2				X			X	X
CO 3				X			X	X
CO 4		X	X	X				X