

FACULTY OF COMPUTER SCIENCE & IT

SYLLABUS

of

COMPUTER FOR CHEMISTS

for

Master of Science (Chemistry) Semester-I

Under Credit Based Continuous Evaluation Grading System

(CBCEGS)

Session: 2026-27



The Heritage Institution
KANYA MAHA VIDYALAYA
JALANDHAR
(Autonomous)

Kanya Maha Vidyalaya, Jalandhar (Autonomous)

CURRICULUM AND SCHEME OF EXAMINATIONS OF TWO YEAR MASTER DEGREE PROGRAMME

Master of Science (Chemistry)

Session 2026-27

Master of Science (Chemistry) Semester I

Course Code	Course Title	Course Type	Hours per week	Credit		Marks				Examination Time (in Hours)
			L-T-P	L-T-P	Total	Total	Ext.		CA	
							L	P		
MCHM-1135	Computer for Chemists	C	2-0-2	2-0-1	3	100	40	30	30	3+3

Master of Science (Chemistry) Semester - I
Session 2026-27

COMPUTER FOR CHEMISTS
COURSE CODE: MCHM – 1135

COURSE OUTCOME

After passing this course the student will be able to:

CO1: Comprehend various programming constructs like variables, data-types, operators, etc of C programming language.

CO2: Apply various control statements of C Programming Language for designing solutions to different real-world problems.

CO3: Comprehend signature, declaration, definition and calling of functions in C for modularization of problem.

CO4: Implement single and multidimensional arrays for representing complex data collections and Role of AI in the field of Chemistry.

Master of Science (Chemistry) Semester - I
Session 2026-27

COMPUTER FOR CHEMISTS
COURSE CODE: MCHM - 1135

Examination Time: (3+3) Hours

L-T-P: 2-0-1

Credits: 3

Max. Marks: 100

Theory: 40

Practical: 30

CA: 30

Instructions for Paper Setter -

Eight questions of equal marks (08 marks each) are to set, two in each of the four sections (A-D). Questions of Sections A-D should be set from Units I-IV of the syllabus respectively. Questions may be divided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any section.

UNIT-I

Introduction to programming, algorithms and flowcharts.

Elementary programming, a typical C program, print function.

Introduction of declarations, assignments and variables: concept of an integer, concept of a variable, rules for naming variables, Data Types, assignment statement, arithmetic operators.

Integer arithmetic expressions, relative priority of arithmetic operators, use of parenthesis, modulus operator.

UNIT-II

Input/Output Functions, Decision making in C, relational operators, logical operators, if statement, if else statement, nesting of if statement.

The while loop, do while loop, for loop, nested for loop.

UNIT-III

Type char and ASCII code, character strings and how to print them, octal and hexadecimal notation.

User defined functions, returning value from a function, functions with more than one parameters.

UNIT-IV

Arrays, declaring an array, initializing an array, break statement, strings and character arrays, sorting an array, finding maximum and minimum in an array, multidimensional arrays. Input and output.

Introduction to AI and its role in the field of Chemistry, Role of AI in drug discovery, Ethical AI and Future Trends

References / Textbooks:

1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill, 1993.
2. Henry Mullish, Herbert L. Cooper, The Spirit of C: An Introduction to Modern Programming, Jaico Publications, 1987.
3. Anshuman Sharma, Learn Programming in C, Lakhanpal Publishers, 7th Edition.
4. E Balagurusamy, Programming in ANSI C, Tata McGraw-Hill, 2002.
5. Yashvant Kanetkar, Let Us C, BPB Publications, 2016.
6. Byron Gottfried, Schaum's Outline Programming with C, McGraw Hill, 1996.

Note: The latest editions of the books should be followed.