

**Interdisciplinary Course
Python for Chemistry**

**Semester: II
25MAII03**

**Hours of Instructions/Week : 4
No. of Credits : 4**

Course Objectives:

1. To understand the fundamentals of Python.
2. To Apply Python programming skills to chemical applications
3. To Demonstrate an appreciation for the role of Python in computational chemistry

Unit I: Python Fundamentals: Understanding Data Types and Data Structures -12 Hrs

Introduction - Python Versions - Python Integrated Development Environments-Applications- Software Installation - Jupyter Notebook - How to work in Anaconda Navigator and Jupyter? - How to upload an external file? - Introduction to Data Types - Introduction to Data Structures.

Unit II: Python Control Flow: Conditional Statements, Loops, and Functions -14 Hrs

Control Statements – Looping Statements – Loop Control Statements – Introduction to Python Function - Built-in Functions – String Functions – List Functions – Tuple Functions-Set Functions – Dictionary Functions-User-defined Functions – Docstring - Python Function Arguments –The return Statement – Scope and Life time of Variables – The Anonymous Function - The Recursion Function.

Unit III: Object-Oriented File Management in Python -12 Hrs

Classes and Objects- Class Attributes - Methods - Class Naming Convention - Object Properties -Introduction to Python Operator-Arithmetic Operators-Comparison Operator-Logical Operator - Identity Operator - Membership Operator - Bitwise Operator - Assignment Operator .

Unit IV : Data Handling and Visualization in Python -12 Hrs

Python File Handling - File Operations - File Directory - File Exception –Exception Handling- User-defined Exception - File Methods – NumPy - Pandas library - Seaborn and Matplotlib – Introduction to Python Package for Chemistry - General Chemistry –Simulations - Molecular Descriptor - Molecular Visualization.

Unit V : Case Studies -10 Hrs

Molecular Similarity Search - Predicting Hydrogen - bond Basicity using Machine Learning - Student Information Management System - Library Book Rental System - Sales Data Analysis and Visualization - Employee Record Management System.

Total Hours:60

ReferenceBooks:

1. Python for Chemistry - with simple exercises
2. Python for Chemists, Christian Hill , (2023).
3. Python for Chemistry: An Introduction to Python Algorithms, Simulations, and Programming for Chemistry, Dr. M. Kanagasabapathy.(2023).
4. Python for Quantum Chemistry: A Full Stack Programming Guide, QimingSun(2025).

E-Learning Resources:

1. <https://pubs.acs.org/doi/book/10.1021/acsinfocus.7e5030>
2. https://pythoninchemistry.org/intro_python_chemists/intro.html

Course Outcomes:

- CO1: Develop Proficiency in Python Programming for Chemical Applications.
- CO2: Apply Data Handling and Preprocessing Techniques to Chemical Data.
- CO3: Utilize Python for Chemical Data Analysis and Visualization.
- CO4: Implement Text Mining Techniques for Chemical Literature.
- CO5: Develop and Apply Machine Learning Models to Chemical Datasets.