Semester	**2**
Course	**MULTIDISCIPLINARY**
Paper Code	M1CH250211P
Paper Title	Organic Chemistry 4
No. of Credits	3
Theory / Practical / Composite	Practical
Minimum No. of preparatory hours per week a student has to devote	3
Number of Modules	03
Syllabus	**Module I: Programming Fundamentals (12 Lectures)** 1. Python Basics: •Variables and data types (integers, floats, strings, lists, dictionaries, etc.). •Input and output (e.g., reading and writing files). •Control flow: loops (for, while) and conditional statements (if, elif, else). •Functions and modular programming. 2. Introduction to Jupyter Notebooks: •Setting up and running Jupyter Notebooks. •Markdown for documentation. •Writing and executing Python code interactively. 3. Python Libraries: •NumPy: Arrays, basic mathematical operations, and array manipulation. •Pandas: DataFrames, importing/exporting data, and basic data analysis. •Matplotlib: Creating 2D plots, customizing graphs, and visualizing chemical data. **Module II: Mathematics for Machine Learning (12 Lectures)** 1. Linear Algebra: •Vectors and vector operations. •Matrices, matrix operations, and their properties. •Eigenvalues, eigenvectors, and matrix diagonalization. •Singular value decomposition (SVD) and its applications in dimensionality reduction. 2. Calculus:

	•Differentiation: Derivatives, partial derivatives, and gradients. •Chain rule and backpropagation in neural networks. •Optimization techniques: Gradient descent and its variants. •Taylor series expansion and its role in approximations. 3. Probability and Statistics: •Random variables and probability distributions. •Expected value, variance, and standard deviation. •Bayes' theorem and its applications. •Hypothesis testing and confidence intervals. **Module III: Introduction to Machine Learning and Artificial Intelligence (12 Lectures)** 1. Supervised Learning: • Regression: Linear regression, polynomial regression. • Classification: Logistic regression, decision trees, and support vector machines (SVMs). • Metrics: Mean squared error, accuracy, precision, recall, and F1-score. 2. Unsupervised Learning: • Clustering: K-means clustering, hierarchical clustering. • Dimensionality reduction: Principal component analysis (PCA), t-SNE. 3. Introduction to Neural Networks: • Basics of perceptrons and multi-layer perceptrons (MLPs). • Activation functions: Sigmoid, ReLU, and softmax. • Forward propagation and loss functions.
Learning Outcomes	1) Write Python scripts to solve simple problems. 2) Create a basic data analysis pipeline using Pandas. 3) Plot chemical property trends using Matplotlib. 4) Document code and results using Jupyter Notebooks. 5) Solve linear algebra problems related to data representation and transformations. 6) Compute gradients and optimize simple machine learning cost functions. 7) Analyze datasets using statistical measures and apply probabilistic reasoning to model predictions 8) Implement and evaluate a linear regression model on a dataset. 9) Apply clustering algorithms to chemical datasets (e.g., grouping molecules based on properties). 10) Build a simple neural network using Python libraries such as TensorFlow or PyTorch.

Reading/Reference Lists	Books: 1) Python Crash Course: A Hands-On, Project-Based Introduction to Programming by Eric Matthes. 2) Automate the Boring Stuff with Python by Al Sweigart. 3) Mathematics for Machine Learning by Marc Deisenroth, A. Aldo Faisal, and Cheng Soon Ong. 4) Linear Algebra and Its Applications by Gilbert Strang. 5) All of Statistics: A Concise Course in Statistical Inference by Larry Wasserman. 6) Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow by Aur´elien G´eron. 7) Pattern Recognition and Machine Learning by Christopher M. Bishop. Online Resources: 1) https://www.learnpython.org/ (Free, interactive Python tutorials). 2) https://realpython.com/ (Comprehensive Python tutorials). 3) https://www.khanacademy.org/math/linear-algebra (Linear algebra tutorials). 4) https://www.probabilitycourse.com/ (Comprehensive probability and statistics guide). 5) https://www.coursera.org/learn/mathematics-for-machine-learning (Coursera course on Mathematics for Machine Learning). 6) https://scikit-learn.org/ (Documentation and tutorials for Scikit-learn). 7) https://www.coursera.org/learn/machine-learning (Andrew Ng's Machine Learning course). 8) https://www.tensorflow.org/tutorials (TensorFlow tutorials for beginners).
Evaluation	Practical: 50 Internal: 50 (CA: 45; Other form of Assessment: 2; Attendance: 3)