

Course Code	Course Name	Credits
26CH611	INTRODUCTION TO AI AND ITS ROLE IN CHEMISTRY	04

Course Objectives

- To introduce the fundamental concepts and techniques of Artificial Intelligence and Machine Learning relevant to chemical sciences, understanding of data handling, preprocessing, and analysis of chemical datasets using AI tools.
- To explore the application of AI in drug discovery, materials science, and analytical chemistry, encourages critical thinking regarding ethical, practical, and technological challenges in applying AI to chemistry.

Learning Outcomes

Upon successful completion of this course it is intended that a student will be able to:

- Explain the basic principles of Artificial Intelligence, Machine Learning, and their relevance in chemistry.
- Process, analyze, and visualize chemical datasets using appropriate AI techniques.
- Develop and implement ML models for classification, regression, and clustering of chemical data using tools,
- To predict physicochemical and biological properties of molecules,
- Demonstrate the use of AI tools in drug discovery and materials development using.
- Understand and discuss ethical issues, limitations, and future prospects of AI in chemical sciences

Unit 1 - Fundamentals of Artificial Intelligence (12 Hrs.)

Definition of Artificial Intelligence; History and Scope of AI; Types of AI (Narrow AI vs General AI); Subfields of AI (Machine Learning, Deep Learning, Natural Language Processing); Overview of Algorithms (Supervised Learning, Unsupervised Learning, Reinforcement Learning)

Unit 2 – Machine Learning Techniques for Chemical Data (12 Hrs.)

Data Preprocessing (Normalization, Feature Selection, Dimensionality Reduction); Regression Methods (Linear, Polynomial, Multivariate); Classification Methods (Decision Trees, Support Vector Machines, k-NN); Clustering Methods (k-Means, Hierarchical Clustering); Model Validation and Performance Metrics; Handling Chemical Datasets (Spectral, Chromatographic, Molecular Data)

Unit 3 - AI in Chemical Structure and Property Prediction (12 Hrs.)

Molecular Descriptors and Fingerprints; QSAR and QSPR; Predictive Modeling of Physicochemical Properties; AI in Spectroscopy Analysis (IR, NMR, UV–Vis)

Unit 4 – AI Applications in Drug Discovery and Materials Science (12 Hrs.)

Role of AI in Drug Design and Discovery; Virtual Screening and Molecular Docking; De Novo Drug Design using AI; Case Studies in Pharmaceutical Chemistry; AI in Materials Discovery (Nanomaterials, Polymers, Catalysts)

Unit 5 - Advanced Topics and Emerging Trends (12 Hrs.)

Deep Learning Architectures (Neural Networks, CNNs, RNNs); AI in Green Chemistry and Sustainability; Ethical Considerations and Limitations of AI in Chemistry.

Reference Books:

- Russell, S. & Norvig, P. – Artificial Intelligence: A Modern Approach
- Goodfellow, I., Bengio, Y., Courville, A. – Deep Learning
- Todeschini, R. & Consonni, V. – Molecular Descriptors for Chemoinformatics
- Leach, A. R. – Molecular Modelling: Principles and Applications
- Brown, N. – Chemoinformatics: Concepts, Methods, and Tools

Websites and eLearning Sources:

- <https://nptel.ac.in/courses/106105077>
- https://www.youtube.com/watch?v=oyPIi1dpzHE&list=PLu7-Sp50sShfLBxemFQQ_o8wTrpQ_9VzB

COs and Bloom's Taxonomy Mapping – 26CH611

Course Outcomes	On completing P.G. program the students will be able to	BTL
CO1	Recall fundamental concepts of Artificial Intelligence, its history, types, and key subfields relevant to chemistry and explain machine learning techniques and their application in processing and analyzing chemical data.	K1, K2
CO2	Apply regression, classification, and clustering algorithms to solve problems involving chemical datasets.	K3
CO3	Analyze molecular descriptors, QSAR/QSPR models, and interpret AI-based predictions of chemical properties and spectroscopic data.	K4
CO4	Evaluate the effectiveness of AI techniques in drug discovery, virtual screening, and materials science applications.	K5
CO5	Design AI-based approaches or models for solving problems in chemistry, considering ethical aspects and emerging trends.	K6

BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6- Create

Relationship Matrix – 26CH611

Course Outcomes	Programme Outcomes (POs)						Programme Specific Outcomes (PSOs)					Mean Score of Cos
	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	3	3	2	1	1	2	3	2	3	1	2	2.09
CO2	3	3	3	2	1	2	3	2	3	2	1	2.27
CO3	3	3	2	2	1	1	3	3	2	2	1	2.09
CO4	3	3	2	2	2	2	3	3	2	2	1	2.27
CO5	2	3	3	2	2	2	3	3	2	2	3	2.45
Total												2.23

Mean Score: 3- High, 2- Medium/Moderate, 1-Low