

## CH-434 Artificial Intelligence in Chemistry

Credit Hours: 2-1

Pre-requisite: Nil

### **Course Objectives**

1. This course introduces the fundamentals of Artificial Intelligence with a focus on its applications in chemistry. Students will explore machine learning, deep learning, and predictive modeling for molecular analysis, drug discovery, and chemical data interpretation. Emphasis is placed on data preparation, ethical considerations, and applying AI to solve real-world chemical problems.

### **Detailed Contents**

2. Introduction to Artificial Intelligence: Basic definitions and the evolution of AI. Overview of machine learning. Deep learning, pattern recognition, and predictive modeling. Importance and impact of AI in modern science (chemistry) and industry. Ethical considerations and challenges in AI applications. Molecular modeling and simulation. Understanding molecular structures and properties. Drug discovery: role of AI in identifying potential drugs and optimizing molecules. Chemical data analysis: using AI to explain experimental data (spectra, chemical reactions, and properties). Types of chemical data: experimental, computational, and literature data. Introduction to data preparation and quality for AI analysis: cleaning, formatting, and organizing data. Basic AI techniques: machine learning (supervised and unsupervised machine learning) with reference to chemistry. Pattern recognition and classification in chemical datasets. Predictive modeling and its significance in chemistry. Applying AI concepts to solve fundamental chemistry problems: reaction optimization, physical and chemical property prediction of compounds. Interpreting AI results and understanding their limitations

### **Course Outcomes**

3. At the end of the course, Explain the basic concepts of artificial intelligence (AI) and its applications in chemistry, including molecular modeling, drug discovery, and chemical data analysis.
4. Analyze chemical datasets using AI techniques such as machine learning, pattern recognition, and predictive modeling.
5. Apply basic AI-based tools and software to solve fundamental problems in

chemistry, including reaction optimization and property prediction.

### **Relevant Experiments:**

7. AI Assisted: spectral analysis for compound identification. Molecular structure visualization (3D). Drug screening. Reaction outcome prediction. Optimized reaction conditions. Data cleaning for reliable results. Chemical art (formula) from text descriptions (SMILES). Solubility testing. pH prediction with colorimetric strips. Descriptor calculation & boiling point regression.

### **Recommended Books**

2. Cartwright, H. M. (Ed.). (2020). *Machine Learning in Chemistry: The Impact of Artificial Intelligence* (1st ed.). Royal Society of Chemistry. ISBN: 978-1-78801-789-3.
3. Yoon, J.-Y., & Yu, C. (Eds.). (2024). *Machine Learning and Artificial Intelligence in Chemical and Biological Sensing* (1st ed.). Elsevier. ISBN: 978-0-443-22001-2.
4. Kulkarni, S., Bhandari, S., Varshney, D., & William, P. (2025). *Artificial Intelligence for Chemical Sciences: Concepts, Models, and Applications* (1st ed.). CRC Press. ISBN: 9781003569282.
5. Cheng, Y., Wang, T., & Zhang, G. (Eds.). (2021). *Artificial Intelligence for Materials Science* (1st ed.). Springer Nature. ISBN: 978-3-030-68312-2.
6. Janet, J. P., & Kulik, H. J. (2020). *Machine Learning in Chemistry*. American Chemical Society. ISBN: 9780841299009.
7. Grisafi, A., Wilkins, D., Willatt, M., & Ceriotti, M. (2019). *Machine Learning in Chemistry: Data-Driven Algorithms, Learning Systems, and Predictions* (E. O. Pyzer-Knapp, & T. Laino, Eds.). American Chemical Society. ISBN: 9780841235045.
8. Zhu, X. (2024). *AI and Robotic Technology in Materials and Chemistry Research*. John Wiley & Sons. ISBN: 978-3-527-84881-2.
9. Filipovic, N. (Ed.). (2023). *Applied Artificial Intelligence: Medicine, Biology, Chemistry, Financial, Games, Engineering* (1st ed.). Springer Nature. ISBN: 978-3-031-29716-8.
10. Filipović, N. (2024). *Applied Artificial Intelligence 2: Medicine, Biology, Chemistry, Financial, Games, Engineering*. Springer Cham. ISBN: 978-3-031-60839-1.
11. Current Literature and Reviews.