

Course Code	Course Name	Credits
26CH112	ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY	04

Course Objectives

- To introduce fundamentals of AI and its role in modern drug discovery
- To understand computational tools used in pharmaceutical research
- To develop basic skills in data-driven drug design and analysis
- To Explore real-world applications and ethical considerations

Learning Outcomes

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

- Students understand the basics of drug discovery and how AI transforms the process.
- Learn how chemical data is represented and prepared for AI models.
- Can apply basic ML models to predict drug activity.
- Understand advanced AI techniques and molecular modeling tools.
- Gain awareness of real-world applications and ethical challenges.

Unit 1 - Introduction to Drug Discovery and AI (12 Hrs.)

Overview of drug discovery pipeline (target identification → clinical trials); Challenges in traditional drug discovery (time, cost, failure rates); Introduction to artificial intelligence and machine learning; Types of AI: Supervised learning, Unsupervised learning, Reinforcement learning; Role of AI in pharmaceutical sciences.

Unit 2 – Data Handling and Cheminformatics (12 Hrs.)

Types of biological and chemical data; Databases: PubChem, DrugBank, ChEMBL; Molecular descriptors and fingerprints; Data preprocessing: cleaning, normalization, feature selection; Introduction to cheminformatics tools (e.g., RDKit).

Unit 3 - Machine Learning in Drug Discovery (12 Hrs.)

Regression and classification models; Algorithms: Linear regression, Decision trees, Random forest, Support vector machines (SVM); Model evaluation: Accuracy, Precision, Recall, ROC–AUC; Overfitting and cross-validation; Applications: QSAR (Quantitative Structure–Activity Relationship).

Unit 4 – Deep Learning and Molecular Modeling (12 Hrs.)

Introduction to deep learning and neural networks; Applications in drug discovery: Virtual screening, De novo drug design; Molecular docking and simulation; Basics of protein–ligand interactions.

Unit 5 - Advanced Applications and Ethics (12 Hrs.)

AI in personalized medicine; Drug repurposing using AI; Case studies (e.g., COVID-19 drug discovery); Ethical issues in AI: bias, data privacy, reproducibility; Future trends in AI-driven pharmaceutical research.

Reference Books:

1. Ekins, S. – Artificial Intelligence in Drug Discovery
2. Schneider, G. – De Novo Drug Design
3. Brown, N. – Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery
4. Goodfellow, I. et al. – Deep Learning Leach, A.R. – Molecular Modelling: Principles and Applications

Websites and eLearning Sources:

1. <https://www.youtube.com/watch?v=EfdmGc2FvLw&t=36s>
2. https://www.youtube.com/watch?v=7rftflGtc10&list=PLyqSpQzTE6M_U1D_xkcJI4xjH_0FgMBBN
3. <https://nptel.ac.in/courses/103106681>

COs and Bloom's Taxonomy Mapping – 26CH112

Course Outcomes	On completing U.G. program the students will be able to	BTL
CO1	Recall fundamental concepts of drug discovery and its pipeline. Identify basic principles of AI and ML in pharmaceutical sciences.	K1
CO2	Explain types of biological and chemical data and descriptors. Describe cheminformatics databases and tools used in drug discovery.	K2
CO3	Apply data preprocessing techniques and feature selection methods. Analyze model performance using evaluation metrics. Examine overfitting and apply cross-validation techniques.	K3, K4
CO4	Evaluate deep learning and molecular modeling approaches and assesses applications like virtual screening and drug repurposing.	K5
CO5	Design AI-based workflows for drug discovery. Incorporate ethical considerations and future trends in solutions.	K6

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

Relationship Matrix – 26CH112

Course Outcomes	Programme Outcomes (POs)						Programme Specific Outcomes (PSOs)						Mean Score of Cos
	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	
CO1	3	2	1.5	1	2	1	3	1.5	1	2	1	1	1.6
CO2	3	3	2	1	1.5	2	3	2	1.5	1	1	1	1.8
CO3	3	3	3	2	2.5	1.5	3	3	2	2	1	1	2.2
CO4	3	3	3	2	2	1	3	3	2	2	2	1	2.2
CO5	3	3	3	3	2	2	3	3	2	2	2	3	2.5
Total													2.06

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