# Online Workshop on

# Machine Learning for Drug Discovery: Concepts to Applications

*Empowering Drug Discovery with the Intelligence of Machine Learning*

17-20 April 2026, 6:30 PM IST   **Sunday Off**

## About the Workshop

This Workshop offers an in-depth overview of machine learning (ML) methodologies specifically designed for the field of drug discovery. Participants will explore how ML can revolutionize the drug development process by forecasting molecular interactions, refining drug candidates, and interpreting intricate biological data. Through practical sessions and case studies, students will acquire the expertise necessary to construct and assess ML models that tackle significant challenges in drug discovery, including predicting bioactivity and creating efficient drug candidates.

**1.6k+ Participants**

**REGISTER NOW**

**Fee: INR 999 $40US**

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| Online Workshop | E-Certificate |
| Live & Interactive Sessions | 24×7 Support |
| Software & Tools Support | Protocols & Lecture PPTs |
| Session Recordings | Hands-on |

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### Day 1 Module: Introduction to Machine Learning–Part I

- Introduction to Machine Learning
- Feature extraction
- Data partition
- Feature selection
- *Tools & Hands-on*: Introduction of Weka

### Day 2 Module: Introduction to Machine Learning–Part II

- Classification algorithms, Machine learning model generation
- Model performance evaluation
- *Tools & Hands-on*: ML Model on Weka

### Day 3 Module: Applications of Machine Learning in Drug Discovery

- Bioinformatics datasets
- Developing a ML model for the biological activity prediction of compounds
- *Tools & Hands-on*: GEO & PubChem for Data, aDEL for Feature Extraction, Weka for ML Modeling

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**CATR** Centre for Advanced Training and Research

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