

## NPTEL Video Lecture Topic List - Created by LinuXpert Systems, Chennai

NPTEL Video Course - Chemical Engineering - NOC:Artificial Intelligence in Drug Discovery and Development

Subject Co-ordinator - Prof. Rajnish Kumar

Co-ordinating Institute - IIT (BHU) Varanasi

Sub-Titles - Available / Unavailable | MP3 Audio Lectures - Available / Unavailable

- Lecture 1 - Drug Discovery and Development
- Lecture 2 - Overview of Drug Discovery Workflows
- Lecture 3 - Drug Design Strategies
- Lecture 4 - Conventional Methods for Drug Discovery
- Lecture 5 - Riddles in Drug Discovery
- Lecture 6 - History and Evolution of AI in Drug Discovery
- Lecture 7 - Overview of AI Technologies
- Lecture 8 - Key Application of AI Across the Pipeline
- Lecture 9 - Available AI Tools and Platforms
- Lecture 10 - Advantages of AI Integration in Drug Discovery
- Lecture 11 - Introduction to Machine Learning Concepts
- Lecture 12 - Overview of Neural Networks
- Lecture 13 - Feature Engineering and Data Preprocessing
- Lecture 14 - Evaluation Metrics for AI Models
- Lecture 15 - Introduction to Python Libraries for AI in Drug Discovery
- Lecture 16 - introduction to Drug Targets
- Lecture 17 - Basic of Target Identification and Validation
- Lecture 18 - Omics Data Integration for Target Discovery
- Lecture 19 - Binding Site and Proteins Structure Prediction with AI
- Lecture 20 - Hands on Tutorial Protein Structure Prediction
- Lecture 21 - Introduction and Approches to Virtual Screening
- Lecture 22 - AI Tools for Virtual Screening
- Lecture 23 - AI Assisted Molecular Docking
- Lecture 24 - Workflow of High Throughput Virtual Screening
- Lecture 25 - Hands on Tutorial - AI Assisted Molecular Docking
- Lecture 26 - Basics of Lead Optimization
- Lecture 27 - AI for Drug Target Interaction Studies
- Lecture 28 - QSAR Modelling
- Lecture 29 - Introduction to Molecular Dynamic MDSimulation

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- Lecture 30 - Hands on Tutorial MD Analysis
- Lecture 31 - Introduction to ADMET Properties
- Lecture 32 - Importance of ADMET and Its Prediction in Lead Optimization
- Lecture 33 - Conventional Methods for ADMET Prediction
- Lecture 34 - Openly Available Resources for ADMET Prediction
- Lecture 35 - Hands on Tutorial AI Enabled ADMET Prediction
- Lecture 36 - Overview of Clinical Trials
- Lecture 37 - Patient Recruitment, Stratification and Retention
- Lecture 38 - Clinical Trial Protocol Design and Optimization
- Lecture 39 - Predicting Outcomes of Clinical Trials with AI
- Lecture 40 - Data Collection and Monitoring for Regulatory Submissions
- Lecture 41 - Introduction to Generative AI in Drug Design
- Lecture 42 - Deep Generative Models for Drug Design
- Lecture 43 - Benchmarking Generative Models for Drug Design
- Lecture 44 - Molecule Optimization with Generative AI
- Lecture 45 - Hands on Tutorial GNN Based De Novo Drug Design
- Lecture 46 - AI in Genomics for Personalized Treatment
- Lecture 47 - AI in Real Time Monitoring and Feedback
- Lecture 48 - Overview and Data Sources for AI in Drug Repurposing
- Lecture 49 - Integrating Multi Target Drug Discovery
- Lecture 50 - network Pharmacology with AI
- Lecture 51 - Public AI Resources for Drug Discovery
- Lecture 52 - Success Case Studies of AI in Drug Discovery
- Lecture 53 - Challenges in Modern Drug Discovery Realm
- Lecture 54 - Regularory Considerations for AI Implementation
- Lecture 55 - Future Outlook Explainable Artificial Intelligence XAI and Other Emerging Technologies in Drug D
- Lecture 56 - Molecular Structure Representation
- Lecture 57 - Solubility Prediction Using Machine Learning
- Lecture 58 - Bioactivity Prediction
- Lecture 59 - Pharmacophore Based Virtual Screening
- Lecture 60 - Similarity Based Screening