Advanced Drug-Target Interaction Analysis Training Course

Professional Development Training Course Outline

Category	Biotechnology and Pharmaceutical Development	**Duration**	10 Days
Base Fee	$4,000 USD	**Delivery Mode**	Online / On-site Hybrid

Course Introduction

The pharmaceutical industry is under immense pressure to accelerate drug development, reduce exorbitant costs, and overcome the high failure rate in clinical trials. Traditional, low-throughput screening methods are no longer sufficient to navigate the vast chemical space and the complexity of the human proteome. This has necessitated a transformative shift toward in silico drug discovery, with Advanced Drug-Target Interaction Analysis emerging as the critical nexus between data science, structural biology, and pharmacology. Mastering DTI prediction which moves beyond simple binding to encompass target engagement and polypharmacology is vital for rational drug design, hit-to-lead acceleration, and identifying new therapeutic modalities like PROTACs and covalent inhibitors.

Advanced Drug-Target Interaction Analysis Training Course is explicitly designed to equip modern drug discovery professionals with the cutting-edge computational skills needed to thrive in this AI-driven era. It provides deep, practical expertise in applying Machine Learning and Deep Learning, specifically Graph Neural Networks and Transformer architectures, to predict, validate, and interpret DTIs from massive multi-omics and high-throughput screening datasets. By integrating theoretical foundations with hands-on application using industry-standard tools, participants will gain the ability to develop highly predictive models, strategize for drug repurposing, and generate mechanistic clarity for complex biological systems, thereby drastically improving translational predictivity and accelerating the delivery of safe, effective therapeutics.

Programme Curriculum

Advanced Drug-Target Interaction Analysis Training Course

Introduction

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Course Objectives

1. Master Deep Learning and Graph Neural Networks for highly accurate DTI/DTA Prediction.
2. Integrate diverse Multi-Omics Data for advanced Systems Pharmacology analysis.
3. Perform Molecular Dynamics simulations and Advanced Molecular Docking for binding site characterization.
4. Develop robust, reproducible computational pipelines for large-scale DTI data processing and feature engineering.
5. Analyze and Interpret the binding mechanisms of Non-Traditional Modalities
6. Apply Network Pharmacology principles to construct and analyze complex Drug-Target-Disease Networks for combination therapy.
7. Identify and computationally predict Off-Target Effects and the potential for Polypharmacology and Drug-Drug Interactions.
8. Execute Virtual Screening and Target Validation strategies using leading bioinformatics and Chemoinformatics databases.
9. Utilize Explainable AI techniques to ensure the interpretability and mechanistic understanding of complex DTI models.
10. Design and implement efficient Drug Repurposing strategies by mapping known DTIs to disease-specific expression profiles.
11. Evaluate model performance using key metrics and understand the principles of Model Generalizability and Transfer Learning in DTI.
12. Characterize Target Druggability and assess the Pharmacokinetic and ADMET properties of predicted drug candidates in silico.
13. Stay Current with emerging trends like Agentic AI and the application of Large Language Models in De Novo Drug Design.

Target Audience

1. Computational Chemists and Bioinformaticians.
2. Drug Discovery Scientists and Pharmacologists.
3. R&D Data Scientists and Machine Learning Engineers.
4. Principal Investigators and Research Managers.
5. Graduate Students and Post-Doctoral Researchers.
6. Biotech/Pharma Professionals.
7. Toxicology and ADMET Scientists.
8. Clinical Researchers focusing on Drug-Drug Interactions and Personalized Medicine.

Course Modules

Module 1: Foundations of Molecular Data and Chemoinformatics

- Chemical and Protein Data Formats
- Molecular Descriptors and Fingerprints
- Handling and Cleaning High-Throughput Screening Data.
- Chemical Space Exploration and Similarity/Clustering Techniques.
- Case Study: Virtual Screening using Tanimoto similarity for a novel Kinase inhibitor hit in the ChEMBL database.

Module 2: Advanced Molecular Modeling for DTI

- Principles of Structure-Based Drug Design vs. Ligand-Based Drug Design
- Advanced Molecular Docking
- Conformational Sampling and Free Energy Perturbation concepts.
- Predicting and Characterizing Allosteric Binding Sites.
- Case Study: Docking a novel lead compound into a GPCR model to predict binding mode and affinity using AutoDock Vina and analyzing PDB structures.

Module 3: Fundamentals of Machine Learning for DTI

- DTI Prediction as a Classification vs. Regression problem.
- Feature Engineering for Drugs and Targets
- Traditional ML Algorithms for DTI baseline models.
- Model Training, Validation, and Performance Metrics
- Case Study: Developing and evaluating an ML model to predict drug-target interaction probability for a subset of the BindingDB dataset.

Module 4: Deep Learning with Graph Neural Networks

- Representing Molecular Structures as Graphs
- Introduction to GNN architectures for DTI.
- Encoding protein information for DL models.
- Integrating drug and target representations for end-to-end prediction.
- Case Study: Implementing a Graph Convolutional Network using DeepChem/PyTorch to predict DTI affinity.

Module 5: Transformer Architectures and Sequence-Based DTI

- The Attention Mechanism and the original Transformer architecture.

- Application of Self-Attention to protein sequences for feature extraction.
- Developing Sequence-Based DTI Models
- Transfer Learning from large pre-trained protein language models
- Case Study: Using a Transformer model to predict the binding affinity of drugs based solely on their SMILES string and the target's amino acid sequence.

Module 6: Molecular Dynamics Simulations in DTI

- Theory and Application of Classical MD Simulations for DTI.
- Setting up, running, and analyzing an MD simulation
- Calculating Binding Free Energy
- Assessing ligand stability and conformational changes in the binding pocket.
- Case Study: Simulating the binding of a known drug to a target protein and analyzing the RMSD/RMSF over time to confirm stability and key interactions.

Module 7: Systems Pharmacology and Network Analysis

- Constructing Heterogeneous Drug-Target-Disease Networks.
- Network Topology Analysis: identifying Hubs, Motifs, and Key Pathway Crosstalk.
- Network-Based Drug Repurposing and Drug Combination Prediction.
- Algorithms for Community Detection and Sub-network Analysis.
- Case Study: Applying network centrality measures to identify high-leverage targets for a specific disease in a heterogeneous interaction network.

Module 8: Multi-Omics Data Integration for Target Validation

- Overview of Genomics, Transcriptomics, and Proteomics data relevance to DTI.
- Methods for Data Fusion and integration into DTI models
- Connecting DTI predictions with disease-specific Gene Expression profiles.
- Computational tools for Target Druggability assessment.
- Case Study: Validating a computationally predicted novel target by integrating public RNA-Seq data to show its differential expression in disease vs. healthy tissue.

Module 9: Polypharmacology and Off-Target Effects Prediction

- The concept of Polypharmacology and its implications
- Computational prediction of Off-Target Interactions using similarity and ML.
- Drug-Drug Interaction prediction based on metabolic pathways
- Strategies for designing Selective vs. Multi-Target compounds.
- Case Study: Predicting the most likely off-target side effects for a known drug by screening it against a panel of high-interest proteins

Module 10: Advanced Modalities

- Chemical and Biological principles of PROTACs and Molecular Glues.
- Computational challenges in modeling Ternary Complexes
- Modeling Covalent Inhibitors.
- Targeted Protein Degradation.
- Case Study: Designing and computationally modeling a hypothetical PROTAC linker and predicting the stability of the resulting ternary complex.

Module 11: Explainable AI in DTI Modeling

- The necessity of Interpretability and Trust in AI-driven Drug Discovery.
- Feature Importance analysis for DTI models.
- Visualizing Attention Maps in GNNs/Transformers to highlight key atoms/residues.
- Connecting XAI insights back to Mechanistic Pharmacology.
- Case Study: Using SHAP values to explain why a Deep Learning model predicted high affinity for a specific drug-target pair, highlighting the most important molecular features.

Module 12: Drug Repurposing and De Novo Design

- Methodologies for Drug Repurposing using DTI
- Utilizing Public Clinical Data and Literature Mining in DTI.
- Introduction to Generative Models for De Novo Drug Design.
- Optimizing generated molecules based on DTI affinity and ADMET properties.
- Case Study: Executing a Drug Repurposing campaign for an orphan disease using a network-based prediction algorithm on the DrugBank and Disease Ontology databases.

Module 13: Bioinformatics Resources and Data Curation

- Deep Dive into Key DTI Databases.
- Efficiently querying and extracting structured DTI data via APIs
- Data Standardization, Normalization, and Handling of Heterogeneity.
- Ethical and Regulatory Considerations in using AI/ML for Pharmaceuticals.
- Case Study: Curating a clean, high-quality dataset of IC50?Çï values for a protein family from multiple public sources for subsequent ML training.

Module 14: Predictive Toxicology and ADMET

- Absorption, Distribution, Metabolism, Excretion, Toxicity prediction models.
- Predicting Pharmacokinetic properties using molecular descriptors.
- Assessing the Toxicity profile of candidates.
- Designing molecules with improved Drug-Likeness
- Case Study: Using an established open-source tool to calculate ADMET profiles for a virtual screening list and prioritizing the top five candidates.

Module 15: Emerging Trends and Future of DTI Analysis

- The role of Quantum Computing in chemical space exploration.
- Agentic AI and LLMs in automating DTI hypothesis generation.
- Integration of Cryo-EM and AlphaFold structural predictions into DTI workflows.
- Future of Personalized Medicine driven by Patient-Specific DTI Models.
- Case Study: Discussion on the success story of a drug that utilized advanced computational DTI for rapid development during a global health crisis.

Training Methodology

This course utilizes an **Intensive Blended Learning** approach to ensure a deep, practical understanding of advanced computational techniques:

1. Lectures & Case Studies.
2. Hands-on Labs
3. Project-Based Learning.
4. Collaborative Workshops.

5. Expert Q&A/Office Hours.

Register as a group from 3 participants for a Discount

Send us an email: info@fineskilltrainingcenter.org or call +254769199797

Certification

Upon successful completion of this training, participants will be issued with a globally- recognized certificate.

Tailor-Made Course

We also offer tailor-made courses based on your needs.

Key Notes

a. The participant must be conversant with English.

b. Upon completion of training the participant will be issued with an Authorized Training Certificate

c. Course duration is flexible and the contents can be modified to fit any number of days.

d. The course fee includes facilitation training materials, 2 coffee breaks, buffet lunch and A Certificate upon successful completion of Training.

e. One-year post-training support Consultation and Coaching provided after the course.

f. Payment should be done at least a week before commence of the training, to Fineskill Training Center account, as indicated in the invoice so as to enable us prepare better for you.

Upcoming Scheduled Sessions

Start Date	End Date	Location	Price
23 Nov 2026	04 Dec 2026	Online	$2,000
23 Nov 2026	04 Dec 2026	Physical	$3,000
23 Nov 2026	04 Dec 2026	Physical	$6,000
23 Nov 2026	04 Dec 2026	Physical	$6,000
23 Nov 2026	04 Dec 2026	Physical	$12,000
23 Nov 2026	04 Dec 2026	Physical	$9,000
23 Nov 2026	04 Dec 2026	Physical	$12,000

Start Date	End Date	Location	Price
23 Nov 2026	04 Dec 2026	Physical	$12,000

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