Advanced Deep Learning for Molecular Design 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

In the face of an ever-growing need for rapid innovation in Drug Discovery, Materials Science, and Chemical Engineering, traditional, labor-intensive methods of molecule design are proving insufficient. This advanced training course bridges the gap between theoretical Deep Learning expertise and cutting-edge Molecular Design applications. It provides a comprehensive, hands-on masterclass in deploying state-of-the-art Generative AI models, such as Graph Neural Networks, Variational Autoencoders, and Deep Reinforcement Learning, to intelligently navigate the vast Chemical Space. Participants will master the critical techniques of Molecular Representation Learning and De Novo Molecular Generation, enabling the creation and optimization of novel compounds with specific, desirable properties.

Advanced Deep Learning for Molecular Design Training Course is specifically designed to transform computational chemists, data scientists, and R&D professionals into leaders of the AI-Native Discovery era. By focusing on practical application and Cheminformatics integration, the course will impart the skills necessary to build robust, scalable In Silico Screening and optimization pipelines. Upon completion, participants will be able to accelerate Hit-to-Lead timelines, improve Synthetic Accessibility prediction, and deliver more potent, selective, and clinically viable molecules, fundamentally reshaping the future of Precision Medicine and advanced materials development.

Programme Curriculum

Advanced Deep Learning for Molecular Design Training Course

Introduction

In the face of an ever-growing need for rapid innovation in Drug Discovery, Materials Science, and Chemical Engineering, traditional, labor-intensive methods of molecule design are proving insufficient. This advanced training course bridges the gap between theoretical Deep Learning expertise and cutting-edge Molecular Design applications. It provides a comprehensive, hands-on masterclass in deploying state-of-the-art Generative AI models, such as Graph Neural Networks, Variational Autoencoders, and Deep Reinforcement Learning, to intelligently navigate the vast Chemical Space. Participants will master the critical techniques of Molecular Representation Learning and De Novo Molecular Generation, enabling the creation and optimization of novel compounds with specific, desirable properties.

Advanced Deep Learning for Molecular Design Training Course is specifically designed to transform computational chemists, data scientists, and R&D professionals into leaders of the AI-Native Discovery era. By focusing on practical application and Cheminformatics integration, the course will impart the skills necessary to build robust, scalable In Silico Screening and optimization pipelines. Upon completion, participants will be able to accelerate Hit-to-Lead timelines, improve Synthetic Accessibility prediction, and deliver more potent, selective, and clinically viable molecules, fundamentally reshaping the future of Precision Medicine and advanced materials development.

Course Duration

10 days

Course Objectives

1. Master the principles and practical application of Generative AI for De Novo Molecular Design.
2. Implement and fine-tune Graph Neural Networks for highly accurate Molecular Property Prediction.
3. Apply advanced Reinforcement Learning (RL) frameworks for Objective-Directed Molecular Optimization.
4. Develop robust Molecular Representation Learning techniques, including SMILES-based and graph-based encodings.
5. Design and evaluate advanced Variational Autoencoder (VAE) and Generative Adversarial Network (GAN) architectures for molecule generation.
6. Integrate essential Cheminformatics and Computational Chemistry tools for data curation and feature engineering.
7. Build high-throughput In Silico Screening pipelines for rapid identification of potential lead compounds.
8. Evaluate and mitigate model limitations using Explainable AI (XAI) techniques for deep learning in molecular design.
9. Predict critical ADMET properties using advanced QSAR/QSPR deep learning models.
10. Utilize Transfer Learning strategies to accelerate model development across diverse chemical targets.
11. Perform Multi-Objective Optimization to balance desired properties like potency, drug-likeness, and synthetic accessibility.
12. Explore the emerging landscape of Foundation Models and Large Language Models (LLMs) for chemical text and structure generation.
13. Address the ethical and regulatory considerations of deploying AI-Designed Drugs in the drug development pipeline.

Target Audience

1. Computational Chemists and Cheminformaticians
2. Data Scientists and Machine Learning Engineers in Pharma/Biotech
3. R&D Researchers and Scientists

4. Structural Biologists and Medicinal Chemists
5. PhD/Post-doc students in Computational Science, Chemistry, or Bioinformatics
6. AI/ML Specialists
7. Team Leads/Managers
8. Professionals involved in Virtual High-Throughput Screening

Course Modules

Module 1: Foundational Cheminformatics and Molecular Data

- Review of Chemical Representations
- Mastering RDKit for molecular manipulation and feature generation.
- Molecular Fingerprints and Descriptors for Machine Learning.
- Cleaning, standardization, and balancing molecular datasets.
- Case Study: Using RDKit to process and featurize a PubChem bioassay dataset for DL.

Module 2: Advanced Molecular Representation Learning

- Graph-based vs. Sequence-based molecular encoding techniques.
- Developing Molecular Embeddings using Autoencoders.
- Concept of Latent Space and its traversability for design.
- Strategies for Pre-training and Transfer Learning on chemical data.
- Case Study: Implementing a masked-token pre-training strategy for a Transformer on a large SMILES corpus.

Module 3: Graph Neural Networks for Property Prediction

- Architecture of Graph Convolutional Networks (GCNs) and GATs.
- Applying GNNs for quantitative ADMET and Toxicity Prediction.
- Handling diverse graph sizes and heterogeneous node/edge features.
- Benchmarking GNN performance against traditional ML and QSAR models.
- Case Study: Building a GCN to predict the Aqueous Solubility of small molecules from the Tanimoto dataset.

Module 4: Sequence-to-Sequence Models for Generation

- Recurrent Neural Networks and LSTMs for sequence generation.
- Applying Seq2Seq architectures to generate valid SMILES strings.
- Controlling sequence generation using sampling and beam search.
- Handling syntax validity and chemical correctness.
- Case Study: Training an LSTM-based model for de novo generation of novel, drug-like compounds.

Module 5: Variational Autoencoders for Chemical Space Exploration

- Deep dive into Variational Autoencoder (VAE) architecture for molecules.
- Mapping chemical structures to a continuous, meaningful Latent Space.
- Bayesian Optimization and guided search within the VAE latent space.
- Decoding and validating latent vectors back into molecular structures.
- Case Study: Utilizing a VAE to interpolate between two known active molecules to find novel scaffolds.

Module 6: Generative Adversarial Networks for Molecular Synthesis

- Fundamentals of Generative Adversarial Networks (GANs) for discrete data.
- Adapting the Discriminator to penalize chemically invalid structures.
- Using conditional GANs for Targeted Molecule Generation.
- Challenges and strategies for stable training of GANs in cheminformatics.
- Case Study: Implementing a WGAN (Wasserstein GAN) to generate molecules with a target molecular weight range.

Module 7: Deep Reinforcement Learning for Optimization

- Introduction to the RL framework
- Implementing the REINVENT framework for de novo design.
- Designing Custom Reward Functions to guide optimization
- Policy gradient methods for molecular design.
- Case Study: Using RL to optimize a lead compound?ÇÖs structure for improved calculated logP while maintaining high Tanimoto similarity.

Module 8: Multi-Objective Molecular Optimization

- Defining and quantifying Multiple Objectives
- Techniques for combining multiple scores into a single Desirability Function.
- Exploring the Pareto Front of non-dominated solutions.
- Integrating Predictive Models into the generation/optimization loop.
- Case Study: Developing a weighted multi-objective function to simultaneously optimize a compound?ÇÖs binding affinity and synthetic ease.

Module 9: Assessing Synthetic Accessibility and Novelty

- Quantifying the Synthetic Accessibility of generated molecules.
- Integrating Retrosynthesis planning with generative models.
- Metrics for evaluating the Novelty and Diversity of the generated chemical space.
- Filtering and validation of in silico hits for experimental follow-up.
- Case Study: Calculating the SA score for 10,000 generated molecules and filtering for high-value, novel scaffolds.

Module 10: Deep Learning for Structural Biology

- Predicting Protein-Ligand Interaction and Binding Affinity using DL.
- Integrating deep learning with Molecular Docking and scoring.
- Overview of AlphaFold and DL models for protein structure prediction.
- Designing small molecules to bind to a specific protein pocket
- Case Study: Using a 3D GNN to predict the binding affinity of small molecules against a target protein crystal structure.

Module 11: Explainable AI (XAI) in Molecular Design

- The necessity of Interpretability in AI-Driven Drug Discovery.
- Techniques like SHAP and LIME for local model explanation.
- Visualizing Molecular Attention mechanisms in GNNs and Transformers.
- Linking model predictions back to specific substructures or features.
- Case Study: Applying XAI to understand why a GNN model predicted high toxicity for a specific molecule, identifying the key functional group.

Module 12: Advanced Topics: Transformers and Diffusion Models

- Transformer architectures for sequence and graph-based chemical data.
- Introduction to Diffusion Models for 3D and 2D molecule generation.
- The concept of Foundation Models for pre-training on vast chemical data.
- Exploring Large Language Models for chemical text-to-structure tasks.
- Case Study: Experimenting with a small-scale diffusion model to generate drug-like molecular conformations.

Module 13: Data Privacy, Ethics, and Regulatory Landscape

- Managing sensitive Biological and Chemical Data securely.
- Ethical considerations in generating potent or potentially toxic compounds.
- Addressing bias, fairness, and transparency in AI Models.
- The evolving Regulatory Landscape for AI-Designed Drugs.
- Case Study: Discussion on the ethical responsibilities in releasing a generative model trained on proprietary pharmaceutical data.

Module 14: Building and Deploying Deep Learning Pipelines

- MLOps principles for managing deep learning models in R&D.
- Model versioning, tracking, and reproducibility in a chemical context.
- Utilizing Cloud Computing for scalable training.
- Creating a robust API for an In Silico Screening tool.
- Case Study: Containerizing a trained GNN property prediction model using Docker for production deployment.

Module 15: Capstone Project & Emerging Trends

- Applying all learned concepts to a defined Molecular Design Challenge.
- Presentation and defense of the designed AI-Generation Pipeline.
- Future of Multimodal AI
- Briefing on Quantum Machine Learning in chemistry.
- Case Study: Review of a published paper on the integration of Autonomous Robotics and Deep Learning in an AI-Native Lab.

Training Methodology

The course adopts an **Intensive, Project-Based Learning (PBL)** methodology, focusing on bridging theory with practical implementation.

- Hands-on Coding Labs.
- Case Study Analysis.
- Instructor-Led Sessions.
- Capstone Project.
- Peer Collaboration and Review.

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
23 Nov 2026	04 Dec 2026	Physical	$12,000

Ready to enroll or request a customized program? Book online or contact us:

Register Online Now

Email: info@fineskilltrainingcenter.com | Website: www.fineskilltrainingcenter.com