# Advanced In Silico Drug Design Training Course

Professional Development Training Course Outline

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

## Course Introduction

Advanced In Silico Drug Design Training Course offers an intensive, hands-on deep dive into Computer-Aided Drug Design (CADD), a pivotal discipline rapidly transforming the pharmaceutical industry. This discipline leverages sophisticated computational chemistry and bioinformatics tools to significantly accelerate the drug discovery and development pipeline, moving from target identification to lead optimization with unprecedented efficiency. Participants will master cutting-edge methodologies, including Structure-Based Drug Design (SBDD) and Ligand-Based Drug Design (LBDD), focusing on real-world application of molecular modeling, advanced virtual screening, and ADMET prediction. The core objective is to cultivate highly skilled professionals capable of applying these data-driven and AI-powered techniques to address complex challenges in modern therapeutic development.

This advanced curriculum is meticulously structured to bridge the gap between theoretical principles and industrial practice, emphasizing the integration of Machine Learning (ML) and Artificial Intelligence (AI) in predictive pharmacology. Trainees will gain proficiency in using industry-standard software for tasks like molecular docking, free energy perturbation (FEP), and complex molecular dynamics simulations. By focusing on practical case studies across diverse therapeutic areas, the course ensures participants can effectively innovate lead compound identification and optimization, thereby driving cost-efficiency and reducing time-to-market for new, safe, and effective therapeutics.

## Programme Curriculum

**Advanced In Silico Drug Design Training Course**

**Introduction**

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**Course Duration**

10 days

**Course Objectives**

Upon completion of this advanced training, participants will be able to:

1. Master the principles of Structure-Based Drug Design (SBDD) and Ligand-Based Drug Design (LBDD).
2. Apply Machine Learning (ML) and Artificial Intelligence (AI) algorithms for predictive Absorption, Distribution, Metabolism, Excretion, Toxicity modeling.
3. Perform advanced molecular docking and implement complex virtual screening workflows for hit identification.
4. Conduct and interpret Molecular Dynamics (MD) simulations to analyze protein-ligand binding kinetics and stability.
5. Utilize Free Energy Perturbation (FEP) and Thermodynamic Integration (TI) for accurate binding affinity prediction.
6. Develop and validate robust Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) models.
7. Employ De Novo Design and Fragment-Based Drug Design (FBDD) techniques for novel compound generation.
8. Design and optimize compounds using pharmacophore modeling and scaffold hopping strategies.
9. Navigate and effectively utilize major cheminformatics and bioinformatics databases
10. Integrate target validation data from genomics and proteomics for informed drug design.
11. Critically evaluate and select appropriate computational tools and platforms for specific drug discovery challenges.
12. Design and execute a complete Lead Optimization campaign using a multi-parameter drug-likeness approach.
13. Apply Quantum Mechanics/Molecular Mechanics (QM/MM) methods to refine active site interactions.

**Target Audience**

1. Pharmaceutical & Biotech Researchers.

2. Computational Chemists/Biologists.
3. Medicinal Chemists.
4. Bioinformaticians & Data Scientists.
5. Postdoctoral Fellows & PhD Students.
6. R&D Managers.
7. Academic Faculty.
8. Toxicology Specialists.

**Course Modules**

**Module 1: Foundations of CADD & Target Validation**

- Review of the modern drug discovery pipeline and CADD's role.
- Introduction to Structure-Based Drug Design and Ligand-Based Drug Design
- Navigating key databases.
- Principles of Target Validation using genomics and proteomics data.
- Case Study: Validating a novel GPCR target for an oncology indication using bioinformatics data mining.

**Module 2: Advanced Protein and Ligand Preparation**

- Handling complex protein structures.
- Protein optimization, energy minimization, and active site identification.
- Advanced ligand perception, tautomer/protonation state analysis, and 3D conformer generation.
- Use of force fields in molecular modeling.
- Case Study: Preparing a membrane protein-ligand complex for a demanding simulation.

**Module 3: Molecular Docking: Beyond the Basics**

- In-depth analysis of scoring functions and their limitations.
- Advanced docking algorithms.
- Re-docking, cross-docking, and enrichment factors.
- Parallelization and high-throughput execution of docking campaigns.
- Case Study: Virtual screening of a one-million-compound library to identify novel hits against a viral protease.

**Module 4: High-Throughput Virtual Screening (HTVS)**

- Design and execution of a tiered Hierarchical Virtual Screening (HVS) workflow.
- Ligand filtration using Lipinski's Rule of Five and custom ADMET filters.
- Analysis of virtual screening results.
- Data visualization and analysis of protein-ligand interaction profiles.
- Case Study: Implementing an HTVS campaign to identify drug repurposing candidates for a rare disease.

**Module 5: Pharmacophore Modeling**

- Generation and validation of ligand-based pharmacophore models.
- Generation and validation of structure-based pharmacophore models.
- Using pharmacophores for virtual screening and focused library design.
- Scaffold hopping and lead-likeness prediction using pharmacophores.
- Case Study: Designing a pharmacophore model for a class of kinase inhibitors to guide lead optimization.

**Module 6: Quantitative Structure-Activity Relationship (QSAR)**

- Theoretical foundations.
- Building and validating predictive QSAR/QSPR models.
- Applicability domain and model reliability assessment.
- Interpretation of QSAR results for chemical intuition and lead optimization.
- Case Study: Developing a predictive QSAR model for compound cytotoxicity

**Module 7: Advanced Molecular Dynamics (MD) Simulations**

- Setting up and running production MD simulations
- Analysis of MD trajectories.
- Enhanced sampling techniques.
- Advanced analysis of protein-ligand unbinding pathways.
- Case Study: Investigating the conformational stability and binding kinetics of a ligand in its target pocket over a microsecond simulation.

**Module 8: Free Energy Perturbation (FEP) and Relative Binding Affinity**

- Theoretical background and practical application of FEP calculations.
- Setting up the thermodynamic cycle and pathway for ?öG calculations.
- Best practices for convergence and error estimation in FEP.
- Comparison of FEP with other methods.
- Case Study: Accurately predicting the relative binding affinity of a congeneric series of SARS-CoV-2 main protease inhibitors.

**Module 9: In Silico ADMET Prediction and PK/PD**

- Computational models for Absorption, Distribution, Metabolism, and Excretion
- Predicting chronic and acute Toxicity (T) using chemoinformatics models.
- Integrating multiple ADMET predictions for drug-likeness scoring.
- Introduction to computational Pharmacokinetics and Pharmacodynamics
- Case Study: Using Cyp450 inhibition prediction and in silico cardiotoxicity models to triage lead compounds.

**Module 10: Artificial Intelligence (AI) and Machine Learning (ML) in Drug Discovery**

- Overview of ML algorithms for drug property prediction.
- Training data curation, feature engineering
- Building models for de novo molecular generation.
- Predicting novel drug-target interactions using network biology and graph ML.
- Case Study: Training a Deep Learning model to classify compounds as active or inactive against a therapeutic target.

**Module 11: De Novo Design and Fragment-Based Drug Design (FBDD)**

- Principles and methodologies of De Novo Design
- Introduction to Fragment-Based Drug Design and fragment linking strategies.
- Computational tools for fragment screening and hit expansion.
- Design of targeted compound libraries using generative models.
- Case Study: Applying De Novo Design to generate novel scaffolds with high predicted potency against an enzyme.

**Module 12: Quantum Mechanics/Molecular Mechanics (QM/MM) in CADD**

- Theoretical basis for QM/MM and its application to enzyme reactions.
- Practical considerations for setting up and running QM/MM calculations.
- Calculating reaction energies and transition states in active sites.
- Refining binding geometry and interaction energies using high-level methods.
- Case Study: Analyzing the covalent bond formation mechanism between a drug and its target protein using QM/MM.

**Module 13: Computational Toxicology and Safety Pharmacology**

- Predicting genotoxicity and carcinogenicity using structural alerts.
- Models for predicting hERG inhibition and other cardiotoxicity risks.
- Regulatory requirements and the role of in silico toxicology
- Integration of Toxicity data into the lead optimization funnel.
- Case Study: Building a safety profile for a lead compound by assessing multiple in silico toxicity endpoints.

**Module 14: Protein-Protein Interaction (PPI) Modulators**

- Challenges and strategies for designing small-molecule PPI modulators.
- Virtual Screening and docking approaches for large, flat interaction surfaces.
- Computational hot-spot identification for PPI interfaces.
- Use of MD to understand PPI dynamics and inhibition mechanisms.
- Case Study: Identifying an allosteric inhibitor binding site to disrupt a crucial signaling pathway PPI.

**Module 15: Final Capstone Project and Presentation**

- Project scoping, data collection, and workflow design.
- Executing an end-to-end Advanced ISDD project
- Data analysis, interpretation, and visualization of results.
- Scientific report writing and peer review.
- Case Study: A complete project demonstrating target identification, virtual screening, lead optimization, and ADMET prediction for a chosen therapeutic area.

**Training Methodology**

The course employs a blended and highly practical methodology designed for maximum skill transfer:

- Interactive Lectures.
- Hands-on Workshops.
- Real-World Case Studies & Mini-Projects.
- Group Discussions & Problem-Solving.
- Expert Q&A Sessions.

**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**