Computational Chemistry and Virtual Screening 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 age of Data-Driven Drug Discovery and Rational Drug Design, the integration of computational methods has become indispensable, dramatically accelerating the path from target identification to lead optimization. This course provides a Comprehensive Curriculum in Computational Chemistry and Virtual Screening, two powerful In Silico Techniques that revolutionize Medicinal Chemistry and Pharmaceutical Research. Participants will master the fundamental principles of Molecular Modeling, Quantum Mechanics, and Cheminformatics, gaining practical proficiency in applying these tools to High-Throughput Virtual Screening campaigns. By moving beyond traditional, resource-intensive laboratory experiments, learners will acquire the skills to perform Structure-Based and Ligand-Based Drug Design, enabling the Rapid Identification and prioritization of novel drug candidates.

Computational Chemistry and Virtual Screening Training Course focuses on real-world applications, emphasizing practical, Hands-On Lab Exercises and Industry Case Studies. You will learn to prepare macromolecular targets and vast chemical libraries, execute and analyze Molecular Docking simulations, perform ADMET Prediction, and leverage Machine Learning in Drug Discovery workflows. The course is structured to build a complete In Silico Drug Design Pipeline, ensuring graduates are immediately effective in roles requiring advanced Computer-Aided Drug Design expertise. Ultimately, this program empowers researchers to make Informed, Data-Driven Decisions that significantly cut down on the time, cost, and risk associated with the development of new therapeutics.

Programme Curriculum

Computational Chemistry and Virtual Screening Training Course

Introduction

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Course Duration

10 days

Course Objectives

1. Master the principles of Molecular Modeling and Quantum Chemistry relevant to drug design.
2. Gain proficiency in Structure-Based Virtual Screening methodologies.
3. Execute and interpret Molecular Docking simulations for protein-ligand complexes.
4. Develop expertise in Ligand-Based Virtual Screening, including Pharmacophore Modeling.
5. Apply Quantitative Structure-Activity Relationship models for activity prediction.
6. Perform In Silico ADMET Prediction to assess Drug-Likeness and toxicity profiles.
7. Design and curate Chemical Libraries and prepare biological targets for computational analysis.
8. Utilize Cheminformatics and Bioinformatics tools for data analysis and visualization.
9. Integrate Machine Learning and AI in Drug Discovery workflows for enhanced hit identification.
10. Apply advanced techniques like Free Energy Perturbation and Molecular Dynamics Simulations.
11. Develop a complete, SEO-Friendly In Silico Drug Design Pipeline from target to lead.
12. Critically evaluate and prioritize Virtual Screening Hits using robust scoring functions and enrichment metrics.
13. Troubleshoot and optimize CADD workflows for complex and flexible protein targets.

Target Audience

1. Medicinal Chemists and Pharmaceutical Scientists
2. Computational Biologists and Bioinformaticians
3. R&D Scientists in Drug Discovery and Agrochemical industries
4. Graduate and Post-Graduate Students
5. Biotech and Pharma Researchers
6. Chemists and Biologists seeking to transition into In Silico Modeling
7. Academic Researchers focused on Protein-Ligand Interactions

8. Data Scientists interested in Chemical Informatics applications

Course Modules

Module 1: Foundations of Computational Chemistry & CADD

- Computational Chemistry
- Quantum Mechanics (QM) and Molecular Mechanics (MM)
- Introduction to Computer-Aided Drug Design methodologies.
- Overview of the Drug Discovery Pipeline and the role of In Silico methods.
- Case Study: The historical impact of Captopril design using early CADD principles.

Module 2: Cheminformatics and Chemical Data Handling

- Representation of chemical structures.
- Handling large Chemical Databases
- Calculating molecular descriptors and fingerprints
- Chemical Space exploration and diversity analysis.
- Case Study: Using RDKit/OpenBabel to process and standardize a million-compound library.

Module 3: Protein Target Preparation and Analysis

- Retrieving and validating protein structures from the Protein Data Bank.
- Cleaning, repairing, and optimizing protein structures
- Binding Site Analysis and identification of druggable pockets.
- Cofactor/water molecule handling and their influence on binding.
- Case Study: Preparing the 3D structure of a Kinase enzyme for docking analysis.

Module 4: Ligand Preparation and Drug-Likeness

- Generating 3D conformations and molecular tautomers.
- Applying Lipinski's Rule of Five and other Physicochemical Filters.
- Filtering for Pan-Assay Interference Compounds and toxicophores.
- Predicting pKa and ionization states for physiological conditions.
- Case Study: Optimizing a list of initial hits by filtering for improved Drug-Likeness.

Module 5: Introduction to Virtual Screening (VS) Strategies

- Comparison of High-Throughput Screening (HTS) and Virtual Screening.
- Overview of Ligand-Based, Structure-Based and VS approaches.
- Designing an effective Hierarchical Virtual Screening workflow.
- Key metrics for evaluating VS performance.
- Case Study: Comparing a simple single-step VS with a multi-stage hierarchical approach.

Module 6: Fundamentals of Molecular Docking

- Theory and algorithms.
- Setting up and running a typical Docking Simulation protocol.
- Analyzing and interpreting docking poses and interaction maps.
- Common Docking Software packages
- Case Study: Docking a known inhibitor to a viral protease and validating the predicted pose.

Module 7: Advanced Molecular Docking & Flexible Systems

- Induced-Fit Docking and handling protein flexibility.
- Target-specific scoring function optimization.
- Challenges and strategies for docking into allosteric sites.
- Consensus Docking and pose clustering techniques.
- Case Study: Utilizing induced-fit docking to model a highly flexible binding loop in an enzyme.

Module 8: Ligand-Based Virtual Screening (LBVS) I: Pharmacophores

- Principles of Pharmacophore Modeling for identifying key molecular features.
- Creating 3D Pharmacophore Models from active ligands.
- Searching chemical libraries using Pharmacophore Queries.
- Validation and refinement of pharmacophore models.
- Case Study: Developing a pharmacophore model from a series of highly potent compounds for a GPCR.

Module 9: Ligand-Based Virtual Screening (LBVS) II: Shape & Similarity

- 2D and 3D Molecular Similarity methods
- Shape-Based Screening and alignment methods.
- Field-Based QSAR (3D-QSAR) principles.
- Fingerprint-based similarity searching in large databases.
- Case Study: Identifying novel scaffolds for an existing drug using shape-based screening.

Module 10: ADMET and Toxicity Prediction (In Silico ADMET)

- Introduction to Pharmacokinetics (ADME) and Toxicology in drug design.
- Applying Rule-Based Models for permeability.
- Using computational tools for predicting metabolism
- Toxicology Prediction models
- Case Study: In silico profiling of a lead compound to minimize the risk of cardiotoxicity.

Module 11: Quantitative Structure-Activity Relationship (QSAR)

- The fundamental theory and workflow of QSAR Modeling.
- Selecting appropriate molecular descriptors and data sets.
- Statistical methods in QSAR.
- Model validation, interpretation, and domain of applicability.
- Case Study: Building a robust QSAR model to predict the IC50?Çï of a series of molecules.

Module 12: Molecular Dynamics (MD) Simulations

- MD Simulation principles.
- Setting up and running a basic protein-ligand MD simulation.
- Analyzing Conformational Changes and system stability
- Interpreting MD results for binding stability and water network analysis.
- Case Study: Using MD to assess the stability of a promising ligand-protein complex over 100ns.

Module 13: Advanced Binding Free Energy Calculations

- Limitations of simple docking scores and the need for Free Energy Calculations.
- MM/GBSA and MM/PBSA end-point methods.
- Introduction to alchemical methods
- Practical considerations and best practices for FEP.

- Case Study: Calculating the relative binding free energy for a set of congeneric ligands.

Module 14: Integrating AI and Machine Learning in VS

- The landscape of Machine Learning in Drug Discovery
- Using Deep Learning and Neural Networks for enhanced scoring functions.
- Applying Classification and Regression ML models to virtual screening data.
- Introduction to De Novo Drug Design using generative AI models.
- Case Study: Training a Random Forest model to re-score and prioritize virtual screening hits.

Module 15: Building an Integrated In Silico Pipeline

- Workflow automation using scripting
- Creating a complete, high-throughput Virtual Screening Pipeline.
- Data management, visualization, and reporting of results.
- Strategies for integrating computational and experimental data.
- Case Study: End-to-end execution of a complete virtual screening project against a new cancer target.

Training Methodology

The course utilizes a Blended Learning Approach focusing on practical mastery:

1. Interactive Lectures.
2. Hands-On Lab Exercises
3. Real-World Case Studies.
4. Project-Based Learning.
5. Troubleshooting 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

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