Structural Bioinformatics and Molecular Modeling 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

Structural Bioinformatics and Molecular Modeling is a rapidly advancing field that leverages computational methods to analyze and predict the structures of biological macromolecules. By integrating molecular biology with computational science, this training course aims to empower learners with the knowledge and skills necessary to model biological molecules, understand protein folding, and predict the interaction of drugs with their targets. In the age of personalized medicine and drug discovery, the ability to manipulate and simulate biological structures is invaluable. Structural Bioinformatics and Molecular Modeling Training Course will provide a comprehensive foundation, from basic principles to advanced techniques, in structural bioinformatics, including molecular dynamics simulations, protein-ligand docking, and visualization techniques.

With a strong focus on real-world applications, this course delves into the tools and technologies that are shaping modern biomedical research. Participants will gain hands-on experience with the latest software packages and computational tools used in the study of molecular structures, drug design, and genetic engineering. By the end of the course, learners will be equipped with the expertise needed to contribute to cutting-edge research and development in fields such as biotechnology, pharmaceutical sciences, and academic research.

Programme Curriculum

Structural Bioinformatics and Molecular Modeling Training Course

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Course Objectives

1. Understand the basics of structural bioinformatics and its applications in drug discovery and protein engineering.
2. Learn advanced molecular modeling techniques, including molecular dynamics simulations and quantum chemistry methods.
3. Gain hands-on experience with protein-ligand docking and protein-protein interaction prediction.
4. Understand macromolecular structure prediction and apply various software tools for structure-based drug design.
5. Master key concepts in biomolecular visualization and the use of software like PyMOL and Chimera.
6. Develop a solid understanding of bioinformatics databases, such as PDB, and their role in computational biology.
7. Study the thermodynamics of protein-ligand binding and its impact on drug development.
8. Acquire skills in structure-based virtual screening to identify potential drug candidates.
9. Analyze protein folding and stability through computational techniques.
10. Understand target identification in drug discovery and the role of bioinformatics in precision medicine.
11. Explore machine learning techniques for molecular modeling and structural predictions.
12. Learn the integration of computational biology with experimental methods in drug development pipelines.
13. Study real-world case studies on the optimization of molecular interactions and the discovery of novel therapeutics.

Target Audience

1. Bioinformatics professionals.
2. Biotechnology and pharmaceutical companies looking to improve drug design.
3. Academic researchers in molecular biology and computational biology.
4. Medical scientists.
5. Computational biologists.
6. PhD students and postdocs in structural bioinformatics or molecular biology.
7. Data scientists.

8. Healthcare professionals.

Course Modules

Module 1: Introduction to Structural Bioinformatics

- Overview of the field and its importance in drug discovery
- Key terminology and concepts in molecular modeling
- Introduction to protein structures: Primary, Secondary, Tertiary, and Quaternary
- Overview of structural databases: PDB, UniProt, and others
- Case Study: Predicting protein structures from sequences

Module 2: Protein Structure Prediction

- Methods for predicting 3D protein structures: Homology modeling, ab initio modeling
- Computational tools for structure prediction (MODELLER, I-TASSER)
- Structural alignment techniques for homologous proteins
- Handling structural data and errors in predictions
- Case Study: Structural prediction of a novel enzyme

Module 3: Molecular Dynamics Simulations

- Introduction to molecular dynamics (MD) simulations
- Setting up and running MD simulations (GROMACS, AMBER)
- Analyzing MD trajectories: RMSD, RMSF, and solvent accessibility
- Applications of MD in protein folding and drug design
- Case Study: MD simulation of a protein-ligand complex

Module 4: Molecular Docking and Virtual Screening

- Basics of protein-ligand docking
- Docking software: AutoDock, DOCK, Glide
- Virtual screening to identify lead compounds
- Scoring functions and binding affinity predictions
- Case Study: Virtual screening for drug candidates against COVID-19 targets

Module 5: Protein-Ligand Interactions

- Key principles of protein-ligand interactions
- Understanding binding sites and hot spots
- Computational techniques for optimizing ligand binding
- Role of solvent in protein-ligand interactions
- Case Study: Designing inhibitors for cancer-related proteins

Module 6: Molecular Visualization Techniques

- Introduction to visualization tools: PyMOL, Chimera, VMD
- Visualizing protein structures and molecular interactions
- Structural representation techniques: ribbons, surface, space-filling
- Advanced features in visualization tools: animations, ligand interactions
- Case Study: Visualizing the binding of a drug molecule to a receptor

Module 7: Bioinformatics Databases

- Introduction to bioinformatics databases and resources
- PDB: Structure repository and search techniques
- UniProt: Protein sequence and functional analysis
- Sequence alignment tools: BLAST, ClustalW
- Case Study: Searching for homologous proteins in PDB

Module 8: Advanced Molecular Dynamics

- Techniques for enhanced sampling in MD simulations
- Free energy calculations and binding affinity predictions
- Analysis of protein stability and folding pathways
- Coupled simulations with experimental data
- Case Study: Predicting the effect of mutations on protein stability

Module 9: Integrating Bioinformatics with Experimental Data

- Combining experimental data with computational models
- Homology-based modeling using experimental structures
- Using NMR, X-ray crystallography, and cryo-EM data
- Validation of computational models with experimental results
- Case Study: Combining cryo-EM and computational methods to refine protein structures

Module 10: Machine Learning in Molecular Modeling

- Overview of machine learning applications in bioinformatics
- Training machine learning models for molecular property predictions
- Feature selection and data preprocessing techniques
- Neural networks and deep learning in molecular modeling
- Case Study: Predicting protein-ligand binding affinity using machine learning

Module 11: Drug Discovery and Target Identification

- Identifying potential drug targets using computational methods
- Structure-based drug discovery and screening
- Designing small molecules for target modulation
- ADMET predictions in drug development
- Case Study: Identifying a target for Alzheimer's treatment

Module 12: Computational Approaches for Enzyme Engineering

- Methods for engineering enzymes for industrial applications
- Modifying enzyme active sites using computational techniques
- Stability and activity prediction of engineered enzymes
- Molecular dynamics simulations in enzyme design
- Case Study: Engineering a thermostable enzyme for biofuel production

Module 13: Biomolecular Simulation for Disease Modeling

- Simulating disease-related proteins and mutations
- Predicting drug resistance in viral proteins
- Structural insights into neurodegenerative diseases
- Modeling protein misfolding and aggregation

- Case Study: Simulation of protein aggregation in Alzheimer's disease

Module 14: Advanced Protein-Protein Interactions

- Predicting protein-protein interactions (PPI)
- Tools and methods for PPI prediction: ZDOCK, ClusPro
- Role of PPIs in signaling pathways and disease mechanisms
- Structural and functional analysis of PPIs
- Case Study: Understanding the PPI network in cancer

Module 15: Applications in Precision Medicine

- Using structural bioinformatics for personalized medicine
- Modeling patient-specific mutations and drug responses
- In silico prediction of drug efficacy and toxicity
- Designing patient-tailored therapeutic approaches
- Case Study: Modeling drug interactions for genetic diseases

Training Methodology

This course employs a participatory and hands-on approach to ensure practical learning, including:

- Interactive lectures and presentations.
- Group discussions and brainstorming sessions.
- Hands-on exercises using real-world datasets.
- Role-playing and scenario-based simulations.
- Analysis of case studies to bridge theory and practice.
- Peer-to-peer learning and networking.
- Expert-led Q&A sessions.
- Continuous feedback and personalized guidance.

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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