Advanced Computational Protein Structure Prediction 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 determination of a protein's three-dimensional (3D) structure is the foundational challenge the "Grand Challenge" of structural biology, as structure dictates function. In the current era of AI-driven scientific discovery, traditional experimental methods like X-ray crystallography and Cryo-EM are being dramatically augmented, and in some cases supplanted, by cutting-edge computational techniques. Advanced Computational Protein Structure Prediction Training Course is designed to bridge the growing gap between vast genomic data and the relatively small pool of known protein structures, focusing on the revolutionary impact of Deep Learning and Biomolecular Foundation Models. Participants will move beyond basic bioinformatics to master state-of-the-art platforms, including the AlphaFold ecosystem and next-generation models like Protein Language Models (pLMs) and ESMFold, enabling high-accuracy, high-throughput structural insights.

This course provides a deep dive into the algorithmic core and practical application of modern Computational Structural Biology. It emphasizes hands-on proficiency in building, validating, and interpreting complex protein models, from single chains to large protein-protein interactions (PPIs), multimers, and protein-ligand complexes. Key areas of study include structure-guided Rational Drug Design, advanced Protein Engineering, and high-resolution Molecular Dynamics (MD) Simulations to analyze conformational changes and dynamic function. Graduates will be equipped to lead innovative projects in Precision Medicine, Synthetic Biology, and Biotherapeutics, translating computational models directly into actionable scientific and commercial breakthroughs.

Programme Curriculum

Advanced Computational Protein Structure Prediction Training Course

Introduction

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Course Outline

10 days

Course Objectives

1. Deeply understand the core Transformer-based and Attention mechanisms driving current state-of-the-art structure prediction.
2. Utilize AlphaFold-Multimer and AlphaFold 3 to accurately predict structures of Protein-Protein Interactions (PPIs), multimeric assemblies, and complexes with small molecules and nucleic acids.
3. Apply and fine-tune ESMFold and similar models for fast, single-sequence prediction and gain insight into evolutionary sequence-structure relationships.
4. Critically evaluate predicted structures using metrics like pLDDT, PAE, and TM-score, and advanced tools like PROCHECK and MolProbity.
5. Set up, run, and analyze all-atom and coarse-grained MD simulations to explore conformational dynamics and flexible regions.
6. Master techniques for Virtual Screening, Molecular Docking, and binding affinity prediction for novel compound identification.
7. Utilize computational models for targeted mutagenesis, de novo protein design, and optimizing stability or binding affinity.
8. Combine predicted structures with Genomics, Proteomics, and Single-Cell data for functional annotation and pathway analysis.
9. Automate prediction, refinement, and validation workflows using Python, Jupyter Notebooks, and version control (Git).
10. Apply specialized techniques for challenging targets, including membrane proteins, intrinsically disordered regions (IDRs), and large conformational changes.
11. Identify and characterize druggable pockets, active sites, and allosteric modulators using geometric and energy-based computational methods.

12. Effectively utilize high-performance computing (HPC) and cloud platforms for computationally intensive tasks.
13. Understand the emerging role of Generative AI and large language models in inverse protein folding and sequence-to-function predictions.

Target Audience

1. Bioinformaticians & Computational Biologists.
2. Structural Biologists.
3. Medicinal Chemists & Pharmacologists.
4. Protein Engineers & Biotechnologists.
5. Data Scientists & AI/ML Engineers.
6. PhD/Post-doctoral Researchers.
7. R&D Scientists in Biopharma/Biotech.
8. Computational Chemists.

Course Modules

1. Foundational Principles & Structural Bioinformatics Refresher

- Review of protein primary, secondary, tertiary, and quaternary structure.
- Thermodynamics and kinetics of the protein folding problem.
- In-depth exploration of major databases.
- Visualization tools mastery.
- Case Study: Visualizing structural differences between native and disease-causing mutant proteins

2. Sequence Alignment & Evolutionary Covariation

- Advanced Multiple Sequence Alignment (MSA) generation and filtering techniques.
- Algorithms for identifying co-evolved residues.
- The role of Evolutionary Covariation in distance and contact prediction.
- Understanding the relationship between MSA depth and prediction accuracy.
- Case Study: Generating a high-quality MSA for a protein with low sequence homology to guide AlphaFold prediction confidence.

3. The AlphaFold Ecosystem: Architecture & Implementation

- Detailed breakdown of the AlphaFold 2 architecture.
- Practical usage of ColabFold and local AlphaFold installations.
- Understanding and interpreting confidence metrics.
- Input file preparation and output file interpretation
- Case Study: Predicting the structure of an uncharacterized Mycobacterium tuberculosis protein and assessing its confidence.

4. Predicting Multimers & Protein-Protein Interactions (PPIs)

- Specialized methods for complex prediction: AlphaFold-Multimer and its limitations.
- Preparing multimeric input sequences and defining stoichiometry.
- Interpreting the Interface pLDDT (ipLDDT) and PAE for inter-chain confidence.
- Predicting and validating models of homologous and heterologous complexes.
- Case Study: Modeling the structure of an antibody-antigen complex or a transcription factor dimer using AlphaFold-Multimer.

5. Advanced Biomolecular Foundation Models (pLMs)

- Introduction to Protein Language Models like ESM-1b and ESMFold.
- Sequence-to-structure prediction using single-sequence models for speed.
- Using pLMs for representation learning and feature extraction on protein sequences.
- Transfer learning and fine-tuning pLMs for specific structural tasks.
- Case Study: Comparing the speed, accuracy, and hardware requirements of AlphaFold vs. ESMFold for a set of benchmark targets.

6. Structure Refinement and Quality Assessment

- Advanced metrics for structural quality
- Stereochemical validation using Ramachandran plots, clash scores, and side-chain rotamers.
- Model optimization via energy minimization
- Using experimental data for refinement and fitting.
- Case Study: Refining a low-pLDDT region of an AlphaFold prediction using short-range MD and comparing MolProbity scores.

7. Molecular Dynamics (MD) Simulation Fundamentals

- Theory of MD and the force field concept
- Setting up an MD system: solvation, ionization, and periodic boundary conditions
- Equilibration and production run protocols using GROMACS or NAMD.
- Hardware requirements and best practices for HPC and GPU utilization.
- Case Study: Running an MD simulation on a protein-ligand complex to observe binding stability and conformational flexibility over a 100ns trajectory.

8. MD Trajectory Analysis for Function

- Analyzing RMSD and RMSF for structural stability and local mobility.
- Principal Component Analysis (PCA) or Essential Dynamics (ED) for large conformational changes.
- Calculating free energy landscapes and monitoring hydrogen bonds/salt bridges.
- Conformational sampling and extracting representative structures for further study.
- Case Study: Using PCA on an MD trajectory of an enzyme to identify the primary conformational movements related to substrate binding and release.

9. Structure-Based Drug Design (SBDD): Ligand Docking

- Introduction to the SBDD workflow and its role in modern drug discovery.
- Theory and application of rigid and flexible Molecular Docking
- Preparing protein receptors and small-molecule ligands
- Scoring functions, binding pose prediction, and active site identification.
- Case Study: Docking a known inhibitor into an enzyme's active site and predicting its correct binding pose and estimated affinity

10. SBDD: Virtual Screening & Affinity Prediction

- Techniques for high-throughput Virtual Screening (VS) of chemical libraries.
- Filtering and ranking docking results and calculating consensus scores.
- Introduction to Free Energy Perturbation (FEP) and Molecular Mechanics/Poisson-Boltzmann Surface Area for advanced affinity calculation.
- Identifying and prioritizing hit compounds for experimental validation.

- Case Study: Performing a small-scale VS of a 100-compound library against a predicted SARS-CoV-2 protein structure to identify novel lead candidates.

11. Rational Protein Engineering and Design

- Introduction to the concept of Inverse Protein Folding and De Novo Design.
- Computational tools for stability prediction and mutation analysis
- Targeted mutagenesis to enhance enzyme activity or thermal stability.
- Design of novel interfaces for custom protein-protein interactions.
- Case Study: Using computational tools to design a thermostable variant of an industrial enzyme by predicting favorable single-point mutations.

12. Modeling Complex Systems & Non-Standard Components

- Prediction and refinement techniques for membrane proteins
- Modeling Intrinsically Disordered Regions (IDRs) and their functions.
- Inclusion of Post-Translational Modifications (PTMs) in structural models.
- Handling metal ions, cofactors, and bound nucleic acids in prediction
- Case Study: Modeling a G-Protein Coupled Receptor (GPCR) in a virtual membrane environment and simulating its activation loop.

13. AI for Structure and Function Prediction

- Generative AI models in protein science
- Predicting protein function from structure using geometric deep learning.
- Introduction to Geometric Deep Learning for protein surfaces and binding pockets.
- Using protein embeddings (pLMs) for fast functional classification.
- Case Study: Using a geometric deep learning tool to predict the Enzyme Commission (EC) number or specific binding partner for a newly predicted protein structure.

14. Computational Pipeline Development & Automation

- Mastering the Python ecosystem for structural bioinformatics
- Introduction to Command-Line Interface (CLI) and basic Shell Scripting.
- Developing reproducible workflows using Snakemake or Nextflow.
- Best practices for data management, FASTA handling, and version control (Git).
- Case Study: Building a fully automated Python script that takes a UniProt ID, runs an AlphaFold prediction, validates the output, and stores the results in a structured database.

15. Ethical AI and Future Directions in Structural Biology

- Ethical considerations of using AI in drug design and intellectual property implications.
- The role of CASP and other community assessments in benchmarking new methods.
- Emerging trends: cryo-ET informed modeling and single-cell proteomics applications.
- Integrating Quantum Computing and Multi-Scale Modeling into future workflows.
- Case Study: Critical discussion and analysis of the limitations of AlphaFold and proposing strategies to overcome them.

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

Start Date	End Date	Location	Price
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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