

# EXPLORING THE FRONTIERS OF DRUG DISCOVERY

A 6-MONTH CADD INTERNSHIP IN INDUSTRIAL BIOINFORMATICS





#### **Welcome to Our Program**

At Dr.Omics Labs, we're delighted to offer you an extraordinary journey into the world of Industrial Bioinformatics and Computer-Aided Drug Designing. Join us and make a significant impact on the future of drug discovery and bioinformatics research.



### About us

Dr.Omics Labs is a leading institution dedicated to advancing bioinformatics, genomics, and proteomics research. Their Industrial Bioinformatics Longterm Internship program provides a combination of coursework and handson project experience to equip individuals with the necessary skills and knowledge to excel in the field.

#### **Key Program Features**

- Comprehensive coursework in CADD techniques.
- Hands-on experience with cutting-edge software and tools.
- Real-world drug design projects, and guidance to publish in Scopus indexed journal
- HR sessions to get you ready for interviews.



#### **Coursework Overview**



- Beginners to advanced Bioinformatics
- Linux, Cloud Computing and its application in CADD
- Python and its application in CADD Techniques
- R and its application in CADD Techniques
- Computer Aided Drug Designing (CADD)
- 6. HR Session
- 7 Machine Learning in Drug Designing
- Research Project CADD 2 month

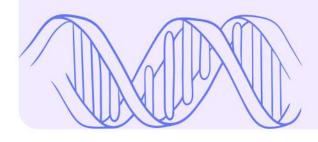


### MODULE 1:

## BEGINNERS TO ADVANCED BIOINFORMATICS

- Introduction to Bioinformatics
- NCBI Database Overview
- Genbank Database Practical Exercises
- UCSC Genome Browser Overview
- UCSC Genome Browser Hands-on Exercises
- Pubmed Database Introduction
- Clinvar Database Overview
- KEGG Database Overview and Exercises
- Protein Databases Overview
- Protein Data Bank (PDB) Overview
- Online BLAST Introduction and Exercises
- Standalone BLAST Setup and Initial Exercises
- Standalone BLAST Advanced Exercises
- Multiple Sequence Alignment with ClustalW
- Multiple Sequence Alignment with MEGA



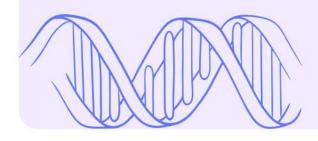




# MODULE 2: LINUX, CLOUD COMPUTING AND ITS APPLICATION IN CADD

- Linux overview and significance
- File and directory operations (create, copy, move, delete)
- Text file editing and creation
- Process management (introduction and termination)
- Basic networking and ownership overview
- Conclusion and further resources
- Basics of Cloud technology (AWS)
- Basics of Pipeline Engineering





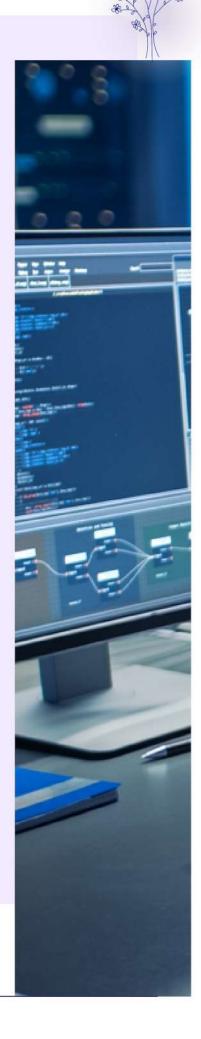
#### **MODULE 3:**

## PYTHON AND ITS APPLICATION IN CADD TECHNIQUES

#### 3.1. Python Programming

- Introduction to Python language
- Role of Programming in Bioinformatics
- Installation of Python on various platforms
- Installation of IDE
- Print function
- Comments
- User input
- Command line arguments
- Data types
- Variables and rules to create a variable
- In-built functions of python
- Slicing and indexing in String
- String and data formatting
- Control statements (if -else, If -elif-else, for loop, etc)
- Python data structure (List, Set, Tuple, etc)
- Methods of data structures
- Function introduction & its requirement
- Exception Handling, File Handling & Pandas Library







#### 3.2. Biopython

- Introduction to Biopython
- Installation of Biopython
- Conversion of a string into a biological sequence
- Obtaining complement, reverse complement, transcribe, reverse transcribe, and translation from a sequence
- Finding GC content from a sequence
- SeqIO object:
- Reading various biological file formats such as Fasta and GenBank
- Analysis of fasta sequences
- Finding GC content of a fasta file containing multiple sequences and storing the data in a file
- Converting a GenBank file into fasta format
- Accessing NCBI's Entrez databases: Entrez Guidelines (Elnfo, ESearch, etc)







#### **MODULE 4:**

## R AND ITS APPLICATION IN CADD TECHNIQUES

#### 4.1. R Programming

- Introduction to the R language
- Importance of R in Bioinformatics
- Installation of R
- Installation of IDE (R studio)
- Print, cut, and paste functions
- Comments
- Variables
- Data types
- Functions of math
- Operators
- Installation of packages
- String formatting
- Learning Control Statements (if -else, while loop, lif types == 'loca' domain = [('could break, etc.)
- R Data Structures (Lists, Vectors, Arrays, etc)
- File Handling & User-Defined Functions



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#### 4.2. Introduction to Bioconductor

- Bioconductor package installation
- Sequence analysis
- Basics of seqinr package
- Import and export FASTA sequences
- Reverse complement
- GC content
- Retrieving genbank and fasta files from NCBI
- Statistical study for Analysis (z-test, t-test, etc)
- Plot generation for data visualization (box plot, PCA plot, Heatmap, Volcano Plot)





#### **MODULE 5:**

## COMPUTER AIDED DRUG DESIGN (CADD)

- Introduction to Drug Discovery and Computer Aided Drug Design
  - Overview of drug discovery process
  - Role of computational methods
  - Hands-on: Introduction to ChemDraw or ChemSketch for chemical structure visualization.
- Molecular Biology Fundamentals for Drug Design
  - Biomolecules and their properties
  - Structure of proteins and ligands
  - Hands-on: Utilize PyMOL or Swiss
  - -PdbViewer for protein structure visualization.
- Molecular Modeling Techniques
  - Molecular visualization tools
  - Molecular mechanics and dynamics simulations
  - Hands-on: Use PyMOL, UCSF Chimera, or VMD for molecular visualization.
- Chemical Informatics and Virtual Screening
  - Chemical databases and data mining
  - Ligand and structure-based virtual screening
  - Hands-on: Explore tools like PubChem for chemical data and Autodock Vina for virtual screening



#### **MODULE 6:**

## MACHINE LEARNING IN DRUG

#### **DESIGN**

#### Introduction to Machine Learning

- Basics of machine learning
- Supervised, unsupervised, and reinforcement learning
- Hands-on: Learn the basics with the scikit-learn library in Python.

#### • Data Preprocessing for Drug Design

- Data cleaning and feature selection
- Handling molecular data
- Hands-on: Use Pandas and NumPy for data preprocessing.

#### Machine Learning Models for Drug Design

- Regression and classification algorithms
- Deep learning in drug discovery
- Hands-on: Implement machine learning models using scikit-learn and TensorFlow/Keras.

#### Applications of Machine Learning in Drug Design

- Predicting drug-target interactions
- QSAR modeling
- Hands-on: Apply machine learning to real datasets with RDKit and Cheminformatics.

#### Drug Optimization and Lead Identification

- Structure-activity relationship (SAR) analysis
- De novo drug design using ML
- Hands-on: Use RDKit for SAR analysis and explore de novo design tools









### Program Structure

Duration: 6 months

Coursework: 4 months

Project: 2 months

#### Gain expertise in CADD techniques

#### 4 Months of In-Depth Learning

- Molecular modeling
- Virtual screening
- Drug-target interaction analysis
- Pharmacokinetics and pharmacodynamics

#### 2 Months of Real-World Application

- Collaborate on a cutting-edge research project.
- Apply acquired skills to solve industry challenges.
- Gain hands-on experience with CADD.
- Work closely with mentors and industry professionals.

**HR Session:** Aligning career aspirations with our 6-month CADD course for skill development and growth.



#### FREQUENTLY ASKED QUESTIONS

## Q: Are these courses suitable for those new to the field without prior experience?

A: Yes, our courses are designed to cater to beginners with no prior experience in the field. We provide foundational content suitable for all skill levels.

#### Q: Will I receive a certification upon completing the course?

A: Absolutely, a digital certificate will be awarded upon course completion. You'll receive this certificate via email.

## Q: Do the courses include practical projects and research opportunities?

A: Certainly, our courses incorporate practical projects and research opportunities to ensure hands-on learning and the practical application of acquired knowledge.

#### Q: Can I access class recordings if I miss a class?

A: Yes, class recordings are available. We'll send you the recording link via email if you miss a class, typically on the day following the live session.

## Q: Can I continue to access course materials and resources after finishing the course?

A: Absolutely, you'll retain access to course materials and resources even after completing the course. These materials will be shared with you via email or WhatsApp.





#### **TERMS AND CONDITIONS**

- Maintaining Discipline during the Tenure.
- It is mandatory to maintain 85% attendance for all students.
- Students must maintain an average 'A2' grade throughout their training period.
- Project completion is a must for research.



Need more insight & support?

### **CONTACT US!**



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## Thank you!



**OUR CERTIFICATIONS & GRANTS** 













