Online & Offline

WINTER TRAINING

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DIVERSE RANGE OF MODULES

- **Computational Biochemistry & Computer Aided Drug Design (Code: ST101)**
- **Homology Modelling (Code: ST102)**
- **Molecular Docking (Code: ST103)**
- **Molecular Dynamics Simulation (Code: ST104)**
- **Genomics and Proteomics (Code: ST105)**
- **Bioinformatics Data Resources & Biological Sequence Analysis, Phylogeny (Code: ST106)**
- **Bioinformatic Approaches for Comparative Analysis of Viruses (Code: ST107)**
- **Secondary structure prediction of 16S ribosomal RNA of *E. coli* (Code: ST108)**
- **Bioinformatics: Comparative and Prediction tools (Code: ST109)**
- **Computer-Aided Prediction of Pharmacokinetic (ADMET) Properties (Code: ST110)**

Training Fee (15 Days)
Online-INR 3000 / 50 USD
Offline-INR 3500

Batch Start From
15 Dec 2024,
5 Jan and 10 Jan 2025

6:00 PM IST (Online)
11:00 AM-5:00PM (offline)

Features

Certificate (Hard Copy)
Live Recording of Lectures
Practical based training
Hands-on-sessions
software & Soft copy of Protocols

WHO CAN JOIN?

Graduate / Postgraduate (B.Sc., B. Tech, M.Sc. M. Tech.)/ Research scholars/ Faculty/ Industrialist in the field of Life Sciences (ZBC, Biotechnology, Biochemistry, Microbiology etc.) Pharmacy (D. Pharm, B. Pharm. M. Pharm), Medicine, Medical Professionals, company professionals etc.

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Computational Biochemistry & Computer Aided Drug Design (Code:ST101)

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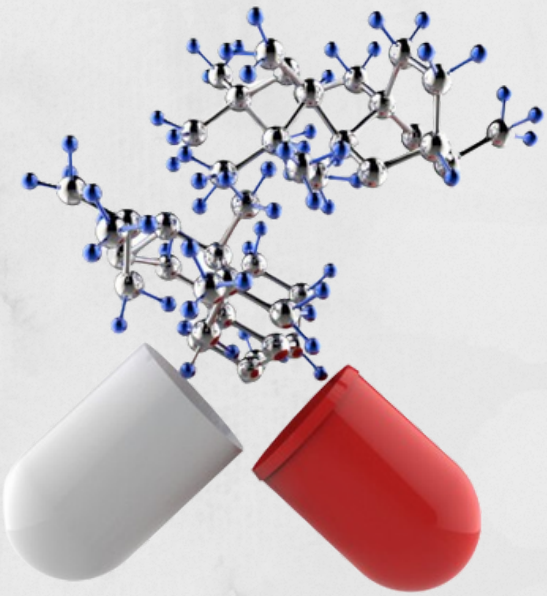
MODULE I

- Introduction of Computational Biochemistry and Bioinformatics
- Protein Structure properties
- Retrieval of data from protein Databases
- Introduction to Molecular modelling techniques
- Molecular Dynamics Simulations
- Medicinal Chemistry Informatics
- Drug discovery Processes



MODULE II

- Introduction to Computer aided drug design (CAAD): Methods-Structure
- Ligand based drug design
- Chemoinformatic for Biomedical drug discovery
- Quantitative Structure Activity Relationship
- Drug Designing approaches to COVID19

MODULE III

- Protein 3D Structure Prediction by software
- Protein structure visualization using PYMOL and Discovery studio software
- Preparation of drug/metabolite ligand
- Active site prediction of enzyme
- Molecular Docking and Drug design software installation and Process
- DLG file analysis
- Result analysis and interpretation

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Homology Modelling (Code:ST102)

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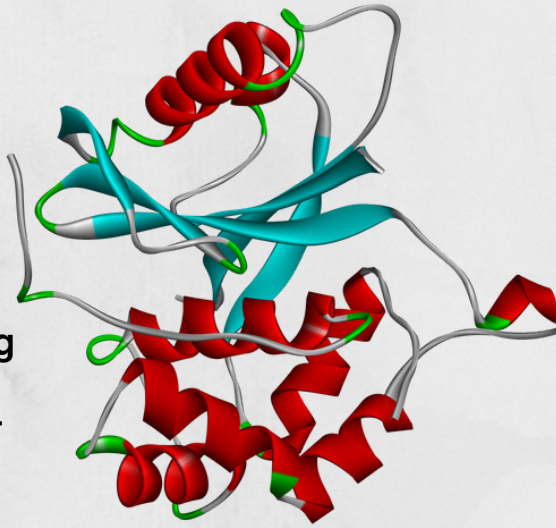
MODULE I

- Basics of Bioinformatics
- Basics of protein & molecular structure of protein
- Protein databases & 3D structure prediction
- Retrieval of data from PDB
- Retrieval of data from PIR and SWISSPROT
- KEGG Server



MODULE II

- Introduction & applications of homology modelling
- Role of homology modelling in virtual drug design
- Online databases of homology modelling (SWISS-MODEL & DALI)
- Understanding of PDB, SDF, Mol files

MODULE III

- Installation of software MODELLER and PYMOL
- Technique for homology modelling employing modeller software
- Preparation of script files and input files
- Template recognition & initial alignment, backbone generation
- Loop modelling, side chain modelling
- Model validation and result analysis

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Molecular Docking (Code:ST103)

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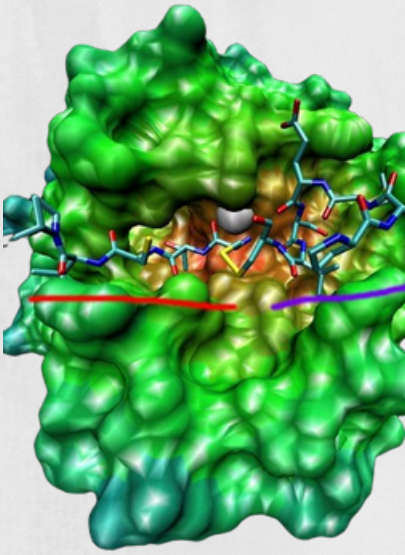
MODULE I

- Overview of Basic Bioinformatics
- Overview of drug discovery and computational methods
- Understand molecular docking & Structure based Drug Design
- Literature study and acquisition of disease target structure
- Lead molecule identification and optimization.



MODULE II

- Understanding of Molecular docking tools and software
- Installation of Software Discovery Studio
- MGL Tool
- Cygwin
- PYMOL

MODULE III

- Protein (disease target) structure validation and Preparation
- Active site Prediction
- Ligand optimization and docking parameters.
- Preparation of PDBQT, DPF and GPF files
- Running docking commands
- Building protein-ligand complex
- Visualization of protein-ligand interactions
- Pose Selection (publication standard)
- Result analysis and interpretation

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Molecular Dynamics Simulation (Code: ST104)

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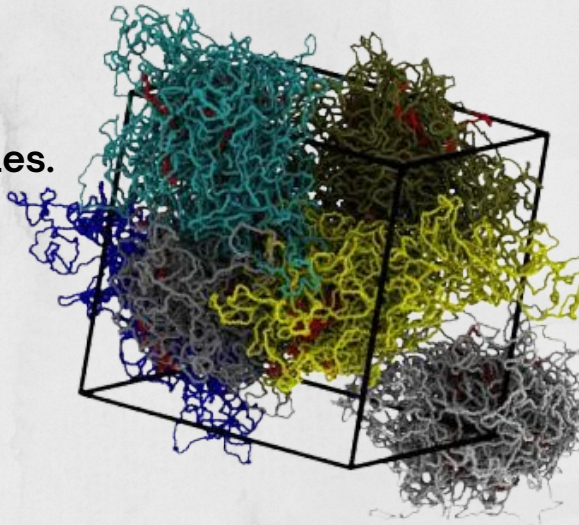
MODULE I

- Introduction to Bioinformatics
- Introduction to Molecular Dynamics Simulation
- Installation of Ubuntu on Window OS
- Installation of software required for simulations (GROMACS)

MODULE II

- Systemic Protocol of Simulation
- Cleaning and preparation of protein and ligand files.
- Solvent selection and solvation box definition.
- Energy minimization and Heating (300K)
- Equilibration (NVT& NPT)



MODULE III

- Role of ions and energy minimization.
- System equilibration and production MD.
- Result analysis by calculating RMSD, RMSF and PCA
- Result Interpretation

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Genomics and Proteomics (Code: ST105)

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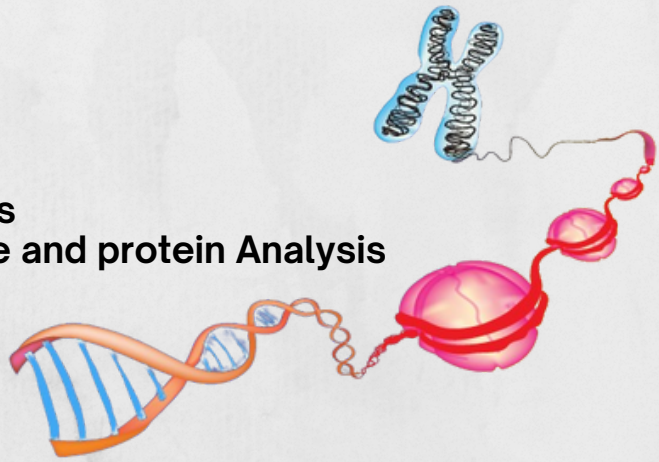
MODULE I



- Introduction to Bioinformatics
- Basics of Molecular Biology
- Understanding of Genomics and Proteomics
- Bioinformatics tools and Server for Genome and protein Analysis

MODULE II

- Genomics Analysis: Gene Structures and Features
- Genomics Analysis: Promoter and Regulatory Elements Analysis
- Genomics Analysis: Genome Assembly and Annotation
- Genomics Analysis: Retrieval of a Gene-Protein-Chromosomal Region
- Genomics Analysis: Transposable Elements Detection
- Genomics Analysis: Regulatory Site Detection and BLAST analysis

MODULE III

- Proteomics analysis: Protein Databases, Retrieval of data and Analysis
- Proteomics analysis: Protein Structure Prediction
- Proteomics analysis: Structure Visualization and Analysis
- Proteomics analysis: Introduction to Molecular Modelling Database (MMDB)
- Proteomics analysis: Active site, binding site and domain analysis of Protein
- Proteomics analysis: Antigenic protein, epitope analysis

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Bioinformatics Data Resources & Biological Sequence Analysis, Phylogeny (Code: ST106)

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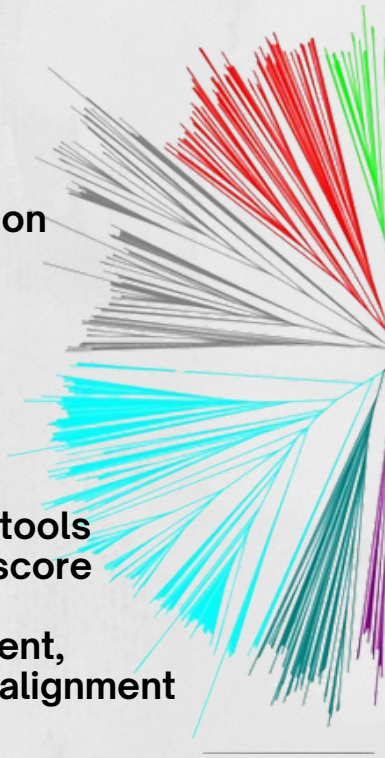
MODULE I

- Importance of Data and Databases in Bioinformatics
- Types of Databases: Primary secondary and Composite
- Nucleotide (DNA & RNA) and Protein Databases
- Structural and Functional Databases
- Major resources and services at NCBI
- ENSEMBL, NCBI-Genome, Gene-Protein-Chromosomal Region
- Molecular Modelling Database (MMDB)
- Introduction to InterPro-Protein Family



MODULE II

- Introduction of Sequence Alignment
- Homology, Similarity & Identity, Scoring matrices, EMBOSS tools
- NCBI Blast programs, Result analysis using E-value and Bit score
- HMMER, Sequence alignment programs
- Different approaches to perform Multiple Sequence Alignment,
- Best strategies to perform pairwise and multiple sequence alignment
- Databases of Multiple sequence alignment

MODULE III

- Principles of molecular phylogeny and evolution
- Stages of Phylogenetic Analysis
- Distance-Based, Character based & Model-Based Phylogenetic Inference
- Model based phylogenetic inference (ML),
- Software installation PHYLIP, & MEGA
- Evaluation of phylogenetic trees, and Phylogenetic networks

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Bioinformatic Approaches for Comparative Analysis of Viruses (Code: ST107)

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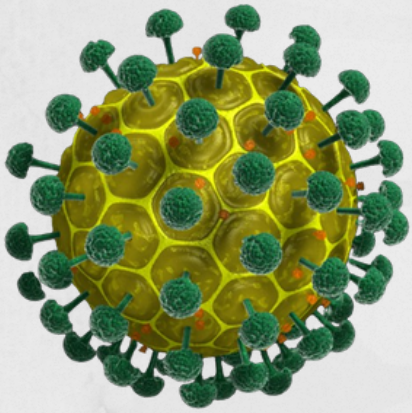
MODULE I

- Virus: Introduction and History
- Bioinformatics resources for Virus
- National Center for Biotechnology Information (NCBI): Viral Genome analysis
- Understanding of Viral Bioinformatics Resource Center (VBRC)
- Metavir Analysis of Viromes server: Annotate Viral Metagenomic Sequences

MODULE II

- Applications of Comparative analysis of Genome
- Grouping of the Viral Genomes by BLAST
- Evalution of Blast Results
- Whole Genome Sequence Analysis of Virus (SARS-CoV2)
- Whole Genome Sequence Alignment
- Result analysis of Sequence Alignment



MODULE III

- Viruses from Environmental Samples
- Access the Metavir Online Platform
- Upload Sequences to Analyze
- Taxonomic Composition Analysis for relative abundance of taxa
- Virome Comparisons and Phylogenetic Analysis

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Secondary structure prediction of 16S ribosomal RNA of Bacteria (Code: ST108)

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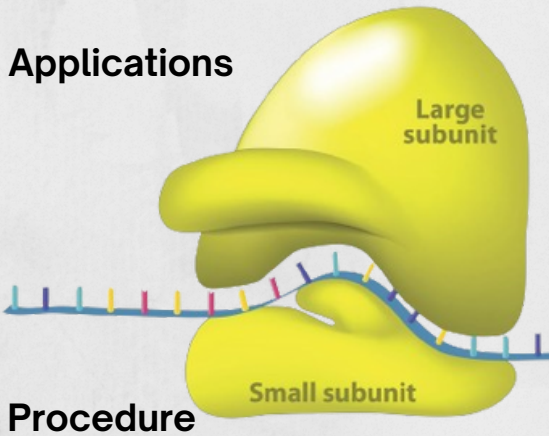
MODULE I

- Introduction to Bioinformatics
- Understanding 16S rRNA: Features, Functions, and Applications
- Detection of 16S rRNA Gene
- Analysis of 16S rRNA Sequence
- rRNA Gene Sequencing
- Databases of 16S rRNA



MODULE II

- Retrieval of 16S rRNA Sequence Methodology and Procedure
- Download of FASTA Sequence of 16S rRNA
- Graphical Analysis of 16S rRNA
- Preparation of 16S rRNA FASTA sequence in Sequence Massager

MODULE III

- Introduction of RNA Fold WebServer
- Analysis procedure of 16S rRNA secondary Structure in RNA Fold WebServer
- Minimum Free Energy Prediction for Secondary Structure
- MFOLD Energy Dot Plot analysis for Secondary Structure
- Graphical Output of Secondary Structure
- Minimum Free Energy (MFE) Structure prediction Using loop-based energy model and the Dynamic Programming Algorithm
- Analysis of thermodynamic Ensemble of RNA structures and the Centroid structure

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Bioinformatics: Comparative and Prediction tools (Code: ST109)

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MODULE I

- Introduction to Bioinformatics
- Nucleotide and Protein Databases
- Major resources and services at NCBI
- Understanding of File Formats in Bioinformatics
- NCBI-BLAST Introduction and Applications

MODULE II

- Introduction of Sequence Alignment and Phylogeny
- Local and Global Sequence Alignment
- BLAST Database Searching
- EMBOSS NEEDLE: Global Alignment of Sequences
- CLUSTAL OMEGA: Most Reliable Multiple Sequence Alignment Tool
- Installation of Mega Software
- MEGA tool: Multiple Sequence Alignment and Phylogenetic Analysis

MODULE III

- Gene Prediction tool and Analysis
- ORF Finder Tool
- GenBank (Sequence Annotation Format), FASTA
- Prediction of potential cleavage sites by ExPasy web tool
- Secondary structure prediction tool
- PubChem and Drug bank Introduction and analysis
- Prediction of Druglike Properties and ADME/T
- Prediction of Toxicity of Chemical Compounds

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Computer-Aided Prediction of Pharmacokinetic (ADMET) Properties (Code: ST110)

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MODULE I

- Introduction to Bioinformatics and Computer-Aided Drug Design
- Introduction of Pharmacokinetics
- Understanding of Lipinski's Rule of Five (Druglikeness)
- Retrieval of 3D structure and Mol file of Chemical Compounds
- Mol file conversion to PDB file by Discovery Studio Software

MODULE II

- Absorption, Distribution, Metabolism and Excretion Analysis
- Understanding of CaCo2 and GI Absorption
- Evaluation of PMDCK, BBB, PPB, HIA
- Cytochrome enzyme Inhibition Analsysis
- Use of ProTox II and ADMET Lab 3.0 Server
- PreADMET and SwissADME Server

MODULE III

- Prediction of Druglike Properties of Drug Candidates
- Prediction of Toxicity of Chemical Compounds
- Prediction of Carcinogenicity and Mutagenicity of Chemical Compounds
- Evaluation of Hepatotoxicity, Nephrotoxicity, Cytotoxicity
- Evaluation of Respiratory toxicity, Neuro and Cardiotoxicity
- Predict Immunotoxicity, BBB-barrier Ecotoxicity of Drug Candidates
- Prediction of Clinical toxicity and Nutritional toxicity
- Study of Tox21 Stress response pathways

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