MODULES & TOPICS

Module-1 Introduction to Bioinformatics and CADD (360 Mins)

- Introduction to CADD and Essentials of Bioinformatics & Cheminformatics
- CADD Databases, tools and Resources: PDB, PubChem, UniProt, KEGG, Zinc, DrugBank, Chembl, MMsINC, STITCH, STRING, GENECARD, MALACARDS

Module-2 Basics of Pharmacology and PharmacoInformatics (780 Mins)

- Basics of Pharmacology: Pharmacokinetics and Pharmacodynamics,
- Molecular Descriptors and Lipinski Rule of five.
- QSAR : 2D and 3D. Applications of QSAR and use in VS.
- ADME and Toxicity properties of drugs
- Chemistry of drug-metabolism, drug deactivation and elimination
- Drug-receptor interactions
- **Tools of Pharmacoinformatics and CADD**
    - Prediction of Physico-chemical properties (VCCLAB,ChEMBL, Chemaxon),
    - Prediction of ADME/T properties (admetSAR, ADMETlab etc).
    - Drug dose Response (EC50, IC50, ED50, TD50, LD50) and Therapeutic index, Lipophilicity (ALOGPS 2.1),
    - Toxicity Analysis and Prediction (protox_II, lazar,ToxiM).

Module-3 Molecular Modelling, Docking and Simulations Techniques (480 Mins)

- Molecular Sketching and SMILES
- Molecular Modelling of Proteins: Prediction Tools
- Molecular Docking: Methods and Principles
- Basics Molecular Simulation Methods: Molecular & Quantum Mechanics

- Molecular Dynamics Simulations: Forcefield and PE functions.
- Fine and Coarse-grain Simulations techniques

Module-4 In-silico Drug Design: Methods (720 Mins)

- Basic of Drug Discovery Process and Clinical Trials
- In-Silico Drug designing approaches: Structure based (Rational), Ligand based, Pharmacophore based methods.
- Drug Targets, Lead Identification & Optimization: Druggable Genome and Known Drug Targets, Pathway Analysis.
- Pharmacophore and Molecular Descriptor Analysis.
- High-throughput Virtual Screening and Combinatorial Library Designing.

Module-5 Artificial Intelligence and Machine learning in CADD (720 Mins)

- Artificial Intelligence(AI) and Machine Learning(ML) in Drug Discovery: Google Collab, Knime, Orange tool etc.
- Data Mining and Image Processing using Python:
- ANN and Deep learning Applications
- NLP and its applications in Drug Discovery

Module-6 Advance Topics (480 Mins)

- Immunoinformatics and Vaccine Design: Reverse Vaccinology.
- Multi-Epitope Vaccine design: Methods and Pipelines
- Drug Repurposing, Scaffold Hopping, Multitarget Analysis
- NGS, Systems Biology and Regulatory Networks in CADD.
- Bioethics and Drug Regulatory Procedures.