TRAINING MODULE – MOLECULAR DOCKING AND DYNAMICS

COURSE DURATION: 7 DAYS

DAY 1: Introduction to Molecular Docking and Computational Biology Tools

- Fundamentals of Molecular Docking and Drug Discovery (MDD)
- Protein structure and functions insights
- Database overview
- Tools and software walkthrough

DAY 2: Protein and Ligand Structure Preparation

- Preparation of the protein and ligand structure using tools like PyMOL or Chimera to optimize protein structures for docking
- Quality control and structure verification for errors or clashes in prepared protein and ligand structures to ensure accuracy in docking studies

DAY 3: Blind Docking and Preliminary Analysis

- Perform Docking with the prepared protein and ligand structure using AutoDock Vina
- Analysis and interpretation of the docked protein and ligand structure using Chimera-X or Discovery Studio

DAY 4: Targeted Docking and Detailed Analysis

- Perform targeted docking with an emphasis on specific binding sites
- Comparing results with blind docking outcomes to assess pose consistency and energy profiles
- Analysis and interpretation of the docked protein and ligand structure
- Visualizing and interpreting protein-ligand complexes using Chimera-X or Discovery Studio and analysing binding site residues

DAY 5: Running MD Simulation

- Preparing the protein-ligand complex for simulation, solvation, ionization, and energy minimization
- Executing the simulation and observing the stability of the protein-ligand interaction over time using GROMACS

DAY 6: Data Analysis and Report Generation

- Analyzing simulation trajectories: RMSD, RMSF, hydrogen bonds, and interaction stability
- Final interpretation of MD simulation results to assess complex stability and binding reliability

DAY 7: Report Submission and Certificate Distribution