Cheminformatics Internship

Research approaches used in the field of applied cheminformatics to address basic, therapeutic, and industrial research at NTHRYS BIOTECH LABS:

QSAR Modeling

Quantitative Structure-Activity Relationship modeling to predict biological activity of molecules.

2.

Molecular Docking

Predicting the binding affinity and mode of interaction between ligands and target proteins.

4.

Molecular Dynamics Simulation

Simulating the motion of molecules over time to study their behavior.

6.

Data Mining

Extracting valuable information from large datasets for insights and trends.

8.

Network Analysis

Studying molecular interactions through network-based approaches.

10.

Therapeutic Research

11.

ADME/Tox Prediction

Assessing Absorption, Distribution, Metabolism, Excretion, and Toxicity properties.

13.

Structure-Based Drug Design

Designing ligands based on target protein structure.

15.

Polypharmacology Prediction

Identifying compounds that can target multiple proteins.

17.

Biological Network Analysis

Integrating chemical and biological networks for drug discovery.

19.

Cheminformatics in Personalized Medicine

Tailoring drug candidates based on individual genetic information.

High-Throughput Screening

Rapidly testing large libraries of compounds for desired properties.

22.

Chemical Process Optimization

Using cheminformatics to optimize chemical synthesis routes.

24.

Predictive Modeling for Material Properties

Designing novel materials with desired properties.

26.

Quality Control

Using cheminformatics to ensure consistency and quality in manufacturing.

28.

Green Chemistry

Applying computational methods to design environmentally friendly chemical processes.

30.