Cheminformatics Training Program

NTHRYS Biotech Labs offers Cheminformatics Training Program under below mentioned protocols. Candidates can opt their interested protocols from the list below. Please click **Join** button to pay the fee for selected protocol. Fees should be paid individually for all the selected protocols separately by clicking the button. Please save the payment proofs and send them as an attachment to
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Please Check Modules as well as individual protocols (if any) under this training program. Module has its fee given in the fee structure table and individual fee in its block. Please communicate with our Help Desk Team via whatsapp on +91-8977624748 for any queries.

Modules

Module I: Molecular Modeling and Drug Design

1. **Introduction to Molecular Modeling**
    - Overview of molecular modeling in drug design
    - Importance of molecular modeling in understanding drug-receptor interactions
2. **Computational Methods in Molecular Modeling**
    - **Quantum Mechanics (QM)**
        - Basics of QM in molecular modeling
        - Application of QM in electronic structure determination
        - **Tools:** Avogadro, Psi4 (for quantum chemical calculations)
    - **Molecular Mechanics (MM)**
        - Force fields in MM
        - Energy minimization and molecular dynamics simulations
        - **Tools:** GROMACS, OpenMM (for molecular dynamics simulations)
    - **Hybrid QM/MM Methods**
        - Principles of QM/MM hybrid methods
        - Applications in studying enzyme mechanisms
        - **Tools:** CP2K (for hybrid QM/MM simulations)
3. **Ligand-Based Drug Design**

- **Pharmacophore Modeling**
  - Identification and analysis of pharmacophoric features
  - Pharmacophore-based virtual screening
  - **Tools:** RDKit, Open3DQSAR (for pharmacophore modeling and analysis)
- **Quantitative Structure-Activity Relationship (QSAR)**
  - Development of QSAR models
  - Application of QSAR in predicting biological activity
  - **Tools:** KNIME, WEKA (for QSAR model development and analysis)

4. **Structure-Based Drug Design**
   - **Docking**
     - Principles of molecular docking
     - Docking methods and scoring functions
     - **Tools:** AutoDock Vina, Dock (for molecular docking studies)
   - **Molecular Dynamics (MD) Simulations**
     - Application of MD in understanding biomolecular interactions
     - Role of MD in drug design
     - **Tools:** NAMD, LAMMPS (for conducting molecular dynamics simulations)
5. **Case Studies and Applications**
   - Detailed walkthroughs of successful drug design projects
   - Analysis of challenges and solutions in molecular modeling

Module II: Chemoinformatics Data Analysis and Machine Learning

1. **Introduction to Chemoinformatics Data**
   - Overview of data types in chemoinformatics
   - Understanding chemical structures and properties
2. **Data Preprocessing and Feature Engineering**
   - Techniques for data cleaning and normalization
   - Feature extraction and selection for chemical data
   - **Tools:** RDKit (for molecular feature extraction), Pandas (for data manipulation)
3. **Machine Learning in Chemoinformatics**
   - **Supervised Learning for Predictive Modeling**
     - Classification and regression models
     - Model evaluation and validation techniques
     - **Tools:** scikit-learn (for building machine learning models), TensorFlow (for deep learning)
   - **Unsupervised Learning and Clustering**
     - Exploratory data analysis and pattern discovery
     - Clustering techniques for chemical data
     - **Tools:** scikit-learn (for clustering algorithms), seaborn (for visualization)
4. **Chemical Databases and Information Retrieval**
   - Overview of major chemical databases (e.g., PubChem, ChEMBL)
   - Techniques for querying and retrieving chemical data

- **Tools:** ChemSpider API, RDKit (for database access and manipulation)

5. **Case Studies in Chemoinformatics**
   - Real-world examples of machine learning applications in chemoinformatics
   - Discussion on the impact of data analysis in drug discovery and development

Module III: Chemical Database Management and Integration

1. **Introduction to Chemical Database Management**
   - Principles of database management in chemoinformatics
   - Types of chemical data and databases
2. **Designing Chemical Databases**
   - Database models and schemas for chemical data
   - Best practices in database design and normalization
   - **Tools:** MySQL, PostgreSQL (for relational database management), MongoDB (for NoSQL databases)
3. **Managing Chemical Data**
   - Data ingestion, storage, and retrieval strategies
   - Ensuring data integrity and security
   - **Tools:** RDKit (for chemical data manipulation), SQLite (for embedded database management)
4. **Integrating Chemical Databases**
   - Strategies for integrating heterogeneous chemical data sources
   - Use of APIs and web services for data access and sharing
   - **Tools:** Open Babel (for data format conversion), Apache NiFi (for data flow automation)
5. **Visualization and Reporting**
   - Techniques for visualizing chemical data and analysis results
   - Tools for generating interactive reports and dashboards
   - **Tools:** Jupyter Notebook (for interactive data analysis and visualization), Dash by Plotly (for creating web-based data dashboards)
6. **Case Studies and Applications**
   - Examples of successful chemical database management projects
   - Lessons learned from challenges in database integration and management

Module IV: Chemical Information Visualization and Chemometrics

1. **Introduction to Chemical Visualization**
   - Importance of visualization in cheminformatics
   - Overview of chemical visualization techniques
2. **Chemical Structure Visualization**
   - Different methods for depicting chemical structures
   - 2D and 3D visualization of molecular structures

    - **Tools:** Avogadro, Jmol (for 3D molecular visualization)
3. **Data Visualization in Chemoinformatics**
    - Visualizing chemical properties and datasets
    - Use of graphs, charts, and heatmaps for data analysis
    - **Tools:** Matplotlib, Seaborn (for data visualization in Python), D3.js (for interactive web visualizations)
4. **Introduction to Chemometrics**
    - Basics of chemometrics and its applications in cheminformatics
    - Preprocessing and analysis of chemical data
5. **Chemometric Methods for Chemical Data Analysis**
    - Principal Component Analysis (PCA) for data dimensionality reduction
    - Cluster analysis for grouping chemical compounds
    - Regression analysis for predicting chemical properties
    - **Tools:** scikit-learn (for PCA and clustering), R (for statistical analysis and visualization)
6. **Case Studies in Chemical Visualization and Chemometrics**
    - Real-world examples of visualization and chemometrics in research
    - Discussion on the impact of these techniques on drug discovery and chemical analysis

Module V: Bioinformatics for Cheminformatics

1. **Introduction to Bioinformatics in Cheminformatics**
    - Overview of bioinformatics and its relevance to cheminformatics
    - Interdisciplinary approaches to studying biological and chemical systems
2. **Sequence Analysis and Cheminformatics**
    - Basics of sequence analysis in bioinformatics
    - Application of cheminformatics tools in analyzing biological sequences
    - **Tools:** BioPython (for sequence analysis), RDKit (for chemical informatics)
3. **Protein-Ligand Interactions and Drug Design**
    - Understanding protein-ligand interactions in drug design
    - Use of cheminformatics and bioinformatics tools to predict binding affinities
    - **Tools:** AutoDock Vina (for docking simulations), PyMOL (for visualizing protein-ligand interactions)
4. **Integrating Chemical and Biological Databases**
    - Strategies for the integration of chemical and biological data
    - Exploring the use of integrated databases in research and development
    - **Tools:** UniProt (for protein sequence and function), PubChem (for chemical structures and properties)
5. **Systems Biology in Cheminformatics**
    - Introduction to systems biology and its applications
    - Modeling and simulation of biological systems using cheminformatics tools
    - **Tools:** Cytoscape (for network visualization), COPASI (for biochemical network simulation)
6. **Case Studies in Bioinformatics and Cheminformatics**

- Examples of successful applications at the intersection of bioinformatics and cheminformatics
- Impact of interdisciplinary research on drug discovery and molecular biology

Module VI: Regulatory Aspects and Data Standards in Cheminformatics

1. **Introduction to Regulatory Compliance**
   - Overview of regulatory landscape in pharmaceuticals and chemicals
   - Importance of compliance in cheminformatics workflows
2. **Regulatory Guidelines and Standards**
   - Key regulatory bodies and their guidelines (FDA, EMA, ICH)
   - Understanding data standards (e.g., CDISC, SEND)
3. **Data Management and Integrity**
   - Principles of good data management practices
   - Maintaining data integrity in cheminformatics databases
   - **Tools:** OpenClinica (for clinical data management), KNIME (for data processing and compliance checking)
4. **Chemical Safety and Reporting**
   - Chemical safety regulations (REACH, GHS)
   - Reporting and documentation requirements
   - **Tools:** IUCLID (for chemical data reporting), OpenTox (for toxicity prediction)
5. **Data Standards and Interoperability**
   - Importance of data standards for interoperability
   - Adopting standard formats (e.g., SMILES, InChI) for chemical data
   - **Tools:** Open Babel (for data format conversion), RDKit (for chemical informatics and standardization)
6. **Case Studies on Regulatory Compliance**
   - Examples of compliance challenges and solutions in cheminformatics
   - Impact of regulatory considerations on drug discovery and chemical safety

Module VII: Emerging Technologies and Future Trends in Cheminformatics

1. **Artificial Intelligence in Cheminformatics**
   - Overview of AI and machine learning applications in cheminformatics
   - Deep learning for structure-activity relationship modeling
   - **Tools:** TensorFlow, PyTorch (for deep learning); RDKit, DeepChem (for cheminformatics)
2. **Blockchain for Chemical Data Security**
   - Understanding blockchain technology and its applications in cheminformatics
   - Use cases for blockchain in ensuring data integrity and security
   - **Tools:** Ethereum, Hyperledger (for blockchain development)
3. **Quantum Computing in Molecular Simulations**

- Basics of quantum computing and its potential impact on cheminformatics
- Quantum algorithms for molecular simulations
- **Tools:** Qiskit, Microsoft Quantum Development Kit (for quantum computing)

4. **Cloud Computing and Big Data in Cheminformatics**
   - Advantages of cloud computing for cheminformatics applications
   - Handling big data in chemical research
   - **Tools:** AWS, Google Cloud Platform (for cloud computing); Apache Hadoop, Spark (for big data)
5. **Personalized Medicine and Cheminformatics**
   - Role of cheminformatics in personalized medicine
   - Integrating chemical and genomic data for personalized drug discovery
   - **Tools:** BioPython (for genomic data analysis); RDKit (for chemical informatics)
6. **Case Studies on Innovative Applications**
   - Exploring cutting-edge research and breakthroughs in cheminformatics
   - Future directions and challenges in the field

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Training based on Individual Protocols

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Rs 480 /-

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