School of Pharmaceutical Sciences & Technology

Curriculum for
Fellowship Program in

PHARMACOINFORMATICS

Malla Reddy Vishwavidyapeeth
(Deemed to be University)
Suraram, Hyderabad Telangana 500055
Email : info@mrvv.edu.in, Phone : 950 777 9999

Course Title: PHARMACOINFORMATICS
Course Type: FELLOWSHIP
Duration: 360 Hours (can be structured as 24 Credits)
Mode: Lectures, Practicals/Hands-on, Project

Overview

The Fellowship in Pharmacoinformatics is a specialized program designed to provide knowledge and practical skills in applying informatics and computational tools to pharmaceutical sciences. The program integrates concepts of drug discovery, bioinformatics, cheminformatics, and data analytics to support modern pharmaceutical research. Delivered over 360 hours (24 credits) through lectures, hands-on practicals, and a project, the fellowship equips participants with industry-relevant skills for careers in pharmaceutical R&D, clinical research, regulatory informatics, and academia.

Objectives:

Upon completion of the course, the fellow shall be able to:

- To provide fundamental and advanced knowledge of pharmacoinformatics and its role in modern drug discovery and development.
- To develop practical skills in using computational tools, databases, and software for pharmaceutical data analysis.
- To train participants in in silico techniques such as molecular modeling, virtual screening, and ADMET prediction.
- To enhance understanding of clinical, pharmacokinetic, and regulatory data management using informatics approaches.
- To foster research aptitude, analytical thinking, and industry readiness through hands-on training and project work.

Course Outcome:

CO1: Explain the principles and applications of pharmacoinformatics in drug discovery, development, and regulatory sciences.
CO2: Apply computational and informatics tools to analyze pharmaceutical, biological, and clinical datasets.
CO3: Perform in silico techniques such as molecular modeling, docking, virtual screening, and ADMET prediction.
CO4: Interpret pharmacokinetic, pharmacodynamic, and clinical data using appropriate data management and analytical approaches.
CO5: Design and execute a project addressing real-world pharmaceutical problems using pharmacoinformatics methodologies.

Teaching & Learning Methods:

Teaching and learning methods include interactive lectures for conceptual clarity, hands-on practical sessions using pharmacoinformatics tools, live demonstrations, project-based learning for real-world application, and self-directed and collaborative activities to enhance analytical and problem-solving skills.

Syllabus

Theory - 10 Credits (150 Lecture Hours)

Module 1: Bioinformatics & Cheminformatics Foundations (30 hours)

- Bioinformatics: Scope, history, and biological databases.
- Sequence Analysis: Global and local alignment algorithms.
- Cheminformatics: Molecular descriptors, representations, similarity, and drug-likeness rules.
- Structural Biology: Protein structure prediction and basics of X-ray and NMR analysis.

Module 2: Computer-Aided Drug Design (CADD) (30 hours)

- Structure-Based Drug Design: Target identification, active site analysis, docking approaches, and scoring functions.
- Ligand-Based Drug Design: Pharmacophore modeling and 2D/3D QSAR techniques.
- Virtual Screening & ADMET: Virtual screening workflows and in silico ADMET prediction.

Module 3: Pharmacogenomics & Genomic Informatics (30 hours):

- Genomic Foundations: Human genetic variations and their role in drug transport and metabolism.
- Pharmacogenomic Applications: Clinical case studies and genomic data integration in therapy decisions.
- NGS Data Analysis: DNA/RNA sequencing workflows, variant annotation, and GWAS interpretation.

Module 4: Clinical Data Management (30 hours):

- Healthcare Data Ecosystem: EHR/CPOE architecture, interoperability standards, and pharmacy information systems.
- Clinical Trial Informatics: Clinical data management systems, regulatory compliance, and data standards.
- Pharmacovigilance Informatics: Signal detection, ADR reporting, and real-world evidence in post-marketing surveillance.

Module 5: Molecular Dynamics & AI in Pharma (30 hours):

- Molecular Dynamics Simulations: Force fields, solvation models, trajectory analysis, and stability metrics.
- AI & Machine Learning: ML methods, deep learning for drug design, and NLP for literature mining.
- Ethics & Regulatory Informatics: Data privacy, ethical AI, and IP considerations in digital health.

Practical/Hands-on Component: 8 Credits (120 Lab Hours)

1. Practical Training in Bioinformatics and Cheminformatics Tools

- Database Mining: Retrieval of 3D protein structures (PDB) and small molecule data (PubChem/ZINC).
- Sequence Analysis: Performing multiple sequence alignment (MSA) and phylogenetic tree construction.
- Cheminformatics Lab: Visualizing chemical spaces, calculating LogP/Rule-of-5 properties, and converting chemical formats using OpenBabel. Tool Focus: NCBI Entrez, PyMOL, ChemDraw.

2. Practical Training in Molecular Docking and Virtual Screening :

- Protein & Ligand Prep: Cleaning PDB files, adding hydrogens, and generating 3D conformations of ligands.
- Molecular Docking: Executing docking simulations between a lead molecule and a disease target (e.g., COX-2 or Protease).
- Virtual Screening: Screening a library of 1,000+ compounds to identify potential hits.
- Analysis: Interpreting binding energy (ΔG) and visualizing H-bond/hydrophobic interactions, Tool Focus: AutoDock Vina, Biovia Discovery Studio, SwissDock.

3. Practical Training in Pharmacogenomics and Genomic Data Analysis

- Variant Analysis: Using Genome Browsers to identify drug-response-related SNPs.
- Clinical Correlation: Navigating PharmGKB to find dosing guidelines based on specific genotypes.
- Pathway Mapping: Visualizing drug action pathways and identifying genetic bottlenecks using KEGG.
- Tool Focus: PharmGKB, UCSC Genome Browser, KEGG Pathway Database.

4. Practical Training in Clinical Data Management and Trial Informatics

- Database Building: Designing an eCRF for a mock Phase II clinical trial.
- Data Cleaning: Performing edit checks, discrepancy management, and query generation.
- Statistical Reporting: Basic data analysis of patient outcomes using R or SAS-lite.
- Tool Focus: REDCap (Open Source), Oracle Clinical (Demo), or OpenClinica.

5. Practical Training in Molecular Dynamics and AI-Based Drug Discovery

- MD Setup: Prepare protein-ligand complex with solvation and neutralization.
- Trajectory Analysis: Calculate RMSD and RMSF to assess stability.
- AI Lab: Predict drug-target interactions using machine learning models.
- Tools: GROMACS, Scikit-learn, Google Colab.

Project: 6 Credits (90 Self Study/Research Hours)

A mandatory Project (6 credits) provides practical application. Projects typically involve database mining, SBDD/LBDD, virtual screening, ADMET prediction, molecular docking, MD simulations, and AI/ML tools to identify potential drug candidates, analyze genetic-drug interactions, and predict pharmacokinetic and pharmacodynamic properties, demonstrating applied computational skills.

References:

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