Course Code	Course Title	L	T	P	C
BABIT309	**Pharmacoinformatics and Pharmacovigilance**	**3**	**0**	**2**	**4**
Pre-requisite	BABIT202 - Fundamentals of Bioinformatics	**Syllabus Version**			
		1			

Course Objectives

1. Outline the drug discovery and development process
2. Understand emerging strategies and tools of computer-aided drug design
3. Illustrate the principles of chemo informatics in drug discovery and understand drug safetyrelated to drug development and use

Course Outcomes

1. Provide deeper understanding of drug discovery process
2. Understand the workflow in structure-based drug design
3. Understand the fundamental issues and challenges of machine learning
4. Identify opportunities for healthcare informatics interventions
5. Identify drug safety and regulation

Module:1	**Introduction to Drug Discovery**	**9 hours**

Drug discovery process; Target identification, Target validation, Hit identification and lead discovery; Lead optimization; Precise medicine; Clinical testing and beyond

Module:2	**Data Types and Resources**	**9 hours**

Chemical compounds - SDF format, InChI and InChI key format, SMILES and SMART formats, Fingerprint format; Other descriptors; Similarity measures; Data resources – Toxicity related database, Drug safety database.

Module:3	**Target Identification and Validation**	**8 hours**

Target identification predictions; Gene prioritization methods; Machine learning and knowledge graphs indrug discovery; Data, Data mining and natural language processing for information extraction.

Module:4	**Hit Discovery and Lean Optimization**	**9 hours**

Chemical space; Screening methods, High-throughput screening, Computer aided drug discovery, Virtual screening; Candidate learning algorithms – Naïve Bayes, k-nearest neighbors, Support vector machine; Lead optimization, Applications of machine learning in lead optimization; Assessing ADMET and biological activities properties; Matched molecular pairs.

Module:5	**Evaluating safety and Toxicity**	**8 hours**

In silico nonclinical drug safety; Machine learning approaches to toxicity prediction, k- nearest neighbors, Logistic regression; Pharmacovigilance and drug safety; Data sources; Disproportionality analysis.		
Module:6	**Contemporary Topics**	**2 hours**
Contemporary Topics		
	Total Lecture Hours:	**45 hours**
Text Book(s)		
Ashenden SK,, "**The Era of Artificial Intelligence, Machine Learning, and Data Science in the Pharmaceutical Industry** ", Academic Press, An imprint of Elsevier, London, UK., 1st Edition, **2021**		
Reference Books		
Wager K A, Lee, F W, & Glaser J P, "**Health care information systems: A practical approach for health care management**", Wiley Brand, San Francisco, California, USA., 4th Edition, **2017**		
Indicative Experiments		
1. Introduction to databases, webservers, tools used in chemo-informatics.		3 hours
2. Introduction to data file types, formatting, retrieval, and processing		3 hours
3. Drug target identification using public databases and tools like DrugBank, DisGeNET, and STRING		3 hours
4. Molecular fingerprint generation, similarity search, and identification of compounds.		3 hours
5. Virtual screening of compounds against a drug target of target disease.		3 hours
6. Evaluation of Drug likeness and ADMET properties, and other toxicity analysis		3 hours
7. Introduction of AI/ML in pharmacoinformatics and pharmacovigilance		3 hours
8. Machine Learning for Drug Activity Classification		3 hours
9. QSAR model development using WEKA or Python ML libraries.		3 hours
10. Pharmacovigilance signal detection: Conduct a disproportionality analysis (e.g., reporting odds ratio, PRR) using simulated or public datasets to detect adverse drug reactions using vigibase data.		3 hours

Total Laboratory Hours:	**30 hours**
Mode of Evaluation : Continuous Assessment Test, Digital Assignment, Quiz, Final Assessment Test, Lab Continuous Assessment, Lab Final Assessment	
Recommended by Board of Studies :	26-05-2025
Approved by Academic Council : No. 78	12-06-2025