VIT
Vellore Institute of Technology
(Deemed to be University under section 3 of UGC Act, 1956)

Office of Academic Research

Details of the Research Scholar					
Name	**Dhivya G**			Register No.	**24PDT0002**
Programme	**Ph. D (Deep Tech)**	School	**SBST**	Category	**IFT**
Topic of Research	**A study on the detection and validation of Protein-Protein Interaction Inhibitors for Cystic Fibrosis treatment using Machine Learning-driven virtual screening approach**				

Details of Special Elective (Self-Study Course/ Guide Course)				
COURSE TITLE:	**Drug Design and Drug Discovery**			
Credit Structure (Common to all Special Elective Courses)	L	T	P	C
	0	3	0	3

Module 1

Introduction to Drug Discovery & Intermolecular Forces

Drug and Drug targets: Cell structure and drug access pathways, Drug targets at the molecular level. Types of Intermolecular Interactions in drug-target binding: Electrostatic (ionic) interactions, Hydrogen bonding, Van der Waals forces, Dipole–dipole and ion–dipole interactions, Hydrophobic interactions and the role of water, Repulsive forces and steric hindrance.

Module 2

Drug Targets — Proteins, Enzymes, Receptors

Proteins: Protein structure: Primary to Quaternary, Post-translational modifications, Functions of proteins: Structural, Transport, Signalling, Immune response, Protein–Protein Interactions (PPIs) as drug targets.

Enzymes: Role in catalysis and biochemical reactions, Active site, substrate binding, enzyme-substrate specificity. Types of enzyme inhibitors: Reversible (competitive, uncompetitive, non-competitive), Irreversible inhibitors. Enzyme kinetics: Michaelis–Menten equation, Lineweaver–Burk plots.

Receptors: Receptor types (GPCRs, ion channels, tyrosine kinases), Neurotransmitters & hormones, Design of agonists vs antagonists, Binding site characteristics: size, shape, pharmacophores, Mechanism of Allosteric modulators: Affinity, efficacy, potency, tolerance, dependence.

Module 3

Lead Identification and Screening Strategies

Drug Discovery Process: Disease selection and target validation, Target specificity and selectivity, Strategies for organ-specific drug delivery, multi-target and polypharmacology approaches.

Assays and Screening: In vitro and in vivo assays, Bioassays for drug activity: High-Throughput Screening (HTS), Surface Plasmon Resonance (SPR), Virtual screening methods.

Lead Compound Identification: Natural product libraries, Synthetic compound libraries, Structure databases, De-novo drug design, Fragment-Based Lead Discovery (FBLD).

Module 4

Drug Design — Optimizing Target Interactions

Structure–Activity Relationships (SAR): Functional group interactions in drug design - Alcohols, phenols, ketones, aldehydes, Amines, amides, carboxylic acids, esters, Aromatics, halides, thiols, ethers.

Pharmacophore identification: SAR-based drug optimization strategies - Improving binding affinity, enhancing selectivity, Minimizing toxicity, Chemical modifications and lead optimization.

Module 5

Computational Tools in Drug Design

Energy minimization and molecular modelling, 3D molecular visualization and alignment, Molecular docking: Predicting binding poses and scores, Molecular dynamics simulations - Assessing stability of ligand–target complexes. Database screening - Automated screening for lead generation, Use of chemical informatics tools (e.g., RDKit, AutoDock).

Module 6

Pharmacokinetics, ADMET & Case Studies

Phases of Drug Action: Agonist/Antagonist behavior, Dose-response curves, potency, efficacy.
Pharmacokinetics & Pharmacodynamics: ADME: Absorption, Distribution, Metabolism, Excretion, Toxicology (Mechanism, prediction), In silico tools for ADMET prediction - SwissADME, pkCSM, PK/PD modelling - Predicting drug behavior in the body.
Case studies: 1. The design of angiotensin converting enzyme (ACE) inhibitors, 2. Artemisinin and related antimalarial drugs, 3. The design of oxamniquine.

References

1. Patrick Graham L., (2009). An Introduction to Medicinal Chemistry. Fifth edition. ND: Oxford university.
2. Mohini Gore., (2024). Computational Drug Discovery and Design. Second edition. Humana press.
3. Richard B. Silverman., (2004). The organic chemistry of drug design. Second edition, Elsevier.

Mode of Evaluation: CAT / Assignment / Quiz / Seminar / Tutorial /FAT

Approval			
S.No	**Name of the Member**	**Role**	**Signature**
1	Dr. ABILASH V G	Dean Nominee	
2	Dr. RM. VIDHYAVATHI	External Member	
3	Dr. C. JAYAPRAKASH	External Member	
4	Dr. KUMAR K	Internal Member	
5	Dr. MANOOV R	Guide	