

**Office of Academic Research**

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| **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** | | | | |

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| 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 | | | | | |

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| **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 |  |