

**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: | **Python Programming for Bio-informatics** | | | | |
| Credit Structure (Common to all Special Elective Courses) | | L | T | P | C |
| 0 | 3 | 0 | 3 |
| **Module 1** | | | | | |
| **Introduction to Python and Basic Programming**  Variables and Data types: Text data type, Numeric data type, Sequence data type, Mapping type. Expressions, Type conversion, Keywords, Operators, Input statement, Conditional statements: if statement, if…else statement. Loops: Definite loop, Indefinite loop in Python, Nested loops. | | | | | |
| **Module 2** | | | | | |
| **String Handling, Modular Programming, and Data Structures**  String Handling: Accessing characters, string slicing, Handling DNA/RNA/protein sequences, String methods, Useful in sequence parsing and mutation handling.  Data Structures: Lists, Tuples, Dictionaries, and Sets essential for storing sequences, annotations, and metadata.  Modular Programming: Writing functions and modules, encourages reusable code in analysis pipelines. | | | | | |
| **Module 3** | | | | | |
| **File Handling and Object-Oriented Programming**  Handling Biological Files: CSV files for gene/protein data, FASTA files, standard format for nucleotide/protein sequences. Working with Directories, sequence datasets.  Object-Oriented Programming: Creation of custom classes for managing sequences, structures, or biological models. | | | | | |
| **Module 4** | | | | | |
| **Module 4: Biopython Module**  Sequence Objects: Seq, SeqRecord, and related operations, Sequence Access from FASTA, GenBank  Database Access: Fetching proteins from NCBI, UniProt, etc. Structure Analysis: Bio.PDB, parse PDB/mmCIF files, extract atoms, compute distances, Integration with PyMOL for 3D visualization. | | | | | |
| **Module 5** | | | | | |
| **Data Handling and Visualization in Bioinformatics**  NumPy: Fast numeric array operations, genome matrices, similarity scores, Pandas: Handling gene expression datasets, mutation tables, annotations, Matplotlib: Plotting gene expression, clustering outputs, and interaction networks, Bar plot: gene expression comparison, Histogram: sequence length distribution, Scatter plot: PCA, t-SNE, or clustering visualization**.** | | | | | |
| **Module 6** | | | | | |
| **Practical Assignment**  Machine Learning with scikit-learn: Principal component analysis, dimensionality reduction in gene/protein data, Clustering, classification of expression data or molecular fingerprints.  Mini Projects: Cluster Analysis of gene expression / sequence similarity, Application of ML in drug discovery to predict bioactivity of small molecules. | | | | | |
| **References** | | | | | |
| 1. Shahnaz Verma, Parul Fatima. (2024). Python For Bioinformatics: using machine learning for drug discovery, cluster analysis, and phylogenetics. First edition. BPB PUBLICATIONS. 2. Youens-Clark, K. (2021). Mastering Python for Bioinformatics. First edition. O'Reilly Media, United states. 3. Idris, I. (2014). Python data analysis: learn how to apply powerful data analysis techniques with popular open-source Python modules. First edition. Packt Pub. | | | | | |
| **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 |  |