AMIRTESH RAGHURAM

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Vellore Institute of Technology, Vellore

Education

B.Tech Biotechnology

Vellore Institute of Technology, Vellore

2023 - 2027 (Expected) | CGPA: 9.01/10

Professional Experience

Summer Research Intern

Strand Life Sciences, Bangalore | May 2025 - July 2025

- Worked on "Identification of Homologous Regions for the Purpose of Variant Verification in NGS Tests"
- Developed automated Bash scripts for NGS data processing pipelines and homology detection workflows
- Utilized BLAST command-line suite for sequence alignment, variant verification, and homologous region identification
- Implemented bioinformatics solutions for high-throughput genomic data analysis and quality control

Ongoing Research Projects

KinaseForge: Generative AI for Kinase Inhibitor Discovery (Manuscript in Submission)

- Fine-tuned NovoMolGen-157M on kinase-like inhibitor datasets to generate 2.8 million novel kinase-like molecules
- Built XGBoost prediction models for 25 kinases to score and rank the generated compounds
- Created a searchable database enabling multi-target queries — filtering compounds active against specified targets and inactive against others
- Platform accepts custom SMILES strings to predict activity profiles across all 25 kinases; deployed at kinaseforge.vit.ac.in

Multi-Target Inhibitors for Triple Negative Breast Cancer Treatment (Manuscript in Submission)

- Independent research screening natural drug-like compounds as multi-target inhibitors for TNBC therapeutic targets
- Performed triplicate molecular dynamics simulations with MMGBSA binding free energy calculations for robust validation

- Evaluated lead compounds for multi-target efficacy using computational screening and pharmacokinetic profiling
- Assessment of compound stability, binding interactions, and drug-likeness properties

Ferroptosis Predictor: Interpretable QSAR Framework (Manuscript in Submission)

- Developed an interpretable QSAR classification framework distinguishing ferroptosis inducers from inhibitors using a curated, balanced dataset of 1,624 compounds
- Engineered 2,092 molecular descriptors and Morgan fingerprints with scaffold-based cross-validation, achieving AUROC 0.9175 and MCC 0.6617
- Applied SHAP analysis to identify 75 key predictive features; translated discriminative fingerprint signals into chemically meaningful functional group enrichment motifs
- Achieved 86.6% alignment when operationalizing discovered patterns as heuristic screening rules applied to drug-like ChEMBL compounds

Natural Plant-Based Inhibitors for Diabetes Treatment (Manuscript in Submission)

- Collaborative research with PhD scholar identifying natural plant compounds as alpha-amylase inhibitors
- Implementation of computational screening methods, molecular docking, and binding affinity calculations
- Molecular dynamics simulations to evaluate stability of protein-ligand complexes
- Identification of lead compounds with potential therapeutic applications through ADMET profiling

Natural Inhibitors for Glaucoma Treatment (Manuscript in Submission)

- Independent research identifying plant-based inhibitors of human carbonic anhydrase II
- Development of computational pipeline for high-throughput virtual screening
- In-depth molecular dynamics simulations to evaluate stability and effectiveness
- Characterization of binding mechanisms and inhibitory potential of lead compounds

Technical Skills

Quantum Chemistry & Biophysics

- Density Functional Theory (ORCA)
- Semi-Empirical QM (xTB)
- Ligand Optimization & Strain Energy
- Conformer & Tautomer Ensembles (CREST)

Programming & Data Science

- Python (NumPy, Pandas, Scikit-learn, BioPython)
- R (dplyr, ggplot2, Bio3D)
- PyTorch & TensorFlow
- Matplotlib/Seaborn
- Statistical Analysis & Machine Learning
- Bash Scripting & Workflow Automation

Structural Bioinformatics

- Protein Structure Analysis (ProDy, Bio3D)
- Protein-Ligand Docking (AutoDock Vina, Smina, QVina, PyRx, AMDock)

- Molecular Dynamics Simulations (GROMACS)
- Binding Free Energy Calculations (gmx_MMPBSA, MMGBSA)
- Protein Modeling (AlphaFold, SWISS-MODEL, I-TASSER, Phyre2)
- Structural Visualization (PyMol, Chimera, Discovery Studio)
- Cheminformatics (RDKit)
- Virtual Screening Workflows

Genomics & Next-Generation Sequencing

- RNA-Seq Analysis
- Single-Cell RNA-Seq (Seurat)
- ChIP-Seq Analysis
- Variant Calling & Genome Assembly
- DNA Methylation Analysis
- GWAS (PLINK)
- Sequence Alignment (BLAST)
- Galaxy, HOMER, BioConductor

Cancer Genomics

- Somatic Mutation Analysis (maftools, oncoplot, lollipopPlot)
- Tumor Heterogeneity and Clonality Assessment
- Mutation Signature Analysis (COSMIC signatures)
- Co-occurrence and Mutual Exclusivity Analysis
- VAF-based Clonal Population Identification
- Oncogenic Driver Identification (Oncodrive)
- rainfallPlot for Mutation Visualization

Computational Drug Discovery & ADMET

- Virtual Screening Pipelines
- In Silico Vaccine Design
- SwissDock, SwissADME, Swiss Target Prediction
- Swiss Similarity, pkCSM, ProTox 3.0
- MolSoft Drug-likeness Assessment
- KEGG Pathway Analysis

Software Contributions

- **DynaMune:** Ensemble-based protein dynamics analysis platform implementing ENM/NMA, PRS, domain–hinge detection and interface stability analysis using ProDy (github.com/Amirtesh/DynaMune)
- **Torchify:** Python library simplifying PyTorch workflows with enhanced model API functions; published on PyPI with 2,500+ downloads (github.com/Amirtesh/Pytorch-Torchify)
- **Automated-Virtual-Screening:** Binary executable automating ligand screening using Vina, Smina, and QVina with features for file conversion, parallel docking, and results management (github.com/Amirtesh/Automated-Virtual-Screening)
- **Pose-Rescorer:** Physics-based post-docking ligand rescoring workflow using deterministic MM/GBSA with Rapid Perturbation Sampling (RPS) for robustness analysis; validated across EGFR kinase, HIV-1 protease, BRD4 bromodomain, and HSP90 systems (amirtesh.github.io/Pose-Rescorer)

Core Competencies & Achievements

- Quantum-mechanical ligand preparation, including conformer/tautomer ensemble generation and strain energy validation using ORCA and xTB-CREST

- Complete computational drug discovery pipelines from virtual screening to molecular dynamics simulations and binding free energy calculations
- Next-generation sequencing data analysis and interpretation including variant calling and clinical genomics
- Cancer genomics data analysis including somatic mutation profiling, tumor evolution assessment, and clonality studies
- Protein structural analysis, comparative modeling, and structure-function relationship investigations
- Development of custom computational workflows for high-throughput data processing and automation
- Implementation of machine learning approaches for biological data analysis and predictive modeling

Bioinformatics Tools & Resources

ORCA, xTB, CREST, SwissDock, SwissADME, Swiss Target Prediction, Swiss Similarity, pkCSM, ProTox 3.0, MolSoft, AlphaFold, SWISS-MODEL, I-TASSER, Phyre2, BLAST, Galaxy, HOMER, KEGG, BioConductor, rainfallPlot, oncoplot, Oncodrive, maftools, ProDy, Bio3D