AMIRTESH RAGHURAM

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EDUCATION

Bachelor of Technology in Biotechnology | *Vellore Institute of Technology, Vellore*   2023 - 2027
- CGPA: 8.99/10

PROFESSIONAL EXPERIENCE

Summer Research Intern | *Strand Life Sciences, Bangalore*   May 2025 - July 2025
- Developed automated Bash pipelines for NGS data processing, homology detection, and variant verification workflows
- Implemented BLAST command-line tools for sequence alignment and homologous region identification in clinical genomics
- Optimized bioinformatics solutions for high-throughput genomic data analysis and quality control processes

TECHNICAL SKILLS

Programming & Data Science: Python (NumPy, Pandas, Scikit-learn, BioPython), R (dplyr, ggplot2), Bash Scripting, PyTorch, TensorFlow, Matplotlib, Seaborn, Statistical Analysis, Machine Learning

Structural Bioinformatics: Protein Structure Analysis (ProDy, Bio3D), Molecular Docking (AutoDock Vina, Smina, QVina, PyRx, AMDock), Molecular Dynamics Simulations (GROMACS), Binding Free Energy Calculations (gmx_MMPBSA), Protein Modeling (AlphaFold, SWISS-MODEL, I-TASSER, Phyre2), Structural Visualization (PyMol, Chimera, Discovery Studio), Cheminformatics (RDKit)

Genomics & NGS Analysis: 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 Assessment, Mutation Signature Analysis (COSMIC), Co-occurrence and Mutual Exclusivity Analysis, VAF-based Clonal Identification, Oncogenic Driver Identification (Oncodrive), rainfallPlot

Drug Discovery & ADMET: Virtual Screening Workflows, SwissDock, SwissADME, Swiss Target Prediction, Swiss Similarity, pkCSM, ProTox 3.0, MolSoft, In Silico Vaccine Design, KEGG Pathway Analysis

ONGOING RESEARCH PROJECTS

Natural Plant-Based Inhibitors for Diabetes Treatment (Manuscript in Submission)
- Identified alpha-amylase inhibitors through computational screening, molecular docking, MD simulations, and ADMET profiling

Natural Inhibitors for Glaucoma Treatment (Manuscript in Submission)
- Developed high-throughput virtual screening pipeline for carbonic anhydrase II inhibitors with MD validation

Multi-Target Inhibitors for Triple Negative Breast Cancer Treatment (Manuscript in Submission)
- Screened natural compounds as multi-target TNBC inhibitors with triplicate MD simulations and MMGBSA calculations

SOFTWARE DEVELOPMENT & PUBLICATIONS

- **Torchify** - Python library published on PyPI with 2,500+ downloads; simplifies PyTorch workflows with enhanced model APIs and training utilities (github.com/Amirtesh/Pytorch-Torchify)
- **Automated-Virtual-Screening** - Binary executable automating ligand screening using Vina, Smina, and QVina with parallel docking capabilities and automated file conversion (github.com/Amirtesh/Automated-Virtual-Screening)

CORE COMPETENCIES

- End-to-end computational drug discovery pipelines from virtual screening to MD simulations and free energy calculations
- Next-generation sequencing data analysis, variant calling, and clinical genomics workflow development
- Cancer genomics analysis including somatic mutation profiling, tumor evolution, and clonality assessment
- Protein structural analysis, comparative modeling, and structure-function relationship studies