AMIRTESH RAGHURAM

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EDUCATION

Bachelor of Technology in Biotechnology | *Vellore Institute of Technology, Vellore* 2023 - 2027

- CGPA: 9.01/10

PROFESSIONAL EXPERIENCE

Summer Research Intern | *Strand Life Sciences, Bangalore* May 2025 - July 2025

- Automated Bash pipelines for high-throughput NGS data processing, quality control, and clinical genomics workflows.
- Utilized BLAST CLI for rapid sequence alignment and precise homolog detection for variant verification.

TECHNICAL SKILLS

Quantum Chemistry: ORCA (DFT Ligand Optimization), xTB & CREST (Ensembles, Tautomers, Strain Energy)

Programming: Python (NumPy, Pandas, BioPython), R, Bash, PyTorch, TensorFlow

Docking & MD: AutoDock Vina, Smina, QVina; GROMACS, gmx_MMPBSA

Structural Bioinformatics: ProDy, Bio3D; PyMol, Chimera, Discovery Studio; RDKit

Genomics: RNA-Seq, scRNA-Seq, ChIP-Seq, Variant Calling, GWAS, DNA Methylation

ONGOING RESEARCH PROJECTS

KinaseForge: Generative AI for Kinase Inhibitor Discovery

- Fine-tuned NovoMolGen-157M to generate 2.8M kinase-like molecules; built XGBoost models for 25 kinases and deployed as a searchable web platform.

Multi-Target Inhibitors for TNBC Treatment

- Validated multi-target efficacy using triplicate MD simulations (MMGBSA free energy estimation) alongside PCA/FEL conformational dynamics analysis.

Ferroptosis Predictor: Interpretable QSAR Framework

- Classified 1,624 ferroptosis modulators using 2,092 descriptors + Morgan fingerprints (AUROC 0.9175); translated SHAP feature importance into chemical motifs.

Natural Plant-Based Inhibitors for Diabetes Treatment

- Evaluated natural alpha-amylase inhibitors via AutoDock Vina, GROMACS MD stability simulations, and SwissADME/pkCSM ADMET profiling.

Natural Inhibitors for Glaucoma Treatment

- Developed virtual screening pipelines and executed in-depth MD-based stability analysis for plant-based Carbonic Anhydrase II inhibitors.

SOFTWARE DEVELOPMENTS

- **DynaMune** - ENM/NMA-based protein dynamics platform using ProDy (github.com/Amirtesh/DynaMune)
- **Torchify** - PyTorch workflow utility library; 2,500+ PyPI downloads (github.com/Amirtesh/Pytorch-Torchify)
- **Automated-Virtual-Screening** - Parallel docking pipeline for Vina, Smina, and QVina (github.com/Amirtesh/Automated-Virtual-Screening)
- **Pose-Rescorer** - Deterministic single-frame MM/GBSA rescoring workflow with Rapid Perturbation Sampling (RPS), validated on EGFR, HIV-1 protease, BRD4, and HSP90 ligand-binding systems (amirtesh.github.io/Pose-Rescorer)

CORE COMPETENCIES

- **Quantum-Validated Ligand Design:** Generating high-fidelity tautomer/conformer ensembles and calculating precise strain energies to ground drug discovery in thermodynamic reality.
- **Computational Drug Discovery & MD:** Executing end-to-end pipelines from high-throughput virtual screening to triplicate MD simulations and MMGBSA binding free energy estimation.
- **NGS & Cancer Genomics:** Analyzing complex genomic landscapes, including variant calling, somatic mutation profiling, and tumor clonality assessment.
- **Structural Bioinformatics:** Investigating protein structure-function relationships through ensemble-based dynamics, comparative modeling, and custom automated workflows.