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 NGS data processing
- BLAST CLI for sequence alignment and homolog detection
- High-throughput genomic data analysis and QC workflows

TECHNICAL SKILLS

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

Protein Modeling: AlphaFold, SWISS-MODEL, I-TASSER

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

ONGOING RESEARCH PROJECTS

Natural Plant-Based Inhibitors for Diabetes Treatment

- AutoDock Vina docking for natural compound binding affinity evaluation
- GROMACS MD simulations for ligand–protein complex stability assessment
- ADMET profiling using SwissADME and pkCSM

Natural Inhibitors for Glaucoma Treatment

- Virtual screening for carbonic anhydrase II inhibitors
- MD-based stability analysis

Multi-Target Inhibitors for TNBC Treatment

- Triplicate MD simulations with MMGBSA binding free energy estimation
- PCA and FEL analysis for conformational dynamics

SOFTWARE DEVELOPMENTS

- **DynaMune** - ENM/NMA-based protein dynamics platform using ProDy (github.com/Amirtesh/DynaMune)
- **Torchify** - PyTorch workflow utility library (github.com/Amirtesh/Pytorch-Torchify)
- **Automated-Virtual-Screening** - Parallel docking pipeline (github.com/Amirtesh/Automated-Virtual-Screening)

CORE COMPETENCIES

- Computational drug discovery: virtual screening and MD simulations
- NGS data analysis and clinical genomics workflows
- Cancer genomics: somatic mutation and clonality analysis
- Protein structural analysis and comparative modeling