



NIKIL KRISHNA

Undergraduate Student
SASTRA Deemed University



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ABOUT ME

My academic and research interests lie at the intersection of biotechnology and computational biology, where I utilize digital tools to visualize and explore microscopic biological systems.

My experience spans molecular visualization, design, and simulation. I am presently deepening my understanding of artificial intelligence and machine learning applications in in silico drug design and protein binder design, with a particular focus on receptor pocket structure-based modeling.

Beyond academia, I enjoy listening to music, reading, and engaging in various forms of craftwork.

EDUCATION

2026	B.tech Biotechnology <ul style="list-style-type: none">8.57 CGPAResearch Credits
2022	Higher Secondary Certificate <ul style="list-style-type: none">PhysicsChemistryBiologyEnglishMathematics
2020	Secondary School Certificate <ul style="list-style-type: none">EnglishHindiScienceMathematicsSocial Science

EXPERIENCE

2025	Summer Internship <ul style="list-style-type: none">Development of Early Stage Drug Discovery Pipeline Using Machine Learning Models<ul style="list-style-type: none">Conda for virtual environemnt, dependency managementPython for workflowComparision of three SOTA machine learning architectures for protein binder design<ul style="list-style-type: none">Bindcraft (Alphafold2 backpropagation)BoltzDesign1 (Boltz1 backpropagation)Rfdiffusion (Denoising diffusion)
2024	Undergraduate Student Researher <ul style="list-style-type: none">Molecular Motors LaboratoryDrug Design and Protein Engineering

SKILLS

ML Protein Structure Prediction

- AlphaFold
- ESMfold
- Chai-1
- Boltz
- Diffusion Based Models

Molecular Modelling

- ChimeraX
- Pymol
- VMD
- MOE
- Schrodinger Maestro

Drug Design

- Virtual Screening
- Fragment Based Drug Design
- Genetic algorithm/Combinatorial Chemistry
- Lead Optimization
- ADMET analysis

Python

- Molecular Visualization
- Data Analysis
- Machine Learning
- Bioinformatics Pipelines
- Dependency management
- AI Automation

Protein Binder Design

- RFdiffusion
- ProteinMPNN
- Bindcraft
- ColabDesign
- Diffusion & Hallucination ML Models

Molecular Docking and Dynamics

- Autodock
- DiffeDock
- Gromacs
- NAMD
- OpenMM

Bioinformatics

- Linux
- Cryo-EM Modelling using ML
- BLAST, MSA
- Visual Studio Code
- Git version management
- Scientific Computing

Process Simulation

- Aspen Plus
- SuperPro Designer
- DWSIM

CERTIFICATIONS

2025
NPTEL

Aspen Plus Simulation Software - A Basic Course For Beginners

- 90%

2024
SASTRA Deemed
University

Schrodinger Drug Discovery Hackathon Winner

To design a insilico de-novo structure-based drug molecule aimed at executing the dual inhibition of critical protein kinases A and B in Mycobacterium tuberculosis by genetic algorithm and combinatorial chemistry.

2024
NPTEL

Drug Delivery : Principles and Engineering

- 83%

PROJECTS

2025	Building PhageBio A web platform which provides computational biology tools in an interactive online interface https://phage.netlify.app/
2024 SASTRA Deemed University	Research Credits Fragment Based Drug Design of Anthelmintic Using Genetic Algorithm

LANGUAGES

• English	- Professional working proficiency
• Hindi	- Limited working proficiency
• Tamil	- Bilingual proficiency
• Kannada	- Bilingual proficiency
• Telugu	- Elementary proficiency

REFERENCES

Dr.Venkatasubramanian Ulanganathan Supervisor Associate Professor SASTRA Deemed University	Email venkat@scbt.sastra.edu	Dr.Karunanithi Mentor Senior Assistant Professor SASTRA Deemed University	Email karuna@carism.sastra.edu
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