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
SASTRA Deemed University, Thanjavur

B.tech Biotechnology

- 8.57 CGPA
- Honours
- Research Credits

2022
ALPHA Wisdom Vidyashram Tiruchirapalli

Higher Secondary Certificate

- Physics
- Chemistry
- Biology
- English
- Mathematics

2020
ALPHA Wisdom Vidyashram Tiruchirapalli

Secondary School Certificate

- English
- Hindi
- Science
- Mathematics
- Social Science

EXPERIENCE

2025
IIT Dharwad

Summer Internship

- Development of Early Stage Drug Discovery Pipeline Using Machine Learning Models
  - Conda for virtual environemnt, dependency management
  - Python for workflow
- Comparision of three SOTA machine learning architectures for protein binder design
  - Bindcraft (Alphafold2 backpropagation)
  - BoltzDesign1 (Boltz1 backpropagation)
  - Rfdiffusion (Denoising diffusion)

2024
SASTRA Deemed University

Undergraduate Student Researher

- Molecular Motors Laboratory
- Drug Design and Protein Engineering

SKILLS

ML Protein Structure Prediction
- Alphafold
- ESMfold
- Chai-1
- Boltz
- Diffusion Based Models

Protein Binder Design
- RFdiffusion
- ProteinMPNN
- Bindcraft
- ColabDesign
- Diffusion & Hallucination ML Models

Molecular Modelling
- ChimeraX
- Pymol
- VMD
- MOE
- Schrodinger Maestro

Molecular Docking and Dynamics
- Autodock
- Diffdock
- Gromacs
- NAMD
- OpenMM

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

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

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

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

Founder - Biostruct
A web platform which provides computational biology tools in an interactive online interface
https://biostruct.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

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