

GANESH CHANDAN KANAKALA

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Education

International Institute of Information Technology, Hyderabad

Hyderabad, India

Integrated B.Tech in Computer Science and M.S. by Research in Computational Natural Sciences

Aug 2019 – Jul 2024

- **CGPA:** 9.0/10 (M.S.) — 8.7/10 (B.Tech)
- Awarded the **Academic Research Award (2023)** for outstanding contributions to academic research.
- Recognized as a **Dean's List Scholar** and **Merit List Scholar** (2023) for exceptional academic performance.
- Secured **Second Place** in the **ML4SCI 2023 Hackathon** for developing a molecular property prediction model.
- Served as a **Teaching Assistant** at [iHub-Data](#) for the [Executive Training Program on AI/ML](#), organized for Council of Scientific & Industrial Research (CSIR) and Defence Research and Development Organization (DRDO) scientists.
- **Teaching Assistant** for **ML4Chem** (Machine Learning for Chemistry) course.

Experience

Samsung Research India

Bangalore, India

Senior Software Engineer at Advanced Research and Standards Team

July 2024 – Present

- Designed and developed advanced AI/ML algorithms for **Photoplethysmogram** (PPG) signals and developed biosensing solutions to monitor human heart health, hydration levels, and glucose levels using PPG obtained from **Samsung Galaxy watch**.
- Worked on developing **State-of-The-Art** deep learning networks for audio data on machine health monitoring for predictive maintenance and human heart health.
- Optimized algorithms for Samsung wearable edge devices.
- **Filed two Patents:** One **A1** and one **A2** in wearable Biosensing technology.
- Co-authored **two Internal Technical papers** contributing to Samsung's Biosensing R&D.
- Received **Samsung Excellence Award 2024** for our work on Biosensing technology.
- Received **Samsung Spot Award 2025** for achieving the KPIs in non-invasive glucose monitoring technology.

Center for Computational Sciences, IIIT-Hyderabad

Hyderabad, India

Undergraduate Researcher under Prof. U. Deva Priyakumar (CRSI Bronze Medal Awardee)

Mar 2021 - Mar 2024

- Conducted advanced research in **Data-Driven Drug Discovery**, applying deep learning techniques such as Graph Neural Networks (GNNs), GPT models, Diffusion models across diverse molecular data modalities, including absorption spectra, molecular graphs, 2D molecular images, and Functional Magnetic Resonance Imaging (fMRI) data.
- Worked collaboratively within a multidisciplinary research group on multiple projects, and independently led projects from ideation to model development, evaluation and publications.
- Mentored junior researchers and guided project direction in the lab, providing technical support and feedback on deep learning workflows and research methodologies.
- Published research findings in **peer-reviewed journals**, contributing to the advancement of AI applications in computational chemistry and bio-informatics.

Virtual Labs

Hyderabad, India

Software Developer

Aug 2022 - Jan 2023

- Developed interactive web-based 3D simulations of solid-state chemistry experiments using **Three.js**, enabling realistic visualization of complex chemical processes.
- Contributed to the **Indian Ministry of Education (MoE)'s Virtual Labs** initiative, providing scalable, accessible remote learning tools for students across India.

Publications

1. **Ganesh Chandan Kanakala**, Rishal Aggarwal, Divya Nayar and U Deva Priyakumar. *Latent Biases in Machine learning methods for Binding Affinity prediction*. ACS Omega 2023, 8, 2, 2389–2397. [Article](#)
2. **Ganesh Chandan Kanakala**, Sriram Devata, Prathit Chatterjee, U Deva Priyakumar. *Generative artificial intelligence for small molecule drug design*, Current Opinion in Biotechnology, Volume 89, 2024, 103175, ISSN 0958-1669. [Article](#)
3. **Ganesh Chandan Kanakala**, Bhuvanesh Sridharan, U Deva Priyakumar. *Spectra to structure: contrastive learning framework for library ranking and generating molecular structures for infrared spectra*. Digital Discovery, Volume 3, Issue 12, 2024, Pages 2417-2423, ISSN 2635-098X. [Article](#)

Projects

MolGPT2.0

- Enhanced [MolGPT](#) to predict complex molecular properties, extending the original generative model for conditional molecular string (SMILES) generation.
- Integrated **Direct Preference Optimization (DPO)** to improve generation quality and alignment with experimental properties for the molecules achieving a molecule validity and novelty > 95%.
- This work is currently being reviewed for publication.

SMEN (Spectra and Molecule Encoder Network)

- Developed a **State-of-The-Art** multimodal framework to rank and generate molecules from Infrared (IR) spectra using Deep learning networks.
- Combined Equivariant Graph Neural Networks (EGNN) for molecular graphs, Vision Transformers (ViT) for spectral embeddings, and generative transformers for molecule synthesis for achieving Top 1 accuracy of 81% and Top 10 accuracy of 99%.
- This work was published in a peer-reviewed journal. ([Digital Discovery](#))

MolVis

- Built an interactive **VisionOS** XR application to visualize and manipulate molecules using Apple Vision Pro.
- Leveraged RealityKit, Reality Composer Pro, and SwiftUI to create immersive scientific experiences, enabling intuitive exploration of protein molecules in extended reality. [Link to Project](#)

BEDS (Brain Encoding and Decoding of Speech)

- Designed a deep learning pipeline to decode speech from 3D fMRI brain activations.
- Used CNNs for neural data encoding and transformers for speech representation, uncovering correlations between brain activity and speech.
- Demonstrated cross-modal learning between neural signals and sequential data, highlighting potential for neuro-AI interfaces.

Technical Skills

Languages: C/C++, Python, JavaScript/TypeScript, Swift, MATLAB, Shell

Databases/Web: MySQL, ReactJS, ExpressJS, MongoDB, Flask, SwiftUI

AI/ML: PyTorch, Pytorch Mobile, Keras, ONNX, TensorFlow, TFLite, Computer Vision, CNNs, RNNs, GNNs, Natural Language Processing, LLMs

Tools & Concepts: Git, Docker, $\text{\LaTeX}$, Jupyter, CI/CD, JIRA, HPC clusters, Data Structures and Algorithms, Data Systems, Distributed Systems, Statistical Methods in AI