Shreyas V

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EDUCATION

BE Computer Science, *Birla Institute of Technology and Science, Pilani – Goa Campus* 2020-2025(expected)
MSc Chemistry, *Birla Institute of Technology and Science, Pilani – Goa Campus* 2020-2025(expected)

SKILLS

Tools and Languages	Python, Git, LaTeX, C, MySQL, PyTorch, TensorFlow, Pandas, CI/CD Pipelines, AWS, Azure
Quantitative Research	Machine Learning, Drug Discovery, Generative AI, NLP, LLMs

TECHNICAL EXPERIENCE

Visiting Researcher Intern Jun 2024 — Present
Yale University *New Haven, NY*
- Conducting research on **molecule generation** models using **geometric deep learning** with Prof. Smita Krishnaswamy
- Developing novel algorithms to enhance molecular design efficiency

Research Intern Dec 2023 — Present
Harvard Medical School *Remote*
- Investigating the neural mechanisms of language processing using **AI models** under Prof Gabriel Kreiman
- Applying advanced machine learning techniques to analyze neural data, contributing to a deeper understanding of language cognition

Research Fellow Jun 2023 — Present
Deep Forest Sciences *Remote*
- Developed tools for **AI-aided retrosynthesis**, **molecule & materials discovery**
- Built infrastructure to train **Molecular LLMs**
- finalist at the **Standard Industries Chemical Innovation Challenge**, awarded prize money of **$100,000**
- Migrated models in the open-source drug discovery toolkit **DeepChem** from TensorFlow to **PyTorch**, increasing user base by **92%**

Product Engineering Intern Jun 2024 — July 2024
Sprinklr *Gurgaon, India*
- Developed an **ASR transcription evaluation pipeline** using NLP techniques
- Created a custom scoring metric for evaluating transcripts in production, enhancing accuracy
- Improved productivity of product managers by **2x** through streamlined evaluation processes

Student Researcher 2022 — Present
APPCAIR, Birla Institute of Technology & Science, Pilani *Goa*
- Researched the use of **Large Language Models** to generate novel molecules for drug discovery and predict their **synthesizability**
- Devised deep learning methods to predict **protein residue binding** sites
- Evaluated **BERT** and **Transformer**-based architectures for protein residue binding location prediction

Research Intern 2021 — 2023
Amrita Vishwa Vidyapeetham *Bangalore, Karnataka*
- Published a paper titled **"Speech to Equation Conversion using a PoE Tagger"**
- Designed a novel **NLP** architecture to handle variability in spoken mathematical equations

Data Science Intern Jun 2022 — Aug 2022
Skan.ai *Bangalore, Karnataka*
- Implemented **data anonymization** techniques using machine learning for process mining applications
- Developed an AI/ML pipeline for real-time data anonymization, improving processing speed by **30%**

Research Intern Feb 2022 — May 2022
Pixis.ai *Bangalore, Karnataka*
- **Optimised Algorithmic Trading** App to identify **arbitrage opportunities** to do a round trip trading with different currencies from **30 min to 2 sec**

PUBLICATIONS

V. Shreyas, J. Siguenza, K. Bania & B. Ramsundar "Open Source Molecular Processing Pipeline for Generating Molecules" *Molecular Machine Learning Conference (MoML) 2024, Baylearn 2024, ML4PS workshop at NeurIPS 2024*

A. Srinivasan, K. Bania, **V. Shreyas**, H. Mestha, & S. Liu (2024). Implementation and Application of an Intelligibility Protocol for Interaction with an LLM. *arXiv preprint arXiv:2410.20600.*

V. Sathyanarayana and **V. Shreyas** "Prompting with Justification and Confidence: Extracting Information and Relationship using LLMs" (Under Review)

V. Shreyas and A. Swati, "Predicting ATP binding sites in protein sequences using Deep Learning and Natural Language Processing" *3rd Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI2ASE)*, 2024.

Mestha, H., Agrawal, T., Bania, K., **V. Shreyas** & Bhisikar, Y. (2024). "CountCLIP–[Re] Teaching CLIP to Count to Ten". *arXiv preprint arXiv:2406.03586.*

P. Basa Pati and **V. Shreyas**, "Speech to Equation Conversion using a PoE Tagger," *2022 IEEE 7th International conference for Convergence in Technology (I2CT)*, 2022, pp. 1-4, doi: 10.1109/I2CT54291.2022.9824252.

PROJECTS

Metamorph - Generative AI   **May 2023 — July 2023**
Building an **emotionally responsive Humanoid** bot with **knowledge capture , speech text generation** using Generative Large Language Models

ACTIVITIES

ML Lead, Google Developer Student Clubs, BITS Goa   **2022 — 2023**
- Guided a group of 25+ ML enthusiasts , conducted weekly ML training sessions
- Organized hackathons , mentored in ML model building , and fostered exploration in ML research.

Sub-Coordinator, Srutilaya, BITS Goa   **2022 — 2023**
- Awarded Certificate of Recognition by the Chief Minister of Goa for Performing a cultural show in the QS India Summit 2023, held in Goa.
- Organized various classical concerts and Led a team of 25+ to bring in Indian Oil and First Edition Arts as sponsors for the event Sursangam which had a footfall of 500 people and 300 Live-stream attendees . Increased revenue of the club by 100

AWARDS AND RECOGNITIONS

2nd Runner up | *ACM Goa Chapter's event PitchIt!*   *Apr 2024*
Best Logical Thinker | *Sri Kumarans Childrens Home CBSE*   *Feb 2020*
Silver Standard | *The Duke of Edinburgh's International Award*   *Aug 2018*
Runner Up | *Vidyarthi Vigyan Manthan*   *May 2018*
1 out of 50 students chosen to participate in National Camp, Ranked **2nd out of 50 students** in the south Zone at National Camp

CERTIFICATIONS

Machine Learning *Stanford University, Coursera. May 2022*
Neural Networks and Deep Learning *DeepLearning.ai, Coursera. May 2022*
Natural Language Processing with Deep Learning *Stanford University. May 2022*
Fundamentals of Accelerated Data Science with RAPIDS *Nvidia DLI. Issued July 2021* Certificate
Python 3 Programming Specialization *University of Michigan, Coursera. December 2020*
Introduction to Artificial Intelligence (AI) *IBM, Coursera. Issued November 2020* Certificate
What is Data Science? *IBM, Coursera. Issued October 2020* Certificate