




Amitesh Badkul

@ Email |  LinkedIn |  GitHub |  Website

EDUCATION

Birla Institute of Technology and Science, Pilani

Master of Science in Chemistry

Bachelor of Engineering in Electrical and Electronics Engineering

Hyderabad, India

August 2018 - June 2023

- **Thesis:** In-silico prediction of protein-ligand binding affinity using deep learning. [\[Link\]](#)

PUBLICATIONS

- Tian Cai, Li Xie, Shuo Zhang, Muge Chen, Di He, **Amitesh Badkul**, ... and Lei Xie. (2022)., "End-to-end Sequence-Structure-Function Meta-learning Predicts Genome-Wide Chemical-Protein Interactions for Dark Proteins", **PLoS Computational Biology** [DOI: [10.1371/journal.pcbi.1010851](https://doi.org/10.1371/journal.pcbi.1010851)]
- **Amitesh Badkul**, Sonakshi Mishra, and Srinivasa Prasad Kommajosyula (2023)., "A Comparative Study of DeepLabCut and Other Open-Source Pupillometry Data Analysis Algorithms". [Status: Under Review, Image and Vision Computing]
- Vyshnavi S K, **Amitesh Badkul**, Vamsi Inturi, Sudha Radhika., "Comparative Study of DCNN and Image Processing based classification of Chest X-rays for identification of COVID-19 patients using Transfer Learning". [Status: In preparation]

EXPERIENCE

Graduate Center, CUNY

Visiting Researcher (Supervisor: Dr. Lei Xie)

New York City, NY

Aug 2022 – Present

- **Developed** a deep learning framework for predicting protein-ligand binding affinity, incorporating uncertainty. **Achieved** a Pearson correlation of **0.92** and MAE of **0.25** in OOD settings, surpassing state-of-the-art methods.
- **Engineered** and **Integrated** Multi-Task learning-based algorithms with Protein Language Models ([DISAE](#) and [ESM-2](#)) for enhanced chemical protein binding affinity prediction. Utilized deep learning techniques such as Transformers, RNNs, and CNNs, **resulting in** a Pearson correlation of **0.81** and MAE of **0.56**. [\[Thesis\]](#)

Arizona State University

Summer Research Intern (Supervisor: Dr. Ashif Iquebal)

Remote

Jun 2022 – Aug 2022

- **Analyzed** large chemical datasets to **identify** the optimal dataset emphasizing compounds with hydrogen bonding.
- **Optimized** a generative model using LSTM and GRU architectures for self-healing compound generation.
- **Trained** a generative model yielding 98.43% valid compounds, with a higher ease of synthesis on average. [\[Poster\]](#)

Birla Institute of Technology and Science Pilani

Undergraduate Research Assistant (Supervisor: Dr. Srinivas Prasad K)

Hyderabad, India

Jun 2021 – Jun 2022

- **Employed** architectures such as MobileNet, ResNet, and EfficientNet to achieve accurate rat pupil measurements.
- **Achieved** minimal deviation from ground truth, outperforming other state-of-the-art image processing algorithms.

Undergraduate Research Assistant (Supervisor: Dr. Durba Roy)

Aug 2021 - May 2022

- **Simulated** a water box cube using Molecular Dynamics for 20 nsec and **analyzed** positional and energy data.
- **Devised** algorithms for Mean Square Displacement (MSD) and Diffusion Coefficient in water systems; **investigated** Rhodobacter Sphaeroides' Reaction Center. [\[GitHub\]](#) [\[Blog 1\]](#) [\[Blog 2\]](#).

Undergraduate Research Assistant (Supervisor: Dr. Sudha Radhika)

Feb 2021 - April 2022

- **Optimized** pretrained models (ResNet, MobileNet, etc) for CXR classification, **achieving 97%** accuracy. **Enhanced** accuracy by **2%** with a CXR enhancement algorithm.
- **Developed** a novel dataset from CXR using statistical descriptors post wavelet transform. **Achieved 97.46%** accuracy with XGBoost and Random Forest models. [\[GitHub\]](#)

Sensordrops Networks, IIT Kharagpur

Research Intern (Supervisor: Dr. Sudip Misra)

Kharagpur, India

Dec 2020 – Feb 2021

- **Developed** a Graph Neural Networks (GNNs) based algorithm for Contact Tracing of COVID-19 patients.
- **Created** a novel Twitter dataset for training and testing. Used Twitter metadata as features and **deployed** the GNN model. **Obtained** accuracy of **92.31%**.

- **Refactored** and **refined** of existing JavaScript code leading to increased efficiency and usability.
- **Developed** and **enhanced** educational content, **benefiting over 20+ teachers** and **elevating** learning outcomes.

PROJECTS

CYP3A4 Inhibition Classification | [GitHub](#)

- **Curated** and **cleaned** the datasets for improved accuracy of machine learning models.
- **Deployed** machine learning algorithms such as Random Forest, and XGBoost. **Achieved** an accuracy of 77%.

CXR Bit Plane Classification | [GitHub](#)

- **Implemented** CXR classification on bit plane sliced CXRs using MobileNet model.
- **Obtained** a highest accuracy of 95% validating the fact that all layers of a CXR are equally important.

Cdh23EC1 Analysis | [Blog](#)

- **Conducted** thorough and **extensive** analysis of the data obtained from the MD Simulation of Cdh23EC1 protein.
- **Programmed** functionalities+ for calculation of various properties - MSD, Radius of Gyration and more.

SKILLS

Programming Languages: Python, MATLAB, R, Verilog, L^AT_EX, C, Bash, Java, Javascript, HTML, CSS

Software Skills: BLAST, NAMD, VMD, OpenCV, EMU8086, LTSpice, Microsoft Office Suite, Adobe Suite, AutoCAD

Languages: Hindi (Native), English (Professional)

Libraries: PyTorch, PyTorch Geometric, TensorFlow, Keras, OpenCV, RDkit, Scikit-Learn, Biopython, Numpy, Pandas, Matplotlib, Seaborn, DeepLabCut, Networkx, DGL, Pywt, Deepchem

SERVICE

- **Reviewer**, International Journal of Computational Biology and Drug Design (2023)
- **Student Member**, IEEE Organization, BITS-Pilani, Hyderabad (2019-2022)

AWARDS & ACHIEVEMENTS

- **Scholarship for Higher Education (SHE):** Recipient of Scholarship for Higher Education provided by the Indian Government for excellence in academics Higher Secondary School Board examination, given to the top 1% of students, held in month of March 2018 in India.
- **Scholarship for Practice School - 1 (held in the summer of 2020):** industry exposure program, given to the students with excellent performance (highest grade - 'A') in the industry provided by BITS Pilani.