Kusal Debnath

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Profile

Graduate Researcher specializing in AI-driven drug discovery, with expertise in machine learning (ML), deep learning (DL), generative AI (Gen-AI), RNA-Seq analysis, and molecular docking. Experienced in *de novo* drug design and drug-target interaction (DTI) prediction modeling. Passionate about leveraging computational biology and AI to advance precision medicine and cheminformatics. Aspiring to lead interdisciplinary research integrating AI and pharmacogenomics for drug discovery.

Education

Doctor of Philosophy (PhD) in Computer Science *Aug 2023 – Present*
Virginia Commonwealth University *Richmond, Virginia, USA*

- **Coursework:** Deep Learning and Neural Networks, Advanced Natural Language Processing, High Performance Distributed Systems, Advanced Algorithms

Master of Technology (MTech) in Biomedical Engineering *Aug 2021 – June 2023*
Indian Institute of Technology *Kharagpur, India*

- GPA: 8.70/10.0
- **Coursework:** Application of Machine Learning in Biological Systems, Deep Learning Foundations and Applications, Medical Imaging, Medical Biotechnology, Cancer Biology

Bachelor of Technology (BTech) in Biotechnology *Aug 2017 – July 2021*
Haldia Institute of Technology *Haldia, India*

- GPA: 9.43/10.0
- **Coursework:** Introduction to C Programming Language, Data Structures and Algorithms, Database Management Systems, Biochemistry, Microbiology, rDNA Technology, Molecular Biology, Tissue Culture

Research Projects

GramSeq-DTA: A Grammar-based Drug-Target Affinity Prediction Approach Fusing Gene Expression Information *Sep 2023 - Mar 2025*

- Developed a multi-modal deep learning model for drug-target affinity (DTA) prediction by integrating differential gene expression information with drug and protein structural information
- Demonstrated improved performance by 1.2% upon benchmarking
- ***Github Repository***: *https://github.com/debnathk/gramseq*

Skills

Programming Languages: C, C++, Python, R

AI/ML Frameworks: Scikit-learn, PyTorch, TensorFlow

Soft Skills: Critical Thinking, Problem Solving, Interdisciplinary Collaboration, Leadership in AI Research

Research Experience

Research Assistant *Aug 2023 – Present*
Virginia Commonwealth University *Richmond, Virginia, USA*

- Developed comprehensive deep-learning pipelines to investigate drug-target interactions (DTI) for exploring novel drugs for biological targets
- Constructed generative deep-learning models for designing de novo drugs against multiple cancer subtypes

Research Assistant *June 2022 – May 2023*
Indian Institute of Technology, Kharagpur *Kharagpur, India*

- Developed robust RNA-Seq analysis pipelines to uncover and examine primary differential gene expressions contributing to Glioblastoma Multiforme (GBM) progression
- Identified potential protein-protein interactions (PPIs) linked to differentially expressed genes as novel drug targets for treating GBM using classical machine learning algorithms.

Research Intern *Jan 2020 – Feb 2020*
Calcutta National Medical College *Kolkata, India*

- Designed experiments to investigate restriction digestion of PCR-amplified G6PD gene to detect the +563 C/T single nucleotide polymorphism (SNP)

Publications

A survey on deep learning for drug-target binding prediction: models, benchmarks, evaluation, and case studies

Briefings in Bioinformatics, *Oxford University Press (Journal Category: Q1, Impact factor: 7.7)* *Sep 2025*

Kusal Debnath, Pratip Rana, Preetam Ghosh

10.1093/bib/bbaf491

- *Highlighted the chronological evolution of deep learning applications in drug–target binding prediction, and comprehensively evaluated current state-of-the-art approaches using widely adopted benchmarks, evaluation metrics, and performed detailed case studies on representative biological targets.*

24R,25(OH)2D3 Regulates Tumorigenesis in Estrogen Sensitive Laryngeal Cancer Cells via Membrane-Associated Receptor Complexes in ER+ and ER- Cells

International Journal of Cancer, *Wiley (Journal Category: Q1, Impact factor: 4.7)* *Sep 2025*

Cydney Dennis, D. Joshua Cohen, ***Kusal Debnath***, Nofrat Schwartz, Brock Lodato, Jonathan Dillon, Tillat Batool, Matthew Halquist, Preetam Ghosh, Zvi Schwartz, and Barbara Boyan

10.1002/ijc.70141

- *Conducted extensive ligand-protein docking analyses, utilizing advanced computational techniques to predict the binding affinity and interactions between the ligand of interest and numerous target proteins.*

GramSeq-DTA: A Grammar-Based Drug–Target Affinity Prediction Approach Fusing Gene Expression Information

Biomolecules, *MDPI (Journal Category: Q1, Impact factor: 4.8)* *Mar 2025*

Kusal Debnath, Pratip Rana, Preetam Ghosh

10.3390/biom15030405

- *Developed an end-to-end deep learning model to analyze and extract features from drug and protein structural data along with gene expression information, demonstrating proficiency in predictive analysis of drug-target binding*