YASH MATHUR

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Dr. Hassan's Lab,
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A dedicated PhD candidate in Computational Biology at Jamia Millia Islamia, specializing in generative deep learning for drug development. Expertise encompasses the design and implementation of automated in-silico workflows and the contribution to peer-reviewed research aimed at advancing computational methodologies in therapeutic discovery. A strong foundation in bioinformatics and computer science is complemented by extensive experience in integrating open-source tools and modern computational techniques to address complex biological challenges.

EDUCATION

PhD Computational Biology, Jamia Millia Islamia, New Delhi, India, expected August 2026

- Thesis title: Employing Generative Deep Learning Models for Strategic Advancements in Drug Development
- Supervisor: Dr. Md. Imtaiyaz Hassan

M.Sc. Bioinformatics, Jamia Millia Islamia, New Delhi, India [May 2020]

B.Sc. Microbiology, University of Delhi, New Delhi, India [May 2018]

HONORS & REWARDS

UGC NET, Computer Science (Assistant Professor Category) [2024]

SKILLS

As a doctoral candidate specializing in AI-integrated drug discovery, advanced programming proficiency encompasses Python development with specialized libraries including PyQT5, SciPy, Biopython, Scikit-learn, PyTorch, and Chemprop for scientific computing and deep learning applications. Extensive experience in generative deep learning model development focuses on therapeutic candidate identification through automated in-silico pipelines that integrate molecular docking, molecular dynamics simulations, and cheminformatics analyses. Web development capabilities span Django and Flask frameworks for creating scientific interfaces and automated tools, demonstrated through published software including InstaDock and PyPAn. Data visualization expertise leverages Matplotlib, Seaborn, and Plotly for

comprehensive analysis of high-throughput molecular screening results and genomic datasets. Machine learning implementation includes neural networks for protein function prediction, generative adversarial networks for style transfer applications, and ensemble models for clinical prediction tasks.

Proficiency in open-source bioinformatics tools and computational biology techniques is demonstrated through expertise in sequence analysis using BLAST and HMMER and molecular docking with AutoDock, AutoDock Vina, Smina, QuickVina2, and QuickVina-W. Advanced phylogenetic analysis skills are supported by the application of RAxML. Extensive experience with molecular dynamics simulations using GROMACS and protein-ligand interaction analyses with MDAnalysis and PyMol is complemented by modern protein structure prediction methods such as AlphaFold and homology modeling using MODELLER. Containerized deployment via Docker ensures scalable and reproducible research pipelines.

RESEARCH

Publications

Yash Mathur, et al.; Current advancement in AI-integrated drug discovery: Methods and applications; Biotechnology Advances (2025); DOI: 10.1016/j.biotechadv.2025.108642

Yash Mathur, et al.; Genome-Wide Analysis of Kidney Renal Cell Carcinoma: Exploring Differentially Expressed Genes for Diagnostic and Therapeutic Targets; OMICS (2023); DOI: 10.1089/omi.2023.0056

Afsar Alam, Mohammed Shahzeb Khan, Yash Mathur, et al.; Structure-based identification of potential inhibitors of ribosomal protein S6 kinase 1, targeting cancer therapy: a combined docking and molecular dynamics simulations approach; Journal of Biomolecular Structure and Dynamics (2023); DOI: 10.1080/07391102.2023.2228912

Md. Imtaiyaz Hassan, Yash Mathur, et al.; Chapter: Molecular Dynamics Simulation to Study Thermal Unfolding in Proteins; Protein Folding Dynamics and Stability (book) (2023); DOI: 10.1007/978-981-99-2079-2_12

Yash Mathur, et al.; PyPAn: An automated graphical user interface for protein sequence and structure analyses; Protein & Peptide Letters (2022); DOI: 10.2174/0929866529666220210155421

Taj Mohammad, Yash Mathur, et al.; Genomic Variations in the Structural Proteins of SARS-CoV-2 and Their Deleterious Impact on Pathogenesis: A Comparative Genomics Approach; Frontiers in Cellular & Infection Microbiology (2021); DOI: 10.3389/fcimb.2021.765039

Taj Mohammad, Yash Mathur and Md. Imtaiyaz Hassan; InstaDock: A single-click graphical user interface for molecular docking-based virtual high-throughput screening; Briefings in Bioinformatics (2020); DOI: 10.1093/bib/bbaa279

Research Experience

Project Assistant, Dr. Hassan's Lab, Jamia Millia Islamia, New Delhi, India [2020–2023]

At Dr. Hassan's Lab, responsibilities included designing, developing, and deploying automated in-silico pipelines dedicated to drug development. The role involved integrating various open-source tools and techniques, such as molecular docking, dynamics simulations, and cheminformatics analyses, to streamline the process of identifying novel therapeutic targets and potential drug candidates.