YASH MATHUR

Updated: 21/03/2025

Dr. Hassan's Lab,
Centre for Interdisciplinary
Research in Basic Sciences, Jamia
Millia Islamia, New Delhi, India

Email: yash185973@st.jmi.ac.in
Website: https://ym59.github.io
ORCID: 0000-0003-2753-0557
Mob: +91-9811622459

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. 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]

RESEARCH

Publications

Yash Mathur, et. Al; Genome-Wide Analysis of Kidney Renal Cell Carcinoma: Exploring Differentially Expressed Genes for Diagnostic and Therapeutic Targets; OMICS: A Journal of Integrative Biology (2023) 27(8):393-401; DOI: 10.1089/omi.2023.0056

Afsar Alam, 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) 26:1-12; 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; 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) PMID: 35142267; 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. Front. Cell. Infect. Microbiol. (2021) 11, 951; 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) 00, 1-8. (Co-First author) 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. The outcomes of these projects contributed to two peer-reviewed publications and a major conference presentation, reinforcing the lab's commitment to advancing computational methodologies in the field of drug development.

SKILLS

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.

In the realm of programming and data science, Python proficiency is highlighted by the use of libraries such as NumPy, SciPy, Pandas, Scikit-learn, PyTorch, and TensorFlow for scientific computing and deep learning. Cheminformatics applications—including QSAR modeling and virtual screening—are supported by robust data visualization through Matplotlib, Seaborn, and Plotly, while user-friendly scientific interfaces and web-based applications have been developed using PyQt5, Django, and Flask.