

# YASH MATHUR

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Dr. Hassan's Lab,  
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PhD candidate in Computational Biology at Jamia Millia Islamia with a focus on generative deep learning for drug development. Experienced in developing automated in-silico workflows and contributing to peer-reviewed research. Proficient in bioinformatics tools and programming languages such as Python and R, with a strong commitment to advancing computational methodologies in therapeutic discovery.

## 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]

Developed and implemented automated in-silico pipelines for drug development, contributing to two peer-reviewed publications and a major conference presentation.

## SKILLS

### Bioinformatics Skills

Expert in bioinformatics tools and servers including BLAST, MODELLER, PyMol, PyRx, Discovery Studio, AutoDock, and energy minimization using SPDBV. Proficient in specialized applications such as molecular dynamics simulations with GROMACS, molecular visualization with VMD, cheminformatics analysis using Marvin and OpenBabel, and protein model building and refinement with WinCoot. Familiar with emerging techniques including protein structure prediction with AlphaFold, and scalable pipelines using Docker.

### Programming Skills

Python: Proficient in GUI development with PyQt5, web development with Django, and scientific computing using PyTorch, NumPy, SciPy, and Pandas for data manipulation, complemented by visualization tools such as Matplotlib and Seaborn.

R: Skilled in data visualization with ggplot2 and RNA-Seq analysis using limma, DESeq2, and NOISeq.

Perl: Experienced with the BioPerl toolkit for bioinformatics scripting, as well as CGI scripting and database interactions via DBI.