NAGMI BANO

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OBJECTIVES

I am a PhD scholar in Bioinformatics at Jamia Millia Islamia University, India, specialising in integrating artificial intelligence and computational biology. My research focuses on applying AI-driven sequence analysis, molecular enumeration, machine learning, and structural modelling to address critical challenges such as multidrug resistance and cancer resistance—both significant global health issues. I am eager to contribute to projects involving sequence analysis, the development of advanced drug discovery pipelines for personalised medicine, overcoming drug resistance, and building innovative deep-learning models for biomedical applications.

EDUCATION

Jamia Millia Islamia University, New Delhi *[2023-ctd]*
[PhD Bioinformatics]

Jamia Millia Islamia University, New Delhi *[2020-2022]*
[MSc Bioinformatics]

University of Allahabad, UP *[2017-2020]*
[Bachelor of Science]

Research Experiences

Jamia Millia Islamia University, India *[2023-ctd]*
Department of Computer Science, Jamia Millia Islamia, New Delhi.
PhD Scholar | Machine Learning and Multitargeted Drug Designing to Combat AMR in *Enterobacteriaceae*
PhD Supervisor: **Dr Khalid Raza** (Associate Professor)

International Centre for Genetic Engineering and Biotechnology, India *[June 2022 – July 2023]*
Translational Bioinformatics Group (ICGEB, New Delhi, India)
Project Associate | AI and Computational Drug Design Methods for Combating Cervical Cancer Resistance
Group Leader: **Dr Dinesh Gupta**

Jamia Millia Islamia University, India *[September 2021 – May 2022]*
Department of Computer Science, Jamia Millia Islamia, New Delhi.
MSc Dissertation | Role of Drug Enumeration Towards Single Capsule-Based Drug Designing and Development
MSc Supervisor: **Dr Khalid Raza** (Associate Professor)

PUBLICATIONS & SCIENTOMETRIC INDICATORS

- **Journal Articles:** Published- 15, Communicated- 04 | **Book Chapters:** Published- 07, Communicated- 01
- **Google Scholar:** Citations- 274, H-index- 09, i10-index- 08 | **WoS**- Citations- 212, H-index- 09
- **Scopus:** Citations- 228, H-index- 07 | **ResearchGate:** Citations- 295, H-index- 08

PATENT (IPR) (Granted: 1)

1. **Extended-Release Tablet Composition for Multitarget Cancer Therapy**
   Mohamed Abd Elhamid Abbas, Shaban Ahmad, Mohammed Saeed Alqahtani, **Nagmi Bano,** Khalid Raza
   (https://register.dpma.de/DPMAregister/pat/register?AKZ=2020241010280&CURSOR=8)

MEMBERSHIP

1. Contributing **Member of the American Society for Microbiology**, entitled to all the rights and privileges associated therewith as specified by the Bylaws of the Society, in **2025**, as well as in **2026**.

AWARDS/ACHIVEMENTS

1. Certificate of Appreciation as "A Patent Holder in advancing knowledge and fostering excellence in research" on the 1st JMI Innovators Conclave 2024, celebrating the 104th Foundation Day of Jamia Millia Islamia University.
2. Achievers of the Year 2023-2024, awarded by the Vice Chancellor and Provost of the J&K Girls Hostel, Jamia Millia Islamia University, New Delhi, on 04 May 2024.

JOURNAL ARTICLES (Communicated- **03**, Published- **15**)

1. **Bano, N.**, & Raza, K. (2026). FDA-approved inotropic Dopexamine outperforms Nitrofurantoin and Ceftriaxone in overcoming MDR as a standalone multitargeted drug for E. coli-induced UTIs and BSIs. *Journal of Antimicrobial Chemotherapy (JAC).* [Q1, IF: **7**]. (*Submitted, not published yet*).

2. Ahmad, S., **Bano, N.**, Raza, K., (2026). Blind vs LigSite Docking Identifies Oxanthrazole as a Top Multitargeted Lung Cancer Inhibitor from PubChem BioAssays. *(IJBIOMAC-D-25-04108).* [Q1, IF: **8.2**]. (*Submitted, not published yet*).

3. **Bano, N.**, Ahmad, S., Raza, K., (2026). DeepEntXAI: A CNN-LSTM and Hybrid, LIME-Based Explainable Framework for Enterobacteriaceae Drug Activity Classification and Efficacy Prediction. *(Molecular Diversity).* [Q2, IF: **3.8**]. *(2nd round of revision Submitted).*

4. Ahmad, S., Qazi, S, **Bano, N** …., Raza., K., (2026). Multitarget Docking and Molecular Enumeration Reveal DdpMPyPEPhU as a Potent Modulator of Cell Cycle, Glucocorticoid, and Estrogen Signalling in Breast Cancer. *(PlosOne).* [Q2, IF: **3.8**]. *(2nd round of revision Submitted).*

5. Karwasra, R., **Bano, N.**, Ahmad, S., Singh, S., Khanna, K., Sharma, N., Raza, K., Verma, S., (2025). Multimodal evaluation of Mannose Engineered Poly Lactic Glycolic Acid Nanoparticles with Granulocyte Colony Stimulating Factor Focused Delivery to Bone Marrow for Neutropenia. *Nature- Scientific Reports.* https://doi.org/10.1038/s41598-025-29790-w [Q1, IF: **4.6**].

6. **Bano, N.**, & Raza, K. (2025). Unravelling mutation patterns in Extended-Spectrum β-Lactamases for precision drug design against AMR in Enterobacteriaceae. *Molecular Genetics and Genomics*. https://doi.org/10.1007/s00438-025-02300-3 [Q2, IF: **7**].

7. **Bano, N.**, Mohammed, S. A., & Raza, K. (2025). Integrating machine learning and multitargeted drug design to combat antimicrobial resistance: a systematic review. Journal of Drug Targeting. https://doi.org/10.1080/1061186X.2024.2428984 [Q1, IF: **4.5**]

8. **Bano, N.**, Ahmad, S., Gupta, D., Raza, K., (2025). FDA-approved Levophed as an alternative multitargeted therapeutic against cervical cancer transferase, cell cycle, and regulatory proteins. *Elsevier- Computers in Biology and Medicine.* https://doi.org/10.1016/j.compbiomed.2025.110163 [Q1, IF: **7**].

9. Ahmad, S., **Bano, N.**, Raza, K., (2025). Evaluating the polypharmacological potency of FEDPN from ChEMBL BioAssays against lung cancer EGFR, ALK, TrkA and KRAS proteins. *Elsevier- International Journal of Biological Macromolecules*. https://doi.org/10.1016/j.ijbiomac.2025.141703 [Q1, IF: **8.2**].

10. Ahmad, S., **Bano, N.**, Raza, K., (2025). RCSB Protein Data Bank: Revolutionising Drug Discovery and Design for Over Five Decades. *TMR Publishing Group- Medical Data Mining*. https://doi.org/10.53388/MDM202508008. [Q4, IF: **NA**]

11. Zhang, J., Gangwar, S., **Bano, N.**, Ahmad, S., Alqahtani, MS., Raza, K., (2025). Probing the Role of Coniferin and Tetrahydrocurcumin from Traditional Chinese Medicine against PSAT1 in Early-stage Ovarian Cancer. *Plos-PLoS ONE*. http://dx.doi.org/10.1371/journal.pone.0313585 [Q1, IF: **3.3**].

12. Ahmad, S., **Bano, N.**, Khanna, K., Gupta, D., & Raza, K. (2024). Reporting multitargeted potency of Tiaprofenic acid against lung cancer: Molecular fingerprinting, MD simulation, and MTT-based cell viability assay studies.

International Journal of Biological Macromolecules. http://dx.doi.org/10.1016/j.ijbiomac.2024.133872. [Q1, IF: **8.2**].

13. Ahmad, S., Singh, AP., **Bano, N.,** Raza, R., Singh, J., Medigeshi, GR., Pandey, R., Gautam, HK., (2024). Integrative Analysis Discovers Imidurea as a dual multitargeted inhibitor of CD69, CD40, SHP2, Lysozyme, GATA3, cCBL, and S-cysteinase from SARS-CoV-2 and M. tuberculosis. *Elsevier- International Journal of Biological Macromolecules.* http://dx.doi.org/10.1016/j.ijbiomac.2024.132332 [Q1, IF: **8.2**].

14. Faloye, K.O., Ahmad, S., Oyasowo, O.T., Shalom, E. O., **Bano, N.,** Olanudun, E. A., Kelani, T. O., Aliyu, H. E., Raza, K., Makinde, B. I., Alanzi, A. R. (2024). Deciphering the influenza neuraminidase inhibitory potential of naturally occurring bioflavonoids: An in-silico approach. *De Gruyter- Open Chemistry.* https://doi.org/10.1515/chem-2024-0053 [Q3, IF: **2.1**].

15. Noori, R., **Bano, N.,** Ahmad, S., Mirza K., Mazumder JA., Parwez, M., Raza, K., Manzoor, N., Sardar, M., (2024). Microbial biofilm inhibition using magnetic cross-linked polyphenol oxidase aggregates. *ACS- Applied Biomaterials.* http://dx.doi.org/10.1021/acsabm.4c00175 [Q1, IF: **4.7**].

16. Famuyiwa, S.O.*, Ahmad, S.**,** Olufolabo, O. K., Olanudun, E. A., **Bano, N.,** Oguntimehin, S. A., Adesida, S. A., Oyelekan, E. I., Raza, K., Faloye, K. O., (2023). Investigating the multitargeted anti-diabetic potential of cucurbitane-type triterpenoid from *Momordica charantia*: An LC-MS, docking-based MM\GBSA and MD Simulation Study. *T & F- Journal of Biomolecular Structure and Dynamics*. https://doi.org/10.1080/07391102.2023.2291174 [Q1, IF: **5.235**]

17. Ahmad, S., Sayeed, S., **Bano, N.,** Sheikh, K., Raza, K. (2022). In silico analysis reveals Quinic acid as a multitargeted inhibitor against Cervical Cancer. *T & F- Journal of Biomolecular Structure and Dynamics*. https://doi.org/10.1080/07391102.2022.2146202 [Q1, IF: **5.235**].

18. Karwasra, R., Ahmad, S., **Bano, N.,** Qazi, S., Raza, K., Singh, S., & Varma, S. (2022). Macrophage-targeted punicalagin nanoengineering to alleviate methotrexate-induced neutropenia: A molecular docking, DFT, and MD simulation analysis. *Molecules.* https://doi.org/10.3390/molecules27186034. [Q1, IF: **4.6**]

19. Ahmad, S., **Bano, N.,** Qazi, S., Yadav, MK., Ahmad, N., Raza, K. (2022). Multitargeted molecular dynamic understanding of Butoxypheser against SARS-CoV-2: An in-silico study. S*AGE-Natural Product Communications*. https://doi.org/10.1177/1934578X221115499 [Q3, IF: **1.496**].

BOOK CHAPTERS (Communicated- **01**, Published- **07**)

1. **Bano, N.,** Firdaus, S., Parveen, R., Ahmad, S., Raza, K., (2025). Artificial Intelligence in Omics Integration for Precision Drug Design. Published in *AI in Precision Drug Design*. (*E-proof submitted).*

2. **Bano, N**., Sajid, I., Barh, D., Raza, K. (2025). Advancements in artificial intelligence-driven spatial transcriptomics: Decoding cellular complexity. Published in *Deep Learning in Genetics and Genomics*. https://doi.org/10.1016/B978-0-443-27523-4.00006-8

3. Ahmad, S., Bashar, A., Khanna, K., **Bano, N.,** Raza, K. (2025). Deep learning in variant detection and annotation. Published in *Deep Learning in Genetics and Genomics.* http://dx.doi.org/10.1016/B978-0-443-27574-6.00010-2

4. **Bano, N**., Sajid, I., Faizi, S. A. A., Mutshembele, A., Barh, D., & Raza, K. (2024). Computational intelligence methods for biomarkers discovery in autoimmune diseases: case studies. Published in *Artificial Intelligence and Autoimmune Diseases: Applications in the Diagnosis, Prognosis, and Therapeutics*. https://doi.org/10.1007/978-981-99-9029-0_15

5. Ahmad, S., Tanveer, K., **Bano, N.,** Ahmad F., Raza, K., (2024). Artificial Bee Colony Algorithms in Gene Expression Studies: A Case Study. Published in *Solving with Bees.* https://doi.org/10.1007/978-981-97-7344-2_10.

6. Ahmad, S., **Bano, N.,** Sharma, S., Sakina, S., Ahmad, N., and Raza, K. (2024). Generative AI in Drug Designing: Current State-of-the-Art and Perspectives. Published in *Generative AI in Drug Designing: Current State-of-the-Art and Perspectives.* https://doi.org/10.1007/978-981-97-8460-8_20

7. Ahmad, S., Sheikh, K., **Bano, N.,** Rafeeq, M. M., Mohammed, M. R. S., Yadav, M. K., & Raza, K. (2024). Beispielhafte Implikationen von naturinspirierten Berechnungsmethoden auf Therapeutika und computergestützte Arzneimittelentwicklung. Published in *Von der Natur inspirierte intelligente Datenverarbeitungstechniken in der Bioinformatik.* https://doi.org/10.1007/978-981-99-7808-3_15.

8. Ahmad, S., Sheikh, K., **Bano, N**., Rafeeq, M. M., Mohammed, M. R. S., Yadav, M. K., & Raza, K. (2022). Illustrious implications of nature-inspired computing methods in therapeutics and computer-aided drug design. Published in *Nature-inspired intelligent computing techniques in bioinformatics*. https://doi.org/10.1007/978-981-19-6379-7_15

WORKSHOPS ATTENDED

1. A one-week workshop on "Advanced Drug Designing and Computational Biology" organised by the Department of Chemistry, Jamia Millia Islamia University, New Delhi, from 16-22 September 2024.
2. New Education Policy (NEP) 2020, Orientation and Sensitisation Programme under the Malaviya Mission Teacher Training Programme (MM-TTP) of University Grants Commission (UGC) Organised by MMTTC, Jamia Millia Islamia, New Delhi from 10-14 August 2024.
3. Attending "Analysis of Next-Generation Sequencing Datasets from Bulk, Single-Cell, and Spatial Transcriptomics", held at the International Centre for Genetic Engineering and Biotechnology (ICGEB), New Delhi, from 07-09 August 2024.
4. Enabling Technology Training (ETT-5) Workshop, titled "How to calculate accurate binding free energy for drug design", 17 February 2024. School of Computational and Integrative Science (SCIS), Jawaharlal Nehru University, New Delhi.
5. Enabling Technology Training (ETT-3) Workshop, "Predicting Drug Resistance in Tuberculosis From Whole Genome Sequencing", 03 February 2024. School of Computational and Integrative Science (SCIS), Jawaharlal Nehru University, New Delhi.
6. Participated in "Artificial Intelligence in Modern Biology" at the International Centre for Genetic Engineering and Biotechnology (ICGEB), New Delhi, from 23-25 August 2022.
7. AI Workshop 2021, a 7-day International Workshop on Artificial Intelligence, conducted by St. Claret College (SCC), Bangalore, from 15-21 November 2021.
8. Biofisica-2K18 National Workshop on "Recent Challenges to Biophysics and Bioinformatics" organised by Biophysics Society in association with Regional Council UP (RC-4), Indian Association of Physics Teachers (IAPT), and Department of Physics, Ewing Christian College, Allahabad from 19-20 January 2018.

CONFERENCES ATTENDED/PRESENTED

1. Participated and Oral presented on title: *"Dopexamine as a Multitargeted Drug Candidate for E. coli caused Urinary Tract and Bloodstream Infections and Outperforms FDA-approved Drugs Nitrofurantoin and Ceftriaxone"* at the 1st International Electronic Conference on Medicinal Chemistry and Pharmaceutics, Online | 1-30 November 2025.
2. Participated and presented poster on title: *"DeepEntXAI: A CNN-LSTM and Hybrid, LIME-Based Explainable Framework for Enterobacteriaceae Drug Activity Classification and Efficacy Prediction"* at the **AMR Research conference 2025 (ARC 2025)**, jointly organized by the Tata Institute for Genetics and Society, National Centre for Biological Sciences and Alliance for Pathogen Surveillance Initiative on 21st & 22nd August 2025 at Bengaluru.
3. "Economic Botany and Plant Genetic Resources: National Perspective" organised by the Botanical Society of Deshbandhu College, University of Delhi, on 18 January 2022.
4. One-Day Awareness Programme on Research Data Management, Organised by Information and Library Network (INFLIBNET) Centre, Gandhinagar, Gujarat, in collaboration with Jamia Millia Islamia University, New Delhi on 10 December 2024.
5. Attended an online session organised by Springer Nature for One Nation One Subscription Member Institutions entitled How to Navigate the World of Scientific Article Writing: From Manuscript Structure to Publication on 15 May 2025.

SKILLS & PRACTICAL EXPERTISE

- **Research Interest:** Artificial Intelligence in Biology, Antimicrobial Resistance (AMR), Drug Resistance, Cancer Resistance, Machine Learning, Deep Learning, Multitarget Drug Design, Explainable AI (XAI), Personalised Medicine, Computational Drug Discovery, Systems Biology.

- **Operating Systems:** Linux (Ubuntu), Windows (10, 11, Server), Android, macOS.

- **Programming & Scripting Languages:** Python (including libraries such as NumPy, pandas, Matplotlib, Biopython), R (tidy verse, Bioconductor), Perl, MATLAB, Bash scripting, SQL.

- **Web Development:** PHP, Django, Flask, API development.

- **Automation & Workflow Tools:** NextGen Flow, KNIME, Power Automate, GitHub Actions.

- **Data Analysis & Machine Learning:** Weka, TensorFlow, Keras, PyTorch, Scikit-learn, XGBoost, LightGBM, Pandas, NumPy, Matplotlib, Seaborn, Jupyter Notebooks, MS Excel.

- **Bioinformatics & Sequence Analysis:** BLAST, FASTA, Clustal Omega, MEGA, Phylip, EMBOSS, HMMER, Bowtie, SAMtools, BWA, T-Coffee, MAFFT, Geneious Prime, Genome Browsers.

- **Structural Biology & Molecular Modelling:** PyMOL, Chimera, Swiss-PDB Viewer, Modeller, VMD, Rosetta, Chimera.

- **Genomics Tools:** GEO2R, Gene Ontology-based Enrichment Analyzer, SRA Toolkit, Bowtie2, TopHat, Cufflinks, HTSeq, SAMtools, BWA, GATK, Picard, Geneious Prime, DESeq2, EdgeR, Bioconductor packages.

- **Systems Biology:** Cytoscape, KEGG Mapper, Reactome Pathway Browser, STRING, GeneMANIA.

- **Drug Discovery:** AutoDock, SwissDock, InstaDock, GOLD, Glide (Schrödinger Suite) MOE, LigPlot+, and many more.

- **Molecular Dynamics Simulation:** Desmond, GROMACS, NAMD, VMD (visualisation).

- **Free Energy Calculations:** MM/GBSA, MM/PBSA, FEP (Free Energy Perturbation), Umbrella Sampling.

- **Graphics & Visualisation:** BioRender, Adobe Photoshop, Blender (3D modelling, animation), ClipChamp, PowerPoint, Matplotlib, Seaborn, ggplot2.

- **Additional Expertise:** Protein and ligand structure optimisation, multitargeted drug design, virtual screening workflows (VSW), interaction fingerprint analysis, WaterMap, Density Functional Theory (DFT) calculations, molecular docking, molecular dynamics simulation, MMGBSA.

- **Cloud & HPC:** Proficient in managing and configuring cloud servers (AWS, Google Cloud), HPC clusters, and supercomputers; job queue management (SLURM), deployment, and workflow scheduling.

PEER-REVIEWED (28 reviews for 9 Journals)

1. Review activity for *BMC Pregnancy and Childbirth*
2. Review activity for *Archives of Microbiology*.
3. Review activity for *Scientific reports*.
4. Review activity for *PLOS ONE*
5. Review activity for *PeerJ*.
6. Review activity for *Journal of Public Health and Community Medicine.*
7. Review activity for *Journal of Pharmacological and Pharmaceutical Research*.
8. Review activity for *Journal of Drug Targeting*.
9. Review activity for *AIMS molecular science*.

ACADEMIC PROJECTS GUIDED

- Guided 10 MSc and 5 MCA dissertation students during my PhD tenure at JMI.
- Guided and helped junior PhD Students as a mentor about quality research and publication.

PERSONAL DETAILS

Father's Details: Mohd Naim

Mother's Details: Kulsoom Fatima

Marital Status:	Unmarried
Nationality/Sex:	Indian / Female
Language Known:	English, Hindi, Urdu and basic Arabic and Sanskrit

REFEREES

Dr Khalid Raza (PhD Supervisor)
Associate Professor
Department of Computer Science
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Dr Dinesh Gupta (PI @ ICGEB)
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Dr Shaban Ahmad (MSc and PhD mentor)
Postdoc Scientist
Microbial Ecology and Biotechnology Section,
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Dr Md Imtaiyaz Hassan (MSc Mentor and Teacher)
Professor
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Updated on 04 February 2026

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