Dr Shaban Ahmad

Postdoc Researcher at University of Copenhagen, Denmark

PhD (*AI in Biology*), **MIASLC, MESMO, MBDDS**

Born on: **August 12, 2000**
High School (X[th]): **2013**
Intermediate (XII[th]): **2015**
Undergraduate (BSc): **2018**
Postgraduate (MSc): **2020**
PhD: Awarded on **07/02/2025**

PROFILE SUMMARY

CONTACT INFORMATION

Mobile: **+45-91433496** | +91-7065822766 | Email: **Shaban.ucph@gmail.com** | Shaban@plen.ku.dk

SCIENTOMETRIC INDICATORS

- **ResearchGate:** Citations- 1650, H-index- 26 | **Scopus:** Citations- 1238, H-index- 23
- **GoogleScholar:** Citations- 1593, H-index- 26, i10-index- 42 | **WoS**- Citations- 913, H-index- 21

PATENT (IPR)

- **Granted: 01 (German)** | In Pipeline: 06 (05 Indian, 1 US)

PUBLICATIONS

- Published: **74** | Journal Articles: **50** (Mostly Q1/Q2) | Chapters/Proceedings: **24**
- Communicated: **05** | Journal Articles: **05** | Book Chapters: **00**
- Authored/Edited Books: **01** (in the pipeline)

FUNDED RESEARCH PROJECTS

- Yet to Start as PI
- Grant Writing Skills: **BRICS, ICMR, ANRF** (Funded to my PhD Lab- ***Prof Khalid Raza***)

EDITORIAL ACTIVITIES

- Guest Editor: **Frontiers in Oncology** 2025 – till date
- Guest Editor: **Current Genomics** 2025 – till date
- Guest Editor: **Discover Biotechnology** 2025 – till date
- Guest Editor: **Mini-Reviews in Medicinal Chemistry** 2024 – till date
- Guest Editor: **Natural Product Communications** 2024 – till date

SOCIETY MEMBERSHIPS

- **Member of the International Association for the Study of Lung Cancer** (18/10/2024-17/10/2026)
- **Member of the European Society for Medical Oncology** (10/05/2024 - 09/05/2026)
- **Member of the Bioinformatics and Drug Discovery Society** (Life Member)
- **Council Member of the Botanical Society (Sanjeevani), DBC-University of Delhi** (2017-2018)

RESEARCH INTERESTS

Artificial Intelligence in Genomics | Artificial Intelligence in Drug Design | Deep Learning | Bioinformatics | Computer-Aided Drug Design | Computational Genomics | Computational Chemistry | Molecular Dynamics Simulation | DFT | Binding Free Energy | Vaccine Design

AWARDS & RECOGNITIONS

- Recognised among **the World's Top 2% Scientists by Stanford University and Elsevier**.
- **Awarded 13 times** for Best Presentation (poster and oral) and working model (prototype) by various universities, institutions and ministries (DBT, DST).
- Society contributions (Greenest Campus in Delhi) were awarded by WEED (affiliated to the United Nations under ECOSOC, UNDPI, UNICEF, and **UNESCO**) in 2016.

Dr Shaban Ahmad

Postdoc Researcher at **University of Copenhagen**

MSc (Bioinformatics), PhD (AI in Biology)

Member of IASLC, ESMO, BDDS

Recognised among the World's Top 2% Scientists by Stanford/Elsevier.

Contact:

Mobile	**+45-91433496**
	+91-7065822766
Emails	**shaban.ucph@gmail.com**
	shaban@plen.ku.dk
Website	website

About Me

Dr Shaban Ahmad is a Postdoctoral Researcher in Microbial Ecology and Biotechnology Section at the Department of Plant and Environmental Sciences, University of Copenhagen. His research combines AI, bioinformatics, and computational biology to identify PFAS-degrading enzymes in bacteria, addressing critical environmental challenges and advancing sustainable solutions. He earned his MSc and PhD in Bioinformatics from Jamia Millia Islamia University, New Delhi, where he developed AI-based models for drug discovery, focusing on lung cancer therapeutics. Dr Ahmad brings strong expertise in genomics, computational drug design, and machine learning, with developer-level proficiency in Python and a broad command of advanced analytical tools.

His earlier research contributions include the development of several deep learning models/frameworks such as **DrLungker**, **DeepEntXAI**, and **LungXAI**. He has also worked on genome-level projects, including de novo assembly and annotation of *Ralstonia solanacearum UTT-25* and comprehensive analyses of the nuclear and chloroplast genomes of *Vigna umbellata*. These projects were conducted during his tenure at institutions including Jamia Millia Islamia, ICGEB, ICAR-IARI, SRM University, and Jamia Hamdard.

Dr Ahmad is the co-author of over 74+ scientific articles and reviews, an active member of various professional societies and a guest editor for several prestigious journals. In addition to his current role in Denmark, he was also a Visiting Postdoctoral Fellow at the *University of Jyväskylä, Finland,* expanding his research and fostering Nordic scientific collaborations.

RESEARCH TRAINING AND EXPERIENCES

University of Copenhagen, Denmark [June 2025- to date]

Postdoc Scientist: AI and Data-driven strategies to identify PFAS-degrading enzymes in bacteria.

University of Jyväskylä, Finland [January-December 2025]

Visiting Researcher: Artificial Intelligence and Data-driven strategies predicting the colorectal cancer susceptibility.

Jamia Millia Islamia, New Delhi [September 2021-February 2025]

PhD Scholar: AI-based Predictive Modelling and Molecular Enumeration against Lung Cancer

SRM University Delhi-NCR, Sonepat, Haryana [Nov 2020-September 2021]

Project Assistant: Drug repurposing against key COVID-19 Drug Targets using advanced Machine Learning based algorithms

ICAR- Indian Agricultural Research Institute [January–June 2020]

DBT-Studentship: (Fellowship awarded for completion of Dissertation at AKMU-IARI)- Denovo assembly, annotation of *Ralstonia solanacearum UTT-25* (Bacterial genome).

International Centre for Genetic Engineering and Biotechnology [15 May 2019 – 30 December 2019]

Research Trainee (NIC- PMB Group): NGS analysis of WGS, Complete chloroplast genome of *Vigna umbellata*.

Jamia Hamdard University **[**March-April 2019]

DBT-Two-month Studentship (DBT-BIF under Prof. Shakir Ali): Comparative Genomics study of *Plasmodium vivax* and *P. falciparum.*

International Centre for Genetic Engineering and Biotechnology [Jan-Feb 2019]

Research Trainee (NIC-PMB): Tissue culture, Different Media and Hormone preparation

University of Delhi (DBC-301) [15 September 2015 - 15 October 2016]

Research Trainee: Performed the seed sterilisation, sowing, fungus culture, colonial study, the microchemical test of active principle, and the weed-based botanicals test against fungi.

ACADEMIC QUALIFICATIONS

Course	School/Department	Board / University	Year
PhD (AI in Biology)	Computer Science (Gold Medallist)	Jamia Millia Islamia	2025
MSc (Bioinformatics)	Computer Science	Jamia Millia Islamia	2020
BSc Hons (Botany)	Deshbandhu College	University of Delhi	2018
XII (Intermediate)	Jesus and Mary Inter College, Lucknow	UP Board	2015
X (High School)	Jesus and Mary School, Lucknow	UP Board	2013

- Honorary Alumna of *National Institute of Pharmaceutical Education and Research (NIPER)-Ahmedabad* for attending the 7-day SERB (DST-GoI) funded KARYASHALA.

PhD DETAILS

Title: *AI-based Predictive Modelling and Molecular Enumeration against Lung Cancer.*

Summary: My PhD research leveraged artificial intelligence (AI) to accelerate drug discovery, focusing on multitargeted drug identification and repurposing. We identified Imidurea, Tiaprofenic Acid, and Theodrenaline through traditional extensive physics-based computational methods and validated them experimentally. For AI work, the Lung Cancer BioAssays obtained from ChEMBL and PubChem with a 5.0 µM threshold and generated 5,886 descriptors of 26,396 unique compounds to apply advanced deep learning models—Residual Neural Network, Feed Forward Neural Network, and Recurrent Neural Network—which achieved near-perfect accuracy (0.99–1) in predicting highly active

compounds. Multitargeted docking studies against ALK, HSP5, KRas, MMP-8, and tRNA DHDS2 identified three potent candidates (PubChem CIDs 144074375, 440810382, and 48426893) with strong docking and MM/GBSA scores. Molecular enumeration of all 6 compounds led to an extensive compound library, from which Ammetazebenpro, Pheammethpuzetidine, and Amthofluoquinoxaline emerged as top candidates by many downstream studies, and Pheammethpuzetidine emerged with the strongest binding and lowest free energy. These compounds demonstrated up to five times the therapeutic potential of FDA-approved Erlotinib, supporting their advancement to preclinical and clinical stages. All studies were published in reputed journals, and the novel compounds were patented.

Timeline: Admission on 07 September 2021, Submitted on 10 October 2025, Defended on 14 January 2024, and Awarded (Notified) on 07 February 2025 (Duration: 3 Years 5 Months)

LEADERSHIP, EXTRACURRICULAR ACTIVITIES

- Class Representative, PhD (2021-25).
- Class Representative, BSc (Hons.) Botany (2015-18).

ACADEMIC PROJECTS GUIDED (Supervision)

- Currently supervising 3 MSc and 1 BSc dissertation students at the University of Copenhagen, Denmark.
- Guided Junior PhD Students as a mentor on quality research and publication.
- Guided 10 MSc and 5 BSc dissertation students during my PhD tenure at JMI.

EDITORIAL EXPERIENCES

- Guest Editor: **Frontiers in Oncology** 2025 – till date
- Guest Editor: **Current Genomics** 2025 – till date
- Guest Editor: **Discover Biotechnology** 2025 – till date
- Guest Editor: **Mini-Reviews in Medicinal Chemistry** 2024 – till date
- Guest Editor: **Natural Product Communications** 2024 – till date

MEMBERSHIP OF PROFESSIONAL BODIES

- Member of the **International Association for the Study of Lung Cancer** (18/10/2024 to 17/10/2026)
- Member of the **European Society for Medical Oncology** (10/05/2024 to 09/05/2026)
- Member of the **Bioinformatics and Drug Discovery Society** (Life Member)
- Ex-Council Member of the **Botanical Society (Sanjeevani)**, **Deshbandhu College, DU.**

AWARDS / ACHIEVEMENTS

1. Recognised among the World's Top 2% Scientists by Stanford University and Elsevier.
2. Facilitated by the Vice Chancellor and other Academic mentors of Jamia Millia Islamia, New Delhi, on 30 June 2025, for securing a full-time Postdoc Scientist position at the University of Copenhagen, Denmark, and a visiting Postdoc fellow at the University of Jyväskylä, Finland.
3. 'Achievers of the Year 2024-2025' award by the University Registrar and Provost of the Maulana Muhammad Ali Jauhar Hall of Boys Residence, Jamia Millia Islamia, New Delhi, on 09 May 2025.
4. Best Presentation Award at the 3rd International Electronic Conference on Cancers: New Targets for Cancer Therapies. March 16–30, 2023 MDPI-Sciforum (PhD Thesis Work).
5. Best Presentation Award at 21st International Conference on Bioinformatics (InCoB), November 21-23, 2022, organised by APBioNet and King Abdullah University of Science and Technology (KAUST), Kingdom of Saudi Arabia (PhD Thesis Work).
6. Awarded a six-month fellowship from the DBT, GoI, as 'DBT-Studentship' at ICAR-IARI, New Delhi, for a master's dissertation from 15 January to 15 July 2020.
7. Best Oral presentation award in Interdisciplinary Science Conference: Big Data and Computational Biology, organised by CIRBSc Jamia Millia Islamia, New Delhi, October 21-22, 2019.
8. Best Poster Presenter award in National Conference on "Conservation, cultivation and Sustainable Use of Medicinal and Aromatic Plants", at MRRIIRS, February 21-22, 2019.
9. Awarded a two-month fellowship from the DBT, Govt of India, as 'DBT-Studentship' at Jamia Hamdard, New Delhi, to carry out the comparative analysis on Plasmodium vivax from March to April 2019.
10. 1st prize in Working Model Presentation, on 13 April 2018, "PARIVARTAN 2K18" Department of Environmental Science and NSS, Sri Aurobindo College, University of Delhi.
11. Felicitated at the 26th World Environmental Congress, World Environmental and Ecology Development (WEED) (Greening of Education, Employment, Environment, Empowerment, and Entrepreneurship) 08 November 2017, at the Indian International Centre, New Delhi, India.
12. 2nd prize in Explico - Know Your Green in "SANJEEVANI" October 2016, Department of Botany, Deshbandhu College, University of Delhi.
13. Best poster award in ICSSR-sponsored National Seminar on "Emerging Issues of Climate Change: Sustainability and Economic Implications" on October 21-22, 2016, organised by Sri Aurobindo College, University of Delhi.
14. Awarded fellowship for the Research/Innovation Project: Food for the Future: Studies on the nutritional value of *Fagopyrum esculentum* (Kuttu) – a pseudo-cereal and efficacy of weed-based botanicals against its root rot disease from 01 September 2015 to 31 August 2016.

PATENT (IPR)

Granted (1):

Extended-Release Tablet Composition for Multitarget Cancer Therapy
Applicant/Owner: **Shaban Ahmad,** Mohamed Abd Elhamid Abbas, Mohammed Saeed Alqahtani, Nagmi Bano, and Khalid Raza
Country: Germany
(*https://register.dpma.de/DPMAregister/pat/register?AKZ=202024101028O&CURSOR=8*)

In Pipeline (6): Drug Molecules Designed During PhD Tenure (**Shaban Ahmad** & Khalid Raza)

PUBLICATIONS

Submitted Journal Articles (05)

1. **Ahmad, S.,** Bano, N., Raza, K. (2026). DeepEntXAI: A CNN-LSTM and Hybrid, LIME-Based Explainable Framework for *Enterobacteriaceae* Drug Activity Classification and Efficacy Prediction. Submitted: CIBM-D-24-06110. [Q1, IF: **7**].
2. Raza, K., **Ahmad, S.** (2026). **Nature's Pharmacy for the Therapeutics of Lung and Respiratory Diseases.** Editorial, *Submitted: NPX-26-0106 (2026)*
3. **Ahmad, S.,** Bano, N., Raza, K. (2026). Blind vs LigSite Docking Identifies Oxanthrazole as a Top Multitargeted Lung Cancer Inhibitor from PubChem BioAssays. Submitted: IJBIOMAC-D-25-04108. [Q1, IF: **8.2**].
4. **Ahmad, S.,** Qazi, S., Bano, N., Rahiduddin, Gatam, P. K., Raza, K. (2026). Multitarget Docking and Molecular Enumeration Reveal DdpMPyPEPhU as a Potent Modulator of Cell Cycle, Glucocorticoid, and Estrogen Signalling in Breast Cancer. Submitted: IJBIOMAC-D-25-041021. [Q1, IF: **8.2**].
5. Shah, S. N. A., **Ahmad, S.,** Parveen, R. (2026). LUNGXAI: A Deep Learning Framework with LIME-based Interpretability for Gene Expression and Classification. Submitted: INFFUS-D-25-02490 [Q1, IF: **14.8**].

Published Journal Articles (50)

6. **Ahmad, S.,** Raza, K. (2025). DrLungker: A Deep Ensemble Learning Framework for Predicting Anti-Lung Cancer Compound Activity and Validating Multitarget Potency through WaterMap, DFT, MD Simulations, and MM-GBSA Analysis. *Wiley-Advanced Theory and Simulations.* https://doi.org/10.1002/adts.202501550 [Q1, IF: **2.9**].
7. 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**].
8. **Ahmad, S.,** Raza, K. (2025). Evaluating the Polypharmacological Potential of Cosmetic Preservative Imidurea Against Lung Cancer-Associated EGFR, CDK2, STAT3, BCL2, p53, and ABCB1 Proteins. *Elsevier- International Journal of Biological Macromolecules*. https://doi.org/10.1016/j.ijbiomac.2025.146175 [Q1, IF: **8.5**].
9. **Ahmad, S., S**hah, S. N. A., Parveen, R., Raza, K. (2025). Machine Learning for Genomic Profiling and Drug Discovery in Personalised Lung Cancer Therapeutics. *T & F- Journal of Drug Targeting.* http://doi.org/10.1080/1061186X.2025.2530656 [Q1, IF: **4.5**].
10. Khzem, A., Al., **Ahmad, S.** (2025). Correction: Integrative computational approaches identify haptoglobin inhibitors to modulate erythrocyte sedimentation rate in trauma-linked inflammatory and haematological malignancies. *Frontiers in Chemistry - Theoretical and Computational Chemistry.* https://doi.org/10.3389/fchem.2025.1662748 [Q1, IF: **3.8**].
11. 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**]

12. **Ahmad, S.,** Kumar, N., Gautam, H. K., Raza, K. (2025). Probing the Multitargeted Potency of Theodrenaline and Its Comparative Evaluation with Crizotinib Against Transferase, Hydrolase, Signalling, and Apoptosis-Related Proteins to Overcome Lung Cancer Drug Resistance. *Elsevier- International Journal of Biological Macromolecules*. https://doi.org/10.1016/j.ijbiomac.2025.142343 [Q1, IF: **8.2**].
13. Khzem, A., Al., **Ahmad, S.** (2025). Integrative Computational Approaches Identify Haptoglobin Inhibitors to Modulate Erythrocyte Sedimentation Rate in Trauma-Linked Inflammatory and Haematological Malignancies. *Frontiers in Chemistry - Theoretical and Computational Chemistry*. https://doi.org/10.3389/fchem.2025.1611972 [Q1, IF: **3.8**].
14. **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**].
15. **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**]
16. Singh, AP., **Ahmad, S.,** Roy, A., Raza, K., Gautam, HK. (2025). Investigating the Inhibitory Effects of Paliperidone on RAGEs: Docking, DFT, MD Simulations, MMPBSA, MTT, Apoptosis, and Immunoblotting Studies. *MDPI- International Journal of Molecular Sciences*. https://doi.org/10.3390/ijms26031060 [Q1, IF: **4.9**].
17. 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**].
18. Kumar, A., ... **Ahmad, S.,** & Mishra, V. (2025). Molecular Dynamics Simulation and Docking Studies Reveal Inhibition of NF-kB Signalling as a Promising Therapeutic Drug Target for Reduction in Cytokine Storms. *Nature- Scientific Reports*. https://doi.org/10.1038/s41598-024-78411-5 [Q1, IF: **4.6**].
19. **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. *Elsevier- International Journal of Biological Macromolecules*. http://dx.doi.org/10.1016/j.ijbiomac.2024.133872 [Q1, IF: **8.2**].
20. Singh, N., Kumar, P., **Ahmad, S.,** Gupta, J., Raza, K., Hashmi, A. A. (2024). Synthesis, structural elucidation, and antibacterial activities of novel copper(II), cobalt(II), and nickel(II) complexes with a bidentate Schiff base ligand against pathogenic bacteria. *Elsevier- Journal of Molecular Structure*. https://doi.org/10.1016/j.molstruc.2024.139874 [Q1, IF: **4.0**].
21. **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**].
22. 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**].

23. **Ahmad, S.** (2024). Meet the Executive Guest Editor of Mini-Reviews in Medicinal Chemistry (Shaban Ahmad). *Bentham Science- Mini-Reviews in Medicinal Chemistry*. http://dx.doi.org/10.2174/1389557524132404221551 39 [Q2, IF: **3.8**].
24. Noori, R., Bano, N., **Ahmad, S.,** Mirza, K., Mazumder, J.A., 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**].
25. **Ahmad, S.,** Raza, K. (2023). An Extensive Review on Lung Cancer Therapeutics Using Machine Learning Techniques: State-of-the-art and Perspectives. *T & F- Journal of Drug Targeting*. https://doi.org/10.1080/1061186X.2024.2347358 [Q1, IF: **4.5**].
26. Rana, M., Ahmedi, S., Mehandi, R., **Ahmad, S.,** Fatima, T., Raza, K. and Manzoor, N. (2024). 2-hydrazinobenzothiazole-based derivatives: Synthesis, characterisation, antifungal, DNA binding and molecular modelling approaches. Elsevier- *Journal of Molecular Structure*, p.138051.https://doi.org/10.1016/j.molstruc.2024.138051 [Q2, IF: **3.841**].
27. **Ahmad, S.,** Gautam, H., Singh, V., Raza, K. (2023). Multisampling-based docking reveals Imidazolidinyl urea as a multitargeted inhibitor for Lung Cancer: An optimisation followed multi-simulation and *in-vitro* study. *T & F- Journal of Biomolecular Structure and Dynamics*. https://doi.org/10.1080/07391102.2023.2209673 [Q1, IF: **5.235**].
28. Sahu, A., **Ahmad, S.,** Imtiyaz, K., Kumaran, A.K., Islam, M., Raza, K., Easwaran, M., Kunnath, A.K., Rizvi, M.A., Verma, S. (2023). In-silico and in-vitro studies reveal ziprasidone as a potential aromatase inhibitor against breast carcinoma. *Nature- Scientific Reports*. https://doi.org/10.1038/s41598-023-43789-1 [Q1, IF: **4.6**].
29. 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**]
30. **Ahmad, S.,** Raza, K. (2023). Identification of 5-nitroindazole as a multitargeted inhibitor for CDK and transferase kinase in lung cancer: a multisampling algorithm-based structural study. *Springer-Mol Diversity*. https://doi.org/10.1007/s11030-023-10648-0 [Q2, IF: **3.9**].
31. Rana, M., Hungyo, H., Parashar, P., **Ahmad, S.,** Mehandi, R., Tandon, V., Raza, K., Assiri, M., Ali, T., El-Bahy, Z., Rahisuddin (2023). Design, synthesis, X-ray crystal structures, anticancer, DNA binding and modelling studies of pyrazole–pyrazoline derivatives. *RSC-Advances*. https://doi.org/10.1039/d3ra04873j [Q2, IF: 3.9].
32. Bhati, R., Nigam, A., **Ahmad, S.,** Raza, K., Singh, R. (2023). Structural-functional analysis and Molecular characterisation of arsenate reductase from *Enterobacter cloacae* RSC3 for arsenic biotransformation. *Springer- 3-Biotech*. https://doi.org/10.1007/s13205-023-03730-9 [Q2, IF: 2.8].
33. Singh, AP., **Ahmad, S.,** Raza, K., Gautam, HK. (2023). Computational screening and MM\GBSA-based MD simulation studies reveal the high binding potential of FDA-approved drugs against *Cutibacterium acnes* Sialidase. *T & F- Journal of Biomolecular Structure and Dynamics*. http://dx.doi.org/10.1080/07391102.2023.2242950 [Q1, IF: 5.235]
34. Mateev, E., Georgieva, M., Mateeva, A., Zlatkov, A., **Ahmad, S.,** Raza, K., Azevedo, V., Barh, D. (2023). Structure-Based Design of Novel MAO-B Inhibitors: A Review. *MDPI-Molecules*. https://doi.org/10.3390/molecules28124814 [Q1, IF: **4.927**].

35. Rohit, S., **Ahmad, S.,** Raza, K. (2023). Comparative genomic assessment of members of Genus *Tenacibaculum*: An exploratory study. *Springer- Molecular Genetics and Genomics*. https://doi.org/10.1007/s00438-023-02031-3 [Q2, IF: **2.980**].
36. Rana, M., Ahmedi, S., Fatima, A., **Ahmad, S.,** Nouman, Siddiqui, N., Raza, K., Manzoor, N., Javed, S., Rahisuddin, (2023). Synthesis, Single crystal, TD-DFT, Molecular Dynamics Simulation and DNA binding studies of Carbothioamide Analogue. *Elsevier- Journal of Molecular Structure.* https://doi.org/10.1016/j.molstruc.2023.135701 [Q2, IF: **3.841**].
37. Shah, AA., **Ahmad, S.,** Yadav, MK., Raza, K., Kamal, MA., Akhtar, S. (2023). Structure-based virtual screening, molecular docking, molecular dynamics simulation, and metabolic reactivity studies of quinazoline derivatives for their anti-EGFR activity against tumour angiogenesis. *Bentham Science- Current Medicinal Chemistry*. https://doi.org/10.2174/0929867330666230309143711 [Q1, IF: **4.740**].
38. Famuyiwa, S.O., **Ahmad, S.,** Fakola, E.G., Olusola, A.J., Adesida, S.A., Obagunle, F.A., Raza, K., Ugwo, J. P., Oyelekan, E.I., Faloye, K.O. (2023). Comprehensive Computational Studies of Naturally Occurring Kuguacins as Anti-diabetic Agents by Targeting Visfatin. *Springer-Chemistry Africa*. http://dx.doi.org/10.1007/s42250-023-00604-8 [Q3, *ESCI*].
39. Yadav, M. K., **Ahmad, S.,** Raza, K., Kumar, S., Eswaran, M., & Pasha, K. M. (2022). Predictive modelling and therapeutic repurposing of natural compounds against the receptor-binding domain of SARS-CoV-2. *T & F- Journal of Biomolecular Structure and Dynamics*. https://doi.org/10.1080/07391102.2021.2021993 [Q1, IF: **5.235**].
40. Tarique, M., **Ahmad, S.,** Malik, A., Ahmad, I., Saeed, M., Almatroudi, A., ... & Al-Saleh, Y. (2022). Correction to: Novel Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) and Other Coronaviruses: A Genome-wide Comparative Annotation and Analysis. *Molecular and Cellular Biochemistry*, *477*(2), 645. https://doi.org/10.1007/s11010-021-04317-9 [Q2, IF: **3.396**].
41. Barh, D., Tiwari, S., Gomes, L. G. R., Pinto, C. A. H. R., Andrade, B. S., **Ahmad, S.,** et al (2022). SARS-CoV-2 Variants Show a Gradual Declining Pathogenicity and Pro-Inflammatory Cytokine Stimulation, an Increasing Antigenic and Anti-Inflammatory Cytokine Induction, and Rising Structural Protein Instability: A Minimal Number Genome-Based Approach—*Springer- Inflammation.* https://doi.org/10.1007/s10753-022-01734-w [Q2, IF: **4.657**].
42. **Ahmad, S.,** Chitakara, P., Kaul, T., Raza, K. (2022). Comparative insight into Rice chloroplasts genome: Mutational Phylogenomics reveals *Echinochloa oryzicola* as the ongoing progenitor of rice. *Springer- Genetic Resources and Crop Evolution.* https://doi.org/10.1007/s10722-022-01471-x [Q2, IF: **1.876**].
43. 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. *MDPI-Molecules*. https://doi.org/10.3390/molecules27186034 [Q1, IF: **4.927**].
44. **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**].
45. **Ahmad, S.,** Bano, N., Qazi, S., Yadav, M.K., Ahmad, N., Raza, K. (2022). Multitargeted molecular dynamic understanding of Butoxypheser against SARS-CoV-2: An in-silico study. *SAGE-Natural Product Communications*. https://doi.org/10.1177/1934578X221115499 [Q3, IF: **1.496**].

46. **Ahmad, S.,** Pasha, K. M., Raza, K., Rafeeq, M. M., Habib, A. H., Eswaran, M., & Yadav, M. K. (2022). Reporting dinaciclib and theodrenaline as a multitargeted inhibitor against SARS-CoV-2: an in-silico study. *T & F- Journal of Biomolecular Structure and Dynamics*. https://doi.org/10.1080/07391102.2022.2060308 [Q1, IF: **5.235**].
47. Alturki, N. A., Mashraqi, M. M., Alzamami, A., Alghamdi, Y. S., Alharthi, A. A., Asiri, S. A., **Ahmad, S.,** & Alshamrani, S. (2022). In-silico Screening and Molecular Dynamics Simulation of Drug Bank Experimental Compounds against SARS-CoV-2. *MDPI-Molecules*. https://doi.org/10.3390/molecules27144391 [Q1, IF: **4.927**].
48. Youssef, S. A., Mashraqi, M. M. Alzamami, A., Alturki, N. A., **Ahmad, S.,** Alharthi, A. A., Alshamrani, S., & Asiri, S. A. (2022). Unveiling the multitargeted potential of N-(4-Aminobutanoyl)-S-(4-methoxybenzyl)-L-cysteinylglycine (NSL-CG) against SARS-CoV-2: A virtual screening and molecular dynamics simulation study. *T & F- Journal of Biomolecular Structure and Dynamics*. https://doi.org/10.1080/07391102.2022.2110158 [Q1, IF: **5.235**].
49. Alzamami, A., Alturki, N. A., Alghamdi, Y. S., **Ahmad, S.**, Alshamrani, S., Asiri, S. A., & Mashraqi, M. M. (2022). Hemi-Babim and Fenoterol as Potential Inhibitors of MPro and Papain-like Protease against SARS-CoV-2: An In-Silico Study. *MDPI-Medicina*. https://doi.org/10.3390/medicina58040515 [Q2, IF: **2.948**].
50. Hou, J., Bhat, AM., **Ahmad, S.**, Raza, K., Qazi, S. (2022). In silico analysis of the ACE2 receptor to find potential herbal drugs in COVID-19-associated neurological dysfunctions. *SAGE- Nat Product Communications*. https://doi.org/10.1177/1934578X221118549 [Q3, IF: **1.496**].
51. **Ahmad, S.**, Bhanu, P., Kumar, J., Pathak, R.K., Mallick, D., Uttarkar, A., Niranjan, V., Mishra, V. (2022). Molecular dynamics simulation and docking analysis of NF-kB protein binding with sulindac acid. *Bioinformation*. https://doi.org/10.6026%2F97320630018170 [Q4, ***ESCI***].
52. Khuntia, B. K., Sharma, V., Wadhawan, M., Chhabra, V., Kidambi, B., Rathore, S., Agrawal, A., Ram, A., Qazi, S., & **Ahmad, S.** (2022). Antiviral Potential of Indian Medicinal Plants Against Influenza and SARS-CoV: A Systematic Review. *SAGE- Natural Product Communications*. http://dx.doi.org/10.1177/1934578X221086988 [Q3, IF: **1.496**].
53. Tarique, M., **Ahmad, S.,** Malik, A., Ahmad, I., Saeed, M., Almatroudi, A., Qadah, T., Murad, M. A., Mashraqi, M., & Alam, Q. (2021). Novel severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) and other coronaviruses: a genome-wide comparative annotation and analysis. *Springer- Molecular and Cellular Biochemistry*. https://doi.org/10.1007/s11010-020-04027-8 [Q2, IF: **3.396**].
54. Pathak, N., Prajneshu, M., **Ahmad, S.,** Kumar, L., Bhaduri, A., Dhandapani, A., Sharma, O.P. (2020). Phytochemical Analysis and Antifungal Activity of Weed Extracts against Rhizoctonia Root Rot in Buckwheat (*Fagopyrum tataricum*). *Biopesticide International*. https://doi.org/02196.2020.16.125 [Q4, IF: **0.598**].
55. Kaul, T., Eswaran, M., **Ahmad, S.,** Thangaraj, A., Jain, R., Kaul, R., Raman, N.M. and Bharti, J. (2019). Probing the effect of a plus 1bp frameshift mutation in the protein-DNA interface of the domestication gene, NAMB1, in wheat. *T & F- Journal of Biomolecular Structure and Dynamics*. https://doi.org/10.1080/07391102.2019.1680435 [Q1, IF: **5.235**].

*Equal to the first author

Published Book Chapters (24)

1. Gangwar, S., **Ahmad, S.,** Raza, K. (2026). Artificial Intelligence in Molecular Screening: Advances, Challenges, and Future Perspectives. Elsevier- Artificial Intelligence in Precision Drug Design. https://doi.org/10.1016/B978-0-443-44415-9.00017-X
2. Bano, N., Firdaus, S., Parveen, R., **Ahmad, S.,** Raza, K. (2026). Artificial Intelligence in Omics Integration for Precision Drug Design. Elsevier- Artificial Intelligence in Precision Drug Design. https://doi.org/10.1016/B978-0-443-44415-9.00014-4
3. **Ahmad, S.,** Bashar, A., Khanna, K., Bano, N., & Raza, K. (2025). Deep learning in variant detection and annotation. Elsevier- In Deep Learning in Genetics and Genomics. http://dx.doi.org/10.1016/B978-0-443-27574-6.00010-2
4. **Ahmad, S.,** Tanveer, K., Bano, N., Ahmad, F., Raza, K. (2024). Artificial Bee Colony Algorithms in Gene Expression Studies: A Case Study. *Springer Nature- Solving with Bees.* https://doi.org/10.1007/978-981-97-7344-2_10
5. **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. *Springer Nature- Generative AI in Drug Designing: Current State-of-the-Art and Perspectives.* https://doi.org/10.1007/978-981-97-8460-8_20
6. **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. In *Von der Natur inspirierte intelligente Datenverarbeitungstechniken in der Bioinformatik* (pp. 325-341). Singapore: Springer Nature Singapore. https://doi.org/10.1007/978-981-99-7808-3_15
7. Sheikh, K., Sayeed, S., Asif, A., Siddiqui, M. F., Rafeeq, M. M., Sahu, A., & **Ahmad, S.** (2024). Bedeutende Innovationen in naturinspirierten intelligenten Computertechniken zur Identifizierung von Biomarkern und potenziellen therapeutischen Mitteln. In *Von der Natur inspirierte intelligente Datenverarbeitungstechniken in der Bioinformatik* (pp. 273-303). Singapore: Springer Nature Singapore. https://doi.org/10.1007/978-981-99-7808-3_13
8. **Ahmad, S.,** Aslam, D., Ansari, A., Bhat, AM., Raza, K. (2024). Deep learning in computer-aided drug design: a case study. *Elsevier-Deep Learning Applications in Translational Bioinformatics.* https://doi.org/10.1016/B978-0-443-22299-3.00012-8
9. **Ahmad, S.,** Kishan, A., Chitkara, P., Asiri, S.A., Eswaran, M., Mehta, S., Alam, M. (2023). Natural Product-Based Drug Designing for Treatment of Human Parasitic Diseases. *Springer-Natural Product-based Drug Discovery against Human Parasites.* https://doi.org/10.1007/978-981-19-9605-4_3
10. Yadav, M.K., Bhutani, K., **Ahmad, S.,** Raza, K., Singh, A., Kumar, S. (2023). Application of machine learning-based approaches in stem cell research. *Elsevier- Computational Biology for Stem Cell Research*. http://dx.doi.org/10.1016/B978-0-443-13222-3.00007-1
11. **Ahmad, S.,** Raza, K. (2023). 5-Nitroindazole against Lung Cancer: A Multitargeted in-silico Molecular Docking and Molecular Dynamics Simulation Study. In the 3rd International Electronic Conference on Cancers: New Targets for Cancer Therapies (IECC 2023) (Session: Overcoming Therapeutic Resistance), organised by MDPI-Sciforum and published in *MDPI-Medical Sciences Forum journal* (ISSN 2673-9992) https://sciforum.net/paper/view/14216
12. **Ahmad, S.,** Raza, K. (2023). Multialgorithm-based docking reveals Imidazolidinyl urea as a multitargeted inhibitor for Lung Cancer. In the 2nd International Electronic Conference on

Biomedicines (Session: Immune System, Tumour Immunology and Autoimmune Diseases), organised by MDPI-Sciforum and published in *MDPI-Medical Sciences Forum journal* (ISSN 2673-9992). https://doi.org/10.3390/ECB2023-14138

13. **Ahmad, S.,** Dahiya, V., Vibhuti, A., Pandey, R.P., Tripathi, M.K., Yadav, M.K. (2023). Therapeutic Protein-Based Vaccines. *Springer- Protein-based Therapeutics*. https://doi.org/10.1007/978-981-19-8249-1_13

14. **Ahmad, S.,** Khan, F., N., Ramlal, A., Begum, S., Qazi, S., Raza, K. (2023). Nanoinformatics and Nanomodeling: Recent developments in computational nanodrug design and delivery systems. *Elsevier- Emerging Nanotechnologies for Medical Applications*. https://doi.org/10.1016/B978-0-323-91182-5.00001-2

15. **Ahmad, S.,** Sheikh, K., Bano, N., Rafeeq, M., Yadav, M., K., Mohammad, M., R., S., Raza, K. (2022). Illustrious Implications of NIC Methods in Therapeutics and Computer-Aided Drug Design. *Springer- Nature-Inspired Intelligent Computing Techniques in Bioinformatics*. https://doi.org/10.1007/978-981-19-6379-7_15

16. Sheikh, K., Sayeed, S., Asif, A., Siddiqui, M., F., Rafeeq, M., Sahu, A., **Ahmad, S.** (2022). Consequential Innovations in NIC Techniques for Biomarkers and Potential Therapeutics Identification. *Springer- Nature-Inspired Intelligent Computing Techniques in Bioinformatics*. https://doi.org/10.1007/978-981-19-6379-7_13

17. Tripathi, M. K., **Ahmad, S.,** Tyagi, R., Dahiya, V., & Yadav, M. K. (2022). Fundamentals of molecular modelling in drug design. *Elsevier- Computer Aided Drug Design: From Ligand-Based Methods to Structure-Based Approaches*. https://doi.org/10.1016/B978-0-323-90608-1.00001-0

18. Karwasra R., Khanna K., Singh S., **Ahmad S.,** Verma S. (2022). The Incipient Role of Computational Intelligence in Oncology: Drug Designing, Discovery, and Development. *Springer- Computational Intelligence in Oncology*. https://doi.org/10.1007/978-981-16-9221-5_21

19. Khan, F.N., Khanam, A.A., Ramlal, A. and **Ahmad, S.** (2021). A review of predictive systems and data models for COVID-19. In Computational Intelligence Methods in COVID-19: Surveillance, Prevention, Prediction and Diagnosis (pp. 123-164), Springer. https://doi.org/10.1007/978-981-15-8534-0_7

20. **Ahmad, S.,** Chitkara, P., Khan, F.N., Kishan, A., Alok, V., Ramlal, A. and Mehta, S. (2021). Mobile Technology Solution for COVID-19: Surveillance and Prevention. *Springer- Computational Intelligence Methods in COVID-19: Surveillance, Prevention, Prediction and Diagnosis*. https://doi.org/10.1007/978-981-15-8534-0_5

21. Ramlal, A., **Ahmad, S.,** Kumar, L., Khan, F.N., Chongtham, R. (2021). From molecules to patients: The clinical applications of biological databases and electronic health records. *Elsevier- Translational Bioinformatics in Healthcare and Medicine*. https://doi.org/10.1016/B978-0-323-89824-9.00009-4

22. Khan, F.N., **Ahmad, S.** and Raza, K. (2021). Clinical Applications of Next-Generation Sequencing Analysis in Acute Myelogenous Leukaemia. *T & F- Translational Bioinformatics Applications in Healthcare.* https://dx.doi.org/10.1201/9781003146988-4

23. Bharti, J., Mehta, S., **Ahmad, S.,** Singh, B., Padhy, A.K., Srivastava, N. and Pandey, V. (2021). Mitogen-activated protein kinase, plants, and heat stress. *Springer- Harsh Environment and Plant Resilience*. https://doi.org/10.1007/978-3-030-65912-7_13

24. Balasubramanian, B., **Ahmad, S.,** Alok, V., Khan, F.N., Anand, K., Mehta, S., Easwaran, M., Meyyazhagan, A. and Saravanan, M. (2021). Exosomes as an emerging nanoplatform for functional therapeutics. *Elsevier- Handbook on Nanobiomaterials for Therapeutics and Diagnostic Applications*. https://doi.org/10.1016/B978-0-12-821013-0.00002-7

PUBLISHED CODES

1. DrLungker: https://github.com/ShabanAhmad/DrLungker
2. DeepEntXAI: https://github.com/ShabanAhmad/DeepEntXAI
3. LungXAI: https://github.com/SyeddNaseer/LUNGXAI
4. RMSD-RMSF and MMGBSA Plots: https://github.com/ShabanAhmad/RMSD-RMSF-Plots
5. ChEMBL-BioAssays: https://github.com/ShabanAhmad/ChEMBL_LungCancer-BioAssays
6. PubChem-BioAssay: https://github.com/ShabanAhmad/PubChem_LungCancer-BioAssay

PUBLISHED SCIENTIFIC DATA

1. **Article Link:** https://doi.org/10.1002/adts.202501550
   Figshare Project Link: https://figshare.com/projects/DrLungker/268952
   Figshare Individual Repositories: https://doi.org/10.6084/m9.figshare.30763082
   https://doi.org/10.6084/m9.figshare.30763514
   https://doi.org/10.6084/m9.figshare.30763484
   https://doi.org/10.6084/m9.figshare.30763544
2. **Article Link:** http://dx.doi.org/10.1016/j.ijbiomac.2025.146175
   Data Link: http://dx.doi.org/10.13140/RG.2.2.36122.71365
3. **Article Link:** https://doi.org/10.3389/fchem.2025.1611972
   Data Link: Link
4. **Article Link:** http://dx.doi.org/10.1016/j.compbiomed.2025.110163
   Data Link: http://dx.doi.org/10.13140/RG.2.2.17248.34566
5. **Article Link:** http://dx.doi.org/10.1016/j.ijbiomac.2025.142343
6. **Data Link:** http://dx.doi.org/10.13140/RG.2.2.30670.11846,
   http://dx.doi.org/10.13140/RG.2.2.13892.90248
7. **Article Link:** http://dx.doi.org/10.1016/j.ijbiomac.2025.141703
   Data Links: http://dx.doi.org/10.13140/RG.2.2.20603.78884,
   http://dx.doi.org/10.13140/RG.2.2.27314.67529
8. **Article Link:** http://dx.doi.org/10.3390/ijms26031060
   Data Link: https://www.mdpi.com/article/10.3390/ijms26031060/s1
9. **Article Link:** http://dx.doi.org/10.1016/j.ijbiomac.2024.132332
   Data Links: http://dx.doi.org/10.13140/RG.2.2.34025.56164,
   http://dx.doi.org/10.13140/RG.2.2.25636.95361
10. **Article Link:** http://dx.doi.org/10.1080/07391102.2023.2209673
    Data Link: http://dx.doi.org/10.13140/RG.2.2.28992.39680
11. **Article Link:** http://dx.doi.org/10.1007/s10753-022-01734-w
    Data Links: Data File 1, Data File 2, Data File 3,
    Supplementary Docx 1, Supplementary Docx 2
12. **Article Link:** http://dx.doi.org/10.1007/s10722-022-01471-x
    Data Link: Data File, Supplementary Manuscript
13. **Article Link:** http://dx.doi.org/10.1080/07391102.2021.2021993
    Data Link: http://dx.doi.org/10.13140/RG.2.2.18926.06725

WORKSHOPS ATTENDED

1. 2025 Summer School in Applied Deep Learning in Bioinformatics, organised by the Faculty of Health and Medical Sciences, University of Copenhagen, Denmark, from 11-15 August 2025.
2. Clinical Interpretation of Whole Genome Sequences, organised by Knowmics (Online Course), held on 29 June 2025.
3. 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 05-14 August 2024.
4. "Artificial Intelligence in Modern Biology-2" 12-14 September 2023, ICGEB, New Delhi.
5. 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.
6. "Indo-Vietnam Hands-on Workshop on Sequencing Techniques" 02-06 August 2023. CSIR-IGIB, India.
7. Training Programme on Computational Techniques for AI and Data Science Applications (July 25-31, 2023) sponsored by DST (STUTI), Banasthali Vidyapith University, Rajasthan, India.
8. Hands-on Workshop on "Design, Synthesis, Computational Studies and Data Interpretation of Drug-Like molecules" (30th January-5th February 2023), sponsored by SERB (KARYASHALA), New Delhi, India and organised by the NIPER-Ahmedabad, Gujarat, India.
9. Participated in "Accelerate your Research Using Elsevier's Science Direct and Scopus" at NIPER-Ahmedabad on Tuesday, 31 January 2023.
10. Participated in One Day Online Training Program on 'Application of High-Performance Computing in Drug Designing' on 06 August 2022, sponsored by SERB, New Delhi, India and organised by the Department of Biotechnology, MNNIT Allahabad, Prayagraj, UP, India.
11. 'BioC2022- Bioconductor Conference 2022', 27-29 July 2022. Organised at Seattle Children's Hospital, Cure Building, 1920 Terry Ave, Seattle, WA 98101. Attended virtually.
12. "Cloud-based Hands-on Workshop on Molecular Docking, Pharmacophore Modelling and Machine Learning" organised by ICMR – NICPR, Noida and Schrödinger Inc., 15-16 March 2022.
13. International Workshop on – 'Discovery of Vaccines and Drugs for Infectious Diseases', 06-09th December 2021, ICGEB, New Delhi.
14. AI workshop 2021, '7 days International Workshop on Artificial Intelligence', 15th-21st November 2021. Co-organised by AiCHEF and St Claret College, Bengaluru, India.
15. Cloud-based Hands-on Workshop '2-days Cloud-based Hands-on Workshop: Computational SBDD & MD Simulations', 2-3 September 2021. Co-organised by SRM University and Schrödinger LLC, India.
16. Hands-on online workshop on 'Quantitative genetics, genomics and plant breeding', 23-27 November 2020, Department of Biotechnology, Vignan's Foundation for Science, Technology & Research, Vadlamudi-522213, Guntur, Andhra Pradesh, India.
17. DBT Apex Biotechnology Information Centre (DBT-ABTIC) workshop on "Advanced Structural Bioinformatics", 18 - 21 November 2019, ICGEB-New Delhi.

18. One-day workshop on "Deep learning and IoT using MATLAB" on 03 October 2019, Dept. of Computer Science, Jamia Millia Islamia, New Delhi.
19. BioTecNika Schrödinger Joint Workshop on Computer-Aided Drug Discovery, organised by Biotecnika Info Pvt. Ltd from 22 July to 02 August 2019.
20. "Application of Artificial Intelligence in Modern Biology" 28-29 March 2019, ICGEB-New Delhi.
21. 9th DBT-BIF sponsored National Workshop on "Translational Bioinformatics: Guinness Book Recording to Digital Era" 6th-7th March 2019, BIF Centre, Computer Science, Jamia Millia Islamia, New Delhi.
22. DBT GOI Sponsored National-level "Interactive NGS Data Analysis" workshop, 15-17 November 2018, at Bioinformatics Centre, Northeastern Hill University, Shillong, India.

CONFERENCE PRESENTATIONS (Poster / Oral)

1. **Ahmad, S.,** Raza, K. (2023). 5-Nitroindazole against Lung Cancer: A Multitargeted in-silico Molecular Docking and Molecular Dynamics Simulation Study. In the 3rd International Electronic Conference on Cancers: New Targets for Cancer Therapies (IECC 2023) (Session: Overcoming Therapeutic Resistance), organised by MDPI-Sciforum https://sciforum.net/paper/view/14216 (PhD Thesis Work).
2. **Ahmad, S.,** Raza, K. (2023). Multialgorithm-based docking reveals Imidazolidinyl urea as a multitargeted inhibitor for Lung Cancer. The 2nd IECB (Session: Immune System, Tumour Immunology and Autoimmune Diseases) was organised by MDPI-Sciforum. https://doi.org/10.3390/ECB2023-14138 (PhD Thesis Work).
3. **Ahmad, S.,** Raza, K. (2022). 'Multitargeted docking-based simulative understanding of Theodrenaline against lung cancer: an in-silico study' in 21st International Conference on Bioinformatics (InCoB) 21-23 November 2022, organised by APBioNet and King Abdullah University of Science and Technology at Computational Bioscience Research Centre (CBRC-KAUST), Saudi Arabia (PhD Thesis Work).
4. Ankita Sahu, Khalid Raza, **Shaban Ahmad**, Saurabh Varma "In silico study of aromatase inhibitors using computer-aided drug design" in World Congress on Reproductive Health with Emphasis on Reproductive Cancers, Infertility and Assisted Reproduction & 30th Annual Meeting of the Indian Society for the Study of Reproduction and Fertility (ISSRF2020), at Shri Mata Vaishno Devi University Katra, J & K- India, 14 – 16 February 2020.
5. **Shaban Ahmad,** "Rice Bean (Vigna umbellata) draft genome sequence: unravelling the late flowering and unpalatability related genomic resources" in Young Scientist Conference India International Science Festival (YSC- IISF), Kolkata, India, 05-07 November 2019.
6. **Shaban Ahmad,** "Deep learning and Artificial intelligence in Biological sciences" in Interdisciplinary Science Conference: Big Data and Computational Biology, organised by Centre for Interdisciplinary Research in Basic Sciences, Jamia Millia Islamia, New Delhi, 21-22 October 2019.
7. Niti Pathak Bhaduri, Asani Bhaduri, Meenakshi Prajneshu, Faran Salik, A. Ramlal, Avantika Kumari, Laxman, Manshi Gaur, Sonia Suri, **Shaban Ahmad**, Aman Sharma "Study of Bioactive component in Buckwheat and in-silico analysis of Fagopyritol synthase" in "Emerging Issues of Climate change: Sustainability and Economic implications" at Sri Aurobindo College, University of Delhi on 21-22 October 2016, New Delhi India.

8. **Shaban Ahmad,** "Rice Bean (Vigna umbellata) draft genome sequence: unravelling the late flowering and unpalatability related genomic resources" in Interdisciplinary Science Conference: Big Data and Computational Biology organised by CIRBSc, Jamia Millia Islamia, New Delhi, 21-22 October 2019.
9. **Shaban Ahmad,** Niti Pathak, Laxman Kumar, Meenakshi Prajneshu, "Efficacy of Weed-based botanicals against Rhizoctonia root rot in Buckwheat (Fagopyrum sp.) in 1st National Conference on "Neglected and Underutilised Crop Species for Food, Nutrition, Energy and Environment" at NIPGR, New Delhi, 02 August 2019.
10. A. Ramlal, Laxman Kumar, Pooja, Tanuja, Loveleen Kaur and **Shaban Ahmad,** "Sustainable Agriculture and Global Food Security: Perspective, importance and Opinion" in Symposium on "Avenues in Plant Sciences: A Hope for Sustainable Future" at Deshbandhu College, University of Delhi, 8-9 March 2019.
11. Niti Pathak, **Shaban Ahmad,** Meenakshi Prajneshu, "Buckwheat (Kuttu): As food, good health and Medicine" in National Conference on "Conservation, cultivation and Sustainable use of Medicinal and Aromatic Plants (CCSMAP)", at Manav Rachna International Institute of Research and Studies (MRIIRS), 21-22 February 2019.
12. **Shaban Ahmad**, A Ramlal, Laxman Kumar, "Biofuels: A sustainable approach of Futuristic Energy" In Trends in Life Sciences and Biotechnology: Innovation Paradigms at Maitreyi College, University of Delhi, 19-20 February 2019.
13. **Shaban Ahmad**, Biodiversity: Threats and Conservation in Fourth National Symposium on "Environment: Green Technology for Environmental Sustainability", Deshbandhu College, University of Delhi, 25 September 2018.
14. Niti Pathak Bhaduri, Meenakshi Prajneshu, Sonia Suri, **Shaban Ahmad**, A. Ramlal "Role of Nanobiotechnology in Enhancing Crop Production" in "Trends in Nanobiotechnology" at TERI University, 28-29 September 2017.
15. Niti Pathak Bhaduri, **Shaban Ahmad**, Aman Sharma "Study of Bioactive component in Buckwheat and in-silico analysis of Fagopyritol synthase" in "Emerging Issues of Climate change: Sustainability and Economic implications" at Sri Aurobindo College, University of Delhi on 21-22 October 2016, New Delhi, India.

CONFERENCES/SEMINARS/SYMPOSIUM ATTENDED

1. Attended "3rd Symposium on Applied Deep Learning in Bioinformatics", organised by the Faculty of Health and Medical Sciences, University of Copenhagen, Denmark, on 15 August 2025.
2. Attended an online session organised by Springer Nature for One Nation One Subscription Member Institutions entitled "Navigate the World of Scientific Article Writing: From Manuscript Structure to Publication", on 15 May 2025.
3. Attended an online session organised by Springer Nature for One Nation One Subscription Member Institutions entitled "How to Navigate Springer Nature Platforms to Access all Journals", on 19 March 2025.
4. Attended "The 3rd International Electronic Conference on Cancers" organised by MDPI, 16-30 March 2023.
5. Attended "The 2nd International Electronic Conference on Biomedicines" organised by MDPI, 01-31 March 2023.

6. Attended "Topics Webinar | EO&GEO Series: GIS in the Management of Sustainable and Smart Cities" organised by MDPI on 09 March 2023.
7. Attended "Entropy Webinar | Entropy Measures to Assess Irregularity and Complexity of Time Series and Multidimensional Data" organised by MDPI on 09 March 2023.
8. Attended a virtual seminar entitled "Recent Advances in Translational Cancer Research and Regulatory Perspectives" organised by the Department of Pharmacy, Indira Gandhi National Tribal University (IGNTU), Amarkantak, India, on 08 February 2023.
9. Attended 'The Non-coding RNA Journal Webinar Series | Screening for miRNA With Essentiality in Cancer' organised by MDPI on 13 December 2022.
10. Attended the Pharmaceuticals webinar on Cardio-Oncology: From Adverse Outcome Pathways to Treatments to Mitigate Cardiotoxicity of Anticancer Therapies, organised by MDPI on 07 December 2022.
11. Participated in the National Webinar on Emotional Intelligence by Ms Shilpa Somanathan, "Clinical Psychologist and Therapist", on Wednesday, 07 December 2022, at MQI college of management, Bangalore, Karnataka.
12. Attended 21st International Conference on Bioinformatics (InCoB) 21-23 November 2022, organised by APBioNet and King Abdullah University of Science and Technology (KAUST), Kingdom of Saudi Arabia.
13. Attended One Day virtual seminar on "Intellectual Property Rights" (on National Science Day), organised by CIF, Jamia Millia Islamia University, New Delhi. 28 February 2022.
14. Attended the 3rd ICGA 2022 Virtual Conference entitled "Biobanking to Omics: Collecting the Global Experience" January 13-14, 2022.
15. Attended Economic botany and plant genetic resources: National Perspective, Deshbandhu College, University of Delhi, New Delhi, 18 January 2022.
16. Attended Computational Biology connecting Demand of Science, ISCBSC- RSG India Student Symposium 2019, Jawaharlal Nehru University (JNU), New Delhi, 22 November 2019.
17. Selected for the Young Scientist Conference- India International Science Festival (YSC-IISF), 2019, (GoI Funded) Kolkata, India, 5-7 Nov 2019.
18. Attended Interdisciplinary Science Conference: Big Data and Computational Biology, organised by Centre for Interdisciplinary Research in Basic Sciences, Jamia Millia Islamia, New Delhi, October 21-22, 2019.
19. Attended DST-PURSE sponsored National Seminar on Biophysics (Biophysica 2019), Centre for Interdisciplinary Research in Basic Sciences, Jamia Millia Islamia, New Delhi.
20. Attended Mini-Symposium on "Tracking Antimicrobial Drug Resistance Tuberculosis: Novel Approaches" at the Vallabhbhai Patel Chest Institute, University of Delhi.
21. Attended the 20th Distinguished Lecture on "Structure-guided Fragment-based Drug Designing for Cancer and Tuberculosis: Fighting the Emergence of Resistance" by Sir Prof. Tom Blundell at Jamia Hamdard on 20 March 2019.
22. Attended Symposium on "Avenues in Plant Sciences: A Hope for Sustainable Future" at Deshbandhu College, University of Delhi, March 08-09, 2019.
23. Attended National Conference on "Conservation, cultivation and Sustainable use of Medicinal and Aromatic Plants (CCSMAP)" at MRIIRS, February 21-22, 2019.
24. Attended Fourth National Symposium on "Environment: Green Technology for Environmental Sustainability" on 25 September 2018, Deshbandhu College, University of Delhi.
25. Attended National Science Congress Association, Delhi Chapter at Zakir Hussain Delhi College, "Consciousness and Artificial Intelligence" along with a model presentation on 25 October 2017.
26. Participated in the Seminar and Working model presentation on 13 April 2018, "PARIVARTAN 2K18" Department of Environmental Science and NSS, Sri Aurobindo College, University of Delhi.

27. Participated in the 26th World Environmental Congress; World Environmental and Ecology Development (WEED) (Greening of Education, Employment, Environment, Empowerment, and Entrepreneurship) on 08 November 2017 at the India International Centre.
28. Attended two-day seminar and poster presentation "Trends in Nanobiotechnology" 'BIOTIKOS 2017', 28-29 September 2017, Department of Biotechnology, TERI School of Advanced Sciences.
29. Attended Conference on "Growth control in development and disease: From Fruit Fly to Human Cancer" on 07 October 2016, National Institute of Immunology, New Delhi
30. Attended National Conference on "Galapagos Island and Darwin's Theory of Evolution" on 06 October 2016, National Institute of Immunology, New Delhi.
31. Attended ICSSR-sponsored seminar "Emerging Issues of Climate change: Sustainability and Economic implications" in Sri Aurobindo College, the University of Delhi, on 21-22 Oct 2016.
32. Attended Environmental Concerns of the 21st Century: Indian Global Context at Zakir Hussain Delhi College, University of Delhi.

INVITED REVIEWER (420+ verified peer reviews on PUBLONS)

I am a regular reviewer in the following journals-

Archives of Computational Methods in Engineering, Archives of Microbiology, Accreditation and Quality Assurance, Biochemical and Biophysical Research Communications, Biochemical Genetics, Bioinformatics and Biology Insights, Biomedical Reports, BMC Artificial Intelligence, BMC Infectious Diseases, BMC Veterinary Research, Brazilian Journal of Biology, Cancer Investigation, Cell Biochemistry and Biophysics, Computer Methods in Biomechanics and Biomedical Engineering, Computers in Biology and Medicine, Crop Protection, Current Cancer Drug Targets, Current Medicinal Chemistry, Current Plant Biology, Digital Health, Discover Applied Sciences, Discover Oncology, Drug Development Research, European Journal of Medicinal Chemistry, Experimental and Therapeutic Medicine, F1000Research, Frontiers in Dental Medicine, Frontiers in Immunology, Future Medicinal Chemistry, Heliyon, In Silico Pharmacology, International Journal of Oncology, IScience, Journal of Biological Research and Reviews, Journal of Biomolecular Structure and Dynamics, Journal of Chemistry, Journal of Computational Science, Journal of Computer-Aided Molecular Design, Journal of Drug Targeting, Journal of Experimental & Clinical Cancer Research, Journal of Molecular Modeling, Journal of Pharmaceutical Innovation, Journal of Proteins and Proteomics, Journal of the Egyptian National Cancer Institute, Medical Oncology, Molecular Diversity, Molecular Medicine Reports, Natural Resources for Human Health, Naunyn-Schmiedeberg's Archives of Pharmacology, Neural Computing and Applications, Npj Precision Oncology, Oncology Letters, Open Chemistry, PeerJ, Pharmacological Research, PLoS Neglected Tropical Diseases, Plos One, Qeios, Scientific Reports, SN Applied Sciences, Structural Chemistry, VEGETOS, Virology, Virulence.

PRACTICAL EXPERTISE

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

Programming & Scripting Languages: Python (including libraries such as NumPy, pandas, matplotlib, Biopython), R (tidyverse, Bioconductor), Perl, MATLAB, Bash scripting, SQL.

Web Development: PHP, Django, Flask, Node.js, Express.js, React, Angular, Vue.js, RESTful API development.

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

Data Analysis & Machine Learning: Weka, TensorFlow, Keras, PyTorch, Scikit-learn, XGBoost, LightGBM, Pandas, NumPy, Matplotlib, Seaborn, MS Excel (advanced functions, pivot tables)

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

Structural Biology & Molecular Modelling: PyMOL, Chimera, Swiss-PDBViewer, Modeller, VMD, Rosetta, Coot, CCP4 Suite, Phenix, ChimeraX.

Genomics Tools: GEO2R, Gene Ontology-based Enrichment Analyser, 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, BioGRID, OmicsNet.

Drug Discovery & Docking: AutoDock Vina, SwissDock, InstaDock, Glide (Schrödinger Suite), MOE.

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

Free Energy Calculations: MM/GBSA, MM/PBSA, FEP (Free Energy Perturbation), Thermodynamic Integration (TI), Umbrella Sampling.

Graphics & Visualisation: BioRender, Adobe Photoshop, CorelDraw, Blender (3D modelling, animation), ClipChamp, PowerPoint, Illustrator, 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, MD simulation, MMGBSA and many more.
- Proficient in managing and configuring cloud servers (AWS, Google Cloud, Microsoft Azure), HPC clusters, and supercomputers for job queue management (SLURM), deployment, containerisation (Docker), and workflow scheduling.

PERSONAL DETAILS

Father's Details:	Noorain Ahmad
Mother's Details:	Jannatun Nisha
Marital Status:	Unmarried
Nationality/Sex:	Indian / Male
Language Known:	English, Hindi, Urdu, basic Arabic and Sanskrit

REFEREES

Dr Tue K. Nielsen (Postdoc PI)
Associate Professor,
MEB Section, PLEN
University of Copenhagen, Denmark
tkn@plen.ku.dk | +45-30234821

Dr Khalid Raza (PhD Supervisor)
Associate Professor,
Department of Computer Science
Jamia Millia University, New Delhi, India.
kraza@jmi.ac.in | +91-9891478255

Dr Tiina Jokela (JYU Visiting PI)
Research Director
Department of Biological & Env Science
University of Jyväskylä, Finland.
malam2@jmi.ac.in | +91-9810650497

Dr Murugesh Eswaran (MSc PI @ ICGEB)
Tenure Track Faculty
Molecular Biology, Biochemistry Lab
Morehouse School of Medicine, USA.
meswaran@msm.edu | +14708909491

Dr Mansaf Alam (MSc Supervisor)
Professor
Department of Computer Science
Jamia Millia University, New Delhi, India.
malam2@jmi.ac.in | +91-9810650497

Dr Manoj K Yadav (PI- SARS-CoV-2)
Associate Professor
Department of Bioinformatics
SRM University, Sonepat, Haryana, India.
manoj.yadav@srmuniversity.ac.in | +91-7581911917

Updated on **17 February 2026**