Dr. Mohammad Kalim Ahmad Khan
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(Google Scholar, | ORCID ID | Scopus, | Web of Science, | Research Gate, | LinkedIn, |Vidwan, |Sci)

PROFILE

- A research-driven and experienced professional with over 16 years of expertise in Computer-Aided Drug Design, High-throughput Virtual Screening, ADMET profiling, Molecular Dynamics Simulations, Molecular Mechanics Poisson-Boltzmann Surface Area calculation, and Principal Component Analysis.
- Extensive hands-on experience in teaching and conducting research in the fields of Biological Databases, Structural Bioinformatics, and Biomolecular Modeling and Simulation.
- Proficient in adapting to new technologies, with the ability to work effectively in multicultural environments and lead diverse teams.
- Expertise in structure-based inhibitor design, with in-depth knowledge of protein structure prediction, virtual screening, MD simulations, and free energy-based computations.
- Significant experience in publishing research, presenting at conferences, and delivering presentations to establish a robust research network.
- Mentoring various B Tech and M Tech students in Bioinformatics, Biotechnology, and Food Technology.
- NAAC Criteria V In-Charge at the departmental level and participated as a member of NAAC Criteria III at the central level.
- Active member of various committees, including Flying Squads, ACS, Robes and Gown (central).
- Course Coordinator M. Tech Bioinformatics and B.Tech Biotechnology programs.
- In-Charge of the Postgraduate Computational Biology Lab (B220, BT14), in addition to coordinating educational tours for the department.
- Member of the Board of Studies, Faculty Board, and Academic Council of Integral University, Lucknow.
- Departmental Admission Coordinator

RESEARCH INTEREST:

- **Structural Bioinformatics:**
  - High-throughput virtual screening.
  - Molecular Docking, ADME and Toxicity profiling.
  - Molecular Dynamics Simulation, Energy-based calculations and Principal Component Analysis
- **Breast Cancer Informatics:**
  - Inhibitor design against Sterol Regulating Element Binding Protein, Sphingosine Kinases, Ephrin type A Receptors, and Kinesin-like proteins.
- **Vitiligo:**
  - Designing of small molecule therapeutic candidates against C-X-C motif chemokine ligands, and Janus Kinases.

SUMMARY OF RESEARCH ACCOMPLISHMENT:

- Published 83 research papers and 3 book chapters in prestigious peer-reviewed national and international journals.
- Received the International Eminent Award in Engineering, Science, and Medicine on December 17, 2022, in an online event organized by VDGOOD Professional Association, Tamil Nadu, India.
- Evaluated a Ph.D. thesis for La Trobe University, Victoria, Australia, in February 2019.
- Published over 100 abstracts in the abstract books and proceedings of various national and international conferences and seminars.
- Served as an invited reviewer for over 30 peer-reviewed national and international journals.

PROFESSIONAL MEMBERSHIP:

- Member of the International Association of Engineers (IAENG), Code: 125745, Hong Kong.
- Member of the International Association of Computer Science and Information Technology (IACSIT), Code: 80345690, Singapore.
- Member of the International Society for Research and Development (ISRD), Code: SR3140900190, London, United Kingdom.

COURSE TAUGHT:

B.Tech

- Introduction to Bioinformatics
- Structural Bioinformatics and Phylogenetics
- Food Informatics
- Fundamentals of Biochemistry

M.Tech

- Biological Database
- Biomolecular Modeling and Simulation
- Protein Informatics

B.Sc.

- Fundamentals of Bioinformatics

M.Sc.

- Bioinformatics
- Metabolomics

ADMINISTRATIVE/DEPARTMENTAL RESPONSIBILITY

- Course Coordinator of B. Tech Biotechnology Final Year
- In-Charge of Postgraduate Bioinformatics and Computational Biology Lab (BT14: B220)
- Continuous Assessment Examination Coordinator (Departmental)
- NAAC Criteria V In-Charge (Departmental)
- Member of Flying Squads and ACS
- Co-Convener of Robes and Gown Committee, Convocation (Central)
- Educational Tour Coordinator (Departmental)
- Departmental Admission Coordinator
- Member of the Board of Studies, Faculty Board, and Academic Council

STUDENTS SUPERVISION

Doctoral Students

- Shalini Maurya (Enroll. No. 1701120, 2024) – Supervisor: *Subtractive Proteomics to identify drug targets and reverse vaccinology for development of Chimeric vaccine against Burkholderia pseudomallei*.
- Mohd Umar Azeem (Enroll. No. 1502068, 2022) – Supervisor: *Identification, Characterization, and Design of potential leads against Dibenzo[a,l]pyrene-induced mammary cancer*.

- Iffat Azim (Enroll. No. 1502066, 2020) – Supervisor: *Identification, Optimization, and In-vitro Validation of Drug Leads Against Mammary Cancer via Targeting the PI3K/AKT Pathway*.
- Akanksha Sharma (Enroll. No. 1502021, 2020) – Co-Supervisor: *Identification and Validation of Potential Natural Compounds against Tuberculosis: An in-silico and in-vitro approach*.
- Ajijur Rehman (Enroll. No. 10005, 2019) – Supervisor: *Design and Optimization of Leads for Novel Drug Target Against Mycobacterium tuberculosis*.
- Tasneem Bano (Enroll. No. 101008, 2018) – Supervisor: *Computer-Aided Vaccine Designing Against HTLV-1 (Human T-Cell Lymphotropic Virus-1)*.

Postgraduate Students Guided

- Heena Bano (M. Tech Biotechnology, 2022) – Supervisor: *Identifying potential inhibitors of human epidermal growth factor receptor 2 using structure-based virtual screening, docking, molecular dynamics simulation, and principal component analysis*.
- Arjumand Bano (M.Sc. Biotechnology, 2021) – Supervisor: *Virtual Screening of flavonoids as inhibitors of AhR and its implication for bioactivation of dibenzo[a,l]pyrene*.
- Naziya Farheen (B. Tech-M. Tech Biotechnology, 2021) – Supervisor: *Evaluation of terpenoids as dipeptidyl 4 inhibitors: Molecular docking study*.
- Mohammad Armoghan (M. Tech Biotechnology, 2019) – Supervisor: *Virtual screening and molecular docking studies of natural inhibitors against cytochrome P450 1A2*.
- Anubhav (M. Tech Biotechnology, 2019) – Co-Supervisor: *Exploring the anti-angiogenesis potential of brassicanal B and its derivative targeting hsp90 protein: an in-silico perspective*.
- Swaraj Dubey (M. Tech Biotechnology, 2019) – Co-Supervisor: *A neuroinformatics approach towards screening and elucidation of selected alkaloids for their anti-Alzheimer potential targeting AChE protein*.
- Reem Khan (B. Tech-M. Tech Biotechnology, 2018) – Supervisor: *Identification of natural compounds as inhibitors of cytochrome P450 1A1*.
- Shrinarayan Tripathi (M. Tech Bioinformatics, 2018) – Supervisor: *Efficacy of natural inhibition against cytochrome P450 1A2: an in-silico approach to combat mammary cancer*.
- Vertika Singh (B. Tech-M. Tech Biotechnology, 2017) – Supervisor: *Virtual screening of plant-derived natural compounds as inhibitors of cytochrome P450 1A1*.
- Mohd Rahil (M. Tech Bioinformatics, 2017) – Co-Supervisor: *Deciphering the antiangiogenic potential of brassicanal B and its derivatives targeting Hsp90 protein: a novel in-silico multipathway targeted move to refrain angiogenic phenomena*.
- Roohi Kumari Parsad (B. Tech-M. Tech Biotechnology, 2016) – Supervisor: *Efficacy of natural inhibitors against cytochrome P450 1A2: an in-silico approach to combat mammary cancer*.
- Sonee Rajpoot (B. Tech-M. Tech Biotechnology, 2016) – Supervisor: *Insights from the docking simulation of plant-derived natural compounds as cancer prevention through inhibiting hypoxia-inducible factor 1 alpha*.
- Anand Vikram Singh (B. Tech-M. Tech Biotechnology, 2015) – Supervisor: *In-silico evaluation and elucidation of plant-derived natural compounds as potent mammary cancer preventive agents*.
- Farah Khan (M.Sc. Biotechnology, 2013) – Supervisor: *In silico studies of activation pathways of carcinogens*.
- Garima Barnawal (M.Sc. Biotechnology, 2013) – Supervisor: *Structure prediction of 'Catenin beta-1' through homology modeling using modeller9v10*.
- Hakikullah (M.Sc. Biotechnology, 2013) – Supervisor: *Structure prediction of CYP1B1 through homology modeling using modeller9v10*.
- Hamda Siddiqui (M.Sc. Biotechnology, 2013) – Supervisor: *Structure prediction of 'Parkin' through homology modeling using modeller9v10*.
- Hammad Akhtar (M.Sc. Biotechnology, 2013) – Supervisor: *Structure prediction of CYP2B1 through homology modeling using modeller9v10*.
- Ishrat Fatima (M.Sc. Biotechnology, 2013) – Supervisor: *In silico studies of detoxification pathways of carcinogens*.

- Shalini Rai (M.Sc. Biotechnology, 2013) – Supervisor: *Structure prediction of BRD7 (Bromodomain containing 7) through homology modeling using modeller9v10*.
- Priya Yadav (M.Sc. Biotechnology, 2013) – Supervisor: *In silico studies of various IARC-classified carcinogens and their metabolites with different CYP450s*.
- Renu Pandey (M.Sc. Biotechnology, 2013) – Supervisor: *In silico studies of detoxification pathways of carcinogens*.
- Ruby (M.Sc. Biotechnology, 2013) – Supervisor: *Structure prediction of N-1 neuraminidase in H5N1 influenza A virus through homology modeling using modeller9v10*.
- Shikha Singh (M.Sc. Bioinformatics, 2010) – Supervisor: *Homology modeling of CYP1B1 and its docking studies with dibenzo[a,l]pyrene and its metabolites*.
- Sheena Saxena (M.Sc. Bioinformatics, 2010) – Supervisor: *Homology modeling of CYP2B1 and its docking studies with dibenzo[a,l]pyrene and its metabolites*.
- Wahida Rais (M.Sc. Bioinformatics, 2010) – Supervisor: *Molecular docking studies, IARC classified carcinogens and their metabolites with DNA*.
- Bhavana Singh (M.Sc. Bioinformatics, 2010) – Supervisor: *In silico studies of cell cycle checkpoints and their inhibitors*.
- Sandeep Kumar Singh (M.Sc. Bioinformatics, 2010) – Supervisor: *Comparative docking studies of benzo[a]pyrene and its metabolites with different Cytochrome P450A1*.
- Shama Bano (M.Sc. Bioinformatics, 2010) – Supervisor: *In silico studies of dibenzo[a,l]pyrene with glutathione-S-transferase alpha isozymes*.
- Vikas Kumar Srivastava (M.Sc. Bioinformatics, 2010) – Supervisor: *Molecular interaction studies of DBPD with CYP3A4*.

Undergraduate Students Guided

- Guided over 100 undergraduate dissertations in Bioinformatics, providing mentorship and expertise to students on various topics within the field, including molecular modeling, virtual screening, structure-based drug design, and in-silico approaches to biological research.

SLECTED PUBLICATIONS (LAST FIVE YEARS)

- Authored 83 research papers and 3 book chapters published in esteemed peer-reviewed national and international journals.
- Computational insights into inhibiting EphA2: Integrating structure-based virtual screening, docking, and molecular dynamics simulations for small molecule discovery (2024) *Cellular and Molecular Biology* – Impact Factor: 1.5, Q4
- Exploring Therapeutic Approaches for Vitiligo: An inclusive review from translational modalities to alternative therapies (2024) *Current Dermatology Reports* – Impact Factor: 2.4, Q2
- Exploring the potential of EphA2 receptor signaling pathway: A comprehensive review in cancer treatment (2024) *Molecular Biology Reports* – Impact Factor: 2.6, Q2
- Computational Approaches for Lead Discovery against SARS-CoV-2 3C-Like Protease: Virtual screening and molecular dynamics studies (2023) *Journal of Medicine and Health Studies* – Not indexed
- Immunoinformatics Approach for the Design of Chimeric Vaccine Against Whitmore Disease (2023) *The Open Bioinformatics Journal* – Scopus Indexed
- Host Immune Response to B. pseudomallei Infection: Insights for therapeutic strategies and vaccine development (2023) *Bulletin of Environment, Pharmacology and Life Sciences* – WoS Indexed
- Identifying potential inhibitors of C-X-C motif chemokine ligand 10 against vitiligo: Structure-based virtual screening, molecular dynamics simulation, and principal component analysis (2023) *Journal of Biomolecular Structure and Dynamics* – Impact Factor: 2.7, Q2
- Design and Modeling of 4-Anilinoquinazoline Derivatives as Small Molecule Inhibitors of T790M/C797S EGFR Mutations: Targeting tumor angiogenesis (2023) *The Open Bioinformatics Journal* – WoS Indexed
- Evaluation of Terpenoids as Dipeptidyl Peptidase 4 Lead Molecules: Molecular docking and dynamics simulation study (2022) *Biointerface Research in Applied Chemistry* – Q3
- Target-based virtual screening and molecular dynamics simulation of small molecules: Promising drug candidates affecting kinesin-like protein KIFC1 (2022) *Cell Biochemistry & Function* – Impact Factor: 2.8, Q2

- Structure-Based In Silico and In Vitro Analysis of Asiatic Acid: A novel inhibitor of *Mycobacterium tuberculosis* maltosyl transferase (2022) *Current Computer-Aided Drug Design* – Impact Factor: 1.5, Q3
- Comparative Analysis of Autodock Tools and Molegro Virtual Docker: Screening high torsional compounds as tocotrienols with anti-angiogenic potential (2022) *Biochemical and Cellular Archive* – Not Indexed
- Identifying the alpha-glucosidase inhibitory potential of dietary phytochemicals against type 2 diabetes: Molecular interactions and dynamics simulation (2022) *Cellular and Molecular Biology* – Impact Factor: 1.5, Q4
- Identifying Natural Therapeutics against Diabetes via Inhibition of Dipeptidyl Peptidase 4: Molecular docking and MD simulation study (2022) *Indian Journal of Pharmaceutical Education and Research* – Impact Factor: 0.8, Q3
- Lifestyle-based health awareness using digital gadgets and online interactive platforms (2021) *NeuroPharmac Journal* – Not Indexed
- Bioplastics advances and their role in managing plastic pollution (2021) *NeuroPharmac Journal* – Not Indexed
- Elucidation of dibenzo[a,l]pyrene and its metabolites as mammary carcinogens: A comprehensive review (2021) *NeuroPharmac Journal* – Not Indexed
- Bioplastic: An approach towards sustainable development (2021) *NeuroPharmac Journal* – Not Indexed
- A review on COVID-19: Facts and current situation (2021) *NeuroPharmac Journal* – Not Indexed
- Molecular docking approach to elucidate the metabolic detoxification pathway of polycyclic aromatic hydrocarbons (2021) *NeuroPharmac Journal* – Not Indexed
- Identification of Potential Lead Molecules against Dibenzo[a,l]pyrene-induced Mammary Cancer: Targeting cytochrome P450 1A1, 1A2, and 1B1 isozymes (2021) *Biointerface Research in Applied Chemistry* – Q3
- Combinatorial Design to Decipher Novel Lead Molecule against *Mycobacterium tuberculosis* (2021) *Biointerface Research in Applied Chemistry* – Q3
- Computational Exploration of Dibenzo[a,l] Pyrene Interaction with DNA: Possible implications for human health (2020) *Biointerface Research in Applied Chemistry* – Q3
- Structural Perspective on Molecular Interaction of IgG and IgA with Spike and Envelope Proteins of SARS-CoV-2: Implications for non-specific immunity (2020) *Biointerface Research in Applied Chemistry* – Q3
- Design, SAR, and Metabolism Study of Crucifereae Family Compound (Spirobrassinin) and its Analogs for Antiangiogenic Potential: Targeting Hsp90 (2020) *Current Proteomics* – Impact Factor: 0.5, Q4
- Subtractive Proteomics for Identification of Drug Targets in Bacterial Pathogens: A review (2020) *International Journal of Engineering Research & Technology* – Not Indexed
- Identification of Potential Lead Molecule against Sphingosine Kinase-1: An in vitro study (2019) *Journal of Pharmaceutical Sciences and Research* – Not Indexed
- Identifying novel sphingosine kinase 1 inhibitors as therapeutics against breast cancer (2019) *Journal of Enzyme Inhibition and Medicinal Chemistry* – Impact Factor: 5.6, Q1
- Virtual screening, docking, and molecular dynamics simulation of selected phytochemicals bound to receptor tyrosine kinases: Correlative anti-angiogenic study (2019) *Bioinformation* – Not Indexed
- Global and Indian Scenario of Cancer and Side Effects Induced by Various Anti-Cancer Agents: Overview of recent developments in cancer treatment (2019) *International Journal of Biology, Pharmacy, and Allied Sciences* – UG Approved
- Molecular modeling and dynamics simulation of natural compounds: Potential anti-angiogenic agents targeting VEGFR-2 (2019) *Journal of Pharmaceutical Sciences and Research* – Not Indexed
- In Silico Identification of Drug-Like Inhibitors against *MtbDHDPS*: Shape-based approach (2019) *Journal of Pharmaceutical Sciences and Research* – Not Indexed
- In-Depth Computational Study of Sphk1 Inhibitors: Exploring structural insights into molecular interaction mechanisms (2019) *Biochemical and Cellular Archive* – Not Indexed
- Elucidation of marine fungi-derived anthraquinones as mycobacterial mycolic acid synthesis inhibitors: An in-silico approach (2019) *Molecular Biology Reports* – Impact Factor: 2.6, Q2
- Computational Outlook of Marine Compounds as Anti-Cancer Agents Targeting Bcl-2 and Survivin (2019) *Current Computer-Aided Drug Design* – Impact Factor: 1.5, Q3

BOOK CHAPTERS

- Nehal M, Khan I, Khatoon J, Akhtar S, Khan MKA (2023): "Metabolomics of Medicinal and Aromatic Plants." In *Ethnobotany and Ethnopharmacology of Medicinal and Aromatic Plants: Steps Towards Drug Discovery*, pp. 211-228. CRC Press, ISBN 9781032256085.
- Khan MKA, Akhtar S (2021): "Novel Drug Design, and Bioinformatics: An Introduction." *Physical Sciences Reviews*, De Gruyter Berlin Germany. DOI: https://doi.org/10.1515/psr-2018-0158
- Akhtar S, Khan MKA, Osama K (2020): "Machine Learning Approaches to Rational Drug Design." In *Computer-Aided Drug Design*, pp. 279-306. Springer, Singapore.