Dr. Faisal Ahmad

Assistant Professor

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Profile

Dr. Faisal Ahmad is an Assistant Professor of Bioinformatics at the National University of Medical Sciences (NUMS), specializing in bioinformatics and computational biology. His research focuses on molecular modeling, integrative data analytics, and computational approaches in health and life sciences. As a Consultant Bioinformatician, he contributed to an mRNA vaccine project at NIH Pakistan under the World Health Organization (WHO). His expertise spans mRNA vaccine development, multi-omics, next-generation sequencing (NGS) analysis, molecular dynamics simulations, AMR bioburden analysis, cancer genomics, and advanced bioinformatics workflows. He has collaborated with WHO, the Fleming Fund, Georgia Institute of Technology (USA), and the University of Maryland (USA). He has authored over 58 peer-reviewed international publications, with a cumulative impact factor exceeding 800, 1,061+ citations, and an H-index of 14. His expertise includes protein modeling, molecular docking, computer-aided drug design, in silico vaccine development, and AI-driven predictive modeling for precision medicine and antimicrobial resistance.

Research Interest

Computer-Aided Drug Design (CADD), Molecular Dynamics (MD) Simulations, Reverse Vaccinology, Genomic Surveillance, NGS Data & Multi-Omics Integration.

Selected Publications

Ahmad, F., Albutti, A., Tariq, M. H., Din, G., Tahir ul Qamar, M., & Ahmad, S. (2022). Discovery of potential antiviral compounds against hendra virus by targeting its receptor-binding protein (G) using computational approaches. *Molecules*, *27*(2), 554.

Ayaz, H., Nawaz, A., Ahmad, S., **Ahmad, F***., Tariq, A., Ahmad Khan, H., ... & Waheed, Y. (2025). Network-Driven methods using gene expression signatures to find therapeutic targets in breast cancer validated via molecular dynamics studies. *Journal of Chemical Information and Modeling*, *65*(14), 7749-7766.

Ahmad, F., Parvaiz, N., MacKerell Jr, A. D., & Azam, S. S. (2023). Non-β Lactam Inhibitors of the Serine β-Lactamase blaCTX-M15 in Drug-Resistant Salmonella typhi. *Journal of chemical information and modeling*, *63*(21), 6681-6695.

Ahmad, F., Ismail, S., & Azam, S. S. (2025). Discovery of novel inhibitor via molecular dynamics simulations against D-alanyl-D-alanine carboxypeptidase of Enterobacter cloacae. *Journal of Biomolecular Structure and Dynamics*, *43*(13), 6816-6831.

Ahmad, F., Navid, A., Irfan, M., Almajhdi, F. N., Hussain, T., Ozsahin, D. U., ... & Waheed, Y. (2026). Discovery of potential antiviral compounds and accelerating the therapeutic discovery against monkeypox virus. *Scientific Reports*.

Grants/Awards/Achievements

Provide expertise as Whole Genome Sequencing by implementing structured programs for One Health (AMR) surveillance to the Fleming Fund Country Grant Pakistan **under UK aid-Foreign, Commonwealth & Development Office (FCDO) funded Fleming Fund Country Grant, Pakistan.**

By harnessing mRNA technology, to construct a vaccine against rabies virus under **World Health Organization (WHO), Country Office and NIH, Islamabad, Pakistan.**

Worked as a Postdoctoral Fellow during pandemic of Covid-19 by Unveiling the Secrets of Omicron (BA5) and BQ.1.1: Molecular Dynamic Simulations to Combat Receptor Binding Sites at **Fauji foundation Medical University, Islamabad Pakistan**

Six Months of training experience in NIH project based on Mathematical modelling of host-host interaction (Cystic fibrosis patients and their microbiomes interactions among healthy and disease individuals) at **Georgia Institute of Technology Atlanta, Georgia, USA (IRSIP Fellowship Scholar)**

Short term visitor and training experience with novel Drugs designing tool SILCS at **University of Maryland Baltimore, USA.**

Member of American Society of Microbiology

Topic Editor of Frontiers in Immunology, Section “PLOS One