SAMEE ULLAH

✉ s.ullah@nih.org.pk

Github https://ullahsamee.github.io/
Researchgate https://www.researchgate.net/profile/Ullah-Samee
Google Scholar https://scholar.google.com/citations?user=wtuV29QAAAAJ&hl=en
Clarivate https://www.webofscience.com/wos/author/record/3917370
Orcid https://orcid.org/0000-0003-1987-3672

EDUCATION

(completed Sep 2019) **MPhil - Bioinformatics** National Center for Bioinformatics, Islamabad

Thesis: "Proteome wide Analysis for Potential Druggable Candidates against Morganella morganii"

Advisor: Prof. Dr. Syed Sikander Azam

(completed Jan 2016) **M.Sc - Microbiology** Quaid-i-Azam University Islamabad

PROFESSIONAL EXPERIENCE

[18 May 2020 – Feb 2022]
(1.8 Years)

Bioinformatician National Institute of Health (NIH), Islamabad

Project: "Lab Diagnostic and Existing Surveilliance System Strengthening for Pandemic Outbreak Management"

Key activities

- Implemented deep learning techniques for protein structure prediction and characterization such as AlphaFold, ColabFold, Foldseek, and Rosetta

- Employed de novo protein design and molecular dynamics simulations (MDS) to model and evaluate structural properties of proposed SARS-CoV-2 vaccine antigen and peptide scaffolds

- Provided training and supervision to undergraduate students, leading 8-week research projects on structure-based drug design for SARS-CoV-2 utilizing computational structural biology tools and techniques

- Speaker at various virtual workshops and webinars on SARS-CoV-2 protein structure modeling and drug design during the COVID-19 pandemic. Presentations focused on utilizing structure-based drug design, molecular simulations and protein design techniques to study SARS-CoV-2 proteins

- Collaborated with research groups at prestigious institutions including the National Research Council (CNR) Italy, University of Ohio, and King Abdullah International Medical Research Center (KAIMRC) on various research projects. Worked on *"elucidating nucleopeptide interactions and dynamics with DNA/RNA", "identifying potential therapeutic compounds from cannabis for Alzheimer's disease", and "computational de novo design of vaccine scaffolds against emerging COVID-19 variants".* Contributions led to multiple co-authored publications in top-quartile peer-reviewed journals

[1 Aug 2016 – 1 Jul 2017]
(01 Year)

Research Assistant (Internship) Quaid-i-Azam University

Key activities

- Executed independent research and identified the carbapenem resistant *E.coli* genes CTX-M15
- Analyzed the sequences and submitted to the GenBank with accession number MK770327.1
- Instructed undergraduates in a routine molecular biology tools and techniques (e.g., DNA, RNA extraction, Plasmid extraction, bacterial cell culturing, Gel preparation, PCR, microscopy,
- Assisted the principal investigator in the preparations of presentations

PUBLICATIONS

[01] Novel insights on nucleopeptide binding: A spectroscopic and In Silico investigation on the interaction of a thymine-bearing tetrapeptide with a homoadenine DNA
https://www.sciencedirect.com/science/article/abs/pii/S0167732221027008
Journal of Molecular Liquids - **6 impact factor, Q1**
Domenica Musumecia, **Samee Ullah**, Aamer Ikram, Giovanni N.Roviello

[02] Computational Prediction of Potential Drug-like Compounds from Cannabis sativa Leaf Extracts Targeted towards Alzheimer Therapy
https://www.sciencedirect.com/science/article/abs/pii/S016773222200931X
Journal of Molecular Liquids - **6 impact factor, Q1**
Adewale Oluwaseun Fadaka, Odunayo Anthonia Taiwo, Oluwatosin Adebisi Dosumu, Oluwafemi Paul Owolabi, Adebola Busola Ojo,Nicole Remaliah Samantha Sibuyi, **Samee Ullah**, Ashwil Klein, Abram Madimab, Madiehe, Mervin Meyer, Oluwafemi Adeleke Ojo

[03] A Novel De-novo Loss of Function Variant in the DNA Binding Domain of the TBX2 Cause Severe Osteochondrodysplasia
https://www.frontiersin.org/articles/10.3389/fgene.2022.1117500/abstract
Frontiers in Genetics - **3.7 impact factor, Q1**
Misbahuddin Rafeeq, Hussam Murad, Najumuddin, **Samee Ullah**, Zaheer Ahmed, Qamre Alam, Muhammad Bilal, Muhammad J. Khan, Muhammad Umair

[04] Importation of SARS-CoV-2 Variant B.1.1.7 in Pakistan
https://onlinelibrary.wiley.com/doi/10.1002/jmv.26869
Jounal of Medical Virology - **12.7 impact factor, Q1**
Massab Umair, Aamer Ikram, Muhammad Salman, Muhammad Masroor Alam, Nazish Badar, Zaira Rehman, Sana Tamim, Adnan Khurshid, Abdul Ahad, Hamza Ahmad, **Samee Ullah**

PREPRINTS

[01] Computational insights on the destabilizing mutations in the binding site of 3CL-protease SARS-CoV-2 Omicron (VOC)
https://www.biorxiv.org/content/10.1101/2023.05.24.542061v1.full.pdf+html
Samee Ullah*, Afreenish Amir, Aamer Ikram, Giovanni Nicola Roviello, Caterina Vicidomini, Rosanna Palumbo

[02] De novo design of anti-variant COVID-19 Vaccine
https://www.biorxiv.org/content/10.1101/2022.10.20.513049v2
Arpita Goswami, S. Madan Kumar, **Samee Ullah**, Milind M. Gore

TECHNICAL SKILLS

Laboratory
light microscopy, DNA and Plasmid extraction | PCR | Gel electrophoresis | Centrifugation | Bacterial cell culturing & media preparation | Western blot | Sterilization and aseptic techniques | General lab maintenance and safety compliance | Spectrophotometry |

Computational

- **Protein structure modelling:** Highly skilled in deep learning and homology based protein structures modelling using AlphaFold, OmegaFold, IgFold, ColabFold, Rosetta, SwissModel, Modeller, Phyre2 etc

- **De novo protein design:** Proficient in computational protein design using algorithms of ProteinMPNN, RFDiffusion, AlphaDesign, Rosetta, PROSS and ProGen2

- **Molecular dynamics simulations:** Skilled in performing molecular dynamics simulations of biomolecular systems using Desmond, Amber, Gromacs, OpenMM, VMD, CHARMGUI and Siremol

- **Molecular Interactions:** Proficiency in predicting protein-protein, small molecule, and nucleic acids interactions through molecular docking algorithms with GlideXP, CCDC Gold, MOE, Autodock and HADDock

- **Binding energy analysis:** Experience in MMGBSA/MMPBSA, $\Delta\Delta G$, metadaynamics and FEP+

- **Nucleic acids modelling/docking:** Expertise in 3D RNA structure modeling and docking using tools like iFoldRNA, NAST, SimRNA, rDock, RNABuilder, ModeRNA, EvoClustRNA.

- **Programming/Scientific computing:** Proficient in developing workflows and pipelines using Linux, R, NumPy, Scipy, Biopython, Google Colab, CUDA configuration, Docker, Anaconda, Jupyter Notebook, KNIME

- **Data visualizations:** Highly skilled in creating 2D and 3D graphical representations of biological data using Gnuplot, ggplot, Matplotlib, Xmgrace, Stata, Prism, Origin, MATLAB

- **Academic manuscript writing:** Proficiency in critically reviewing, manuscripts drafting, typesetting for Journals using Latex, Overleaf and creating figures for publications via Biorender and Canva

CERTIFICATIONS

[21 July 2023]	Career Essentials in Generative AI - Microsoft and LinkedIn
[24 May 2022]	Focus on Peer Review - SPRINGER NATURE
[24 May 2022]	An Introduction to Peer Review - Clarivate Web of Science
[26 May 2022]	How to peer review a review article - Elsevier
[24 May 2022]	Good Citation Behavior - Clarivate Web of Science
[26 May 2022]	Introduction to the Certified Peer Reviewer Course - Elsevier
[26 May 2022]	ACS Reviewer Lab - American Chemical Society
[4 Sep 2021]	Essentials of Writing and Reviewing Scientific Abstracts a field epidemiology focus - ECDC

WORKSHOPS AND PRESENTATIONS

[2-4 Feb 2022]	Cryo-EM Introductory Workshop 2022 - University of Copenhagen (UCPH)
[3 Feb 2022]	ARC Centre for Cryo-electron Microscopy of Membrane Proteins Research Symposium 2022
[26-29 Apr 2021]	Electron Cryo Microscopy in Structural Biology Workshop 2022 - Diamond light Source UK
[29 Mar 2021]	4th CCPBioSim/CCP5 Multscale Modelling Conference- Science & Technology Facilities Council (STFC) Daresbury Laboratory
[22-23 Mar 2021]	Introduction to electron microscopy Instruments and methods - at UCEM Umeå Centre for EM
[8-9 Apr 2021]	What can cryoelectron tomography and cryo soft X-ray tomography do - iNEXT-Discovery EMBL
[1 Mar 2021]	Instruct-ERIC webinar series: structure meets function - Instruct Centre EMBL
[25 May 2021]	Proteome wide analysis for potential druggable candidates against Morganella morganii Cambridge Crystallographic Data Center(CCDC)
[25 May 2021]	How COVID19 Vaccines Works at National Humanitarian Network Pakistan
[25 July 2020]	Underlying medical conditions and people at higher risk of COVID19 at International Webinar NIH
[01 Apr 2021]	SARS-CoV-2 Vaccines and mechanisms of action at Dow University of Health Sciences Karachi

MEMBERSHIPS

[01 Jan 2023 – Present]	American Chemical Society (ACS) - (Member No. 33104006)
[31 Dec 2020 – Present]	Royal Microscopical Society (RMS) Oxford UK - (Member No. RMS13431)

REFERENCES

[01] **Prof. Dr. Syed Sikander Azam**
Professor (Chairperson)

National Center for Bioinformatics (NCB)
Quaid-i-Azam University (QAU), Islamabad 45320 Pakistan

Tel: +92-051 9064-4130 | ssazam@qau.edu.pk

[02] **Prof. Dr. Sajid Rashid**
Professor

National Center for Bioinformatics (NCB)
Quaid-i-Azam University (QAU), Islamabad 45320 Pakistan

Tel: +92-051 9064-4113 | sajid@qau.edu.pk