SAMEE ULLAH

s.ullah@nih.org.pk
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 Sept 2019] (02 Years) **MPhil Bioinformatics** ***National*** *Center for Bioinformatics, Quaid-i-Azam University*, Islamabad

[Completed June 2016] (02 Years) **M.Sc. Microbiology** ***Quaid-i-Azam University***, Islamabad, Pakistan

PROFESSIONAL EXPERIENCE

[18 May 2020 – Feb 2022] (1.8 Years)

Bioinformatician ***National Institute of Health*** *(NIH), Islamabad 44000, Pakistan*

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

Main activities and responsibilities:

- Applied state-of-the-art deep learning methods and algorithms to model and characterize protein 3D structures in the laboratory using AlphaFold, Rosetta, AlphaFill, ColabFold, and Foldseek.
- Predicted the effects of mutations on the stability of *SARS-CoV-2* proteins by screening their 3D-structures derived from illumina sequences with DynaMut, DEUT and SDM tools.
- Established a computational structural biology unit via open source workflows in linux to perform simulations of proteins and nucleic acids structures with Gromacs, OpenMM and Desmond packages.
- Led and mentored undergraduates on "*SARS-CoV-2* structure based drug design using open source tools" for 8-week projects. Utilized Colab, AutodockGPU, Smina, Jupyter Notebook, and Anaconda to perform computational docking and screening of potential inhibitors.
- Co-authored two high-impact research articles in Q1 journals with an impact factor of 6.6 each.Demonstrated strong writing and analytical skills in producing original and rigorous scientific publications.
- Contributed to the development and submission of grant proposals, maintained accurate and comprehensive laboratory records, and created high-quality presentations, posters, covers and newsletters for professional audiences.

[1 Aug 2016 – 1 Jul 2017] (01 Year)

Research Assistant (Internship) ***Quaid-i-Azam University***

Main activities and responsibilities:

- Analyzed the CTXM-15 gene sequences and submitted to the GenBank with accession number MK770327.1
- Trained undergraduate students on molecular biology tools and techniques, such as DNA/RNA isolation, plasmid purification, cell culture, gel electrophoresis, PCR, microscopy, biosafety cabinets and GLPs.
- Supported the principal investigator in creating and delivering presentations on research findings and progress.

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 6.6 IF, 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 6.6 IF, 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 4.7 IF

Misbahuddin Rafeeq, Hussam Murad, Najumuddin, Samee Ullah, Zaheer Ahmed, Qamre Alam, Muhammad Bilal, Muhammad J. Khan, Muhammad Umair

RESEARCH SKILLS

Laboratory & Biochemistry techniques

-Performing Scanning Electron Microscopy (SEM) and Nuclear Magnetic Resonance Spectroscopy (NMR) to analyze the structure and composition of samples.

- Applying light microscopy, DNA and plasmid extraction, PCR, and gel electrophoresis to study the molecular biology of microbial cells

- Culturing microbial cells in different media and conditions, preparing media and reagents, and conducting Western blot assays to detect proteins.

- Operating centrifuges, broth filters, autoclaves, and other laboratory equipment to prepare and process samples.

- Maintaining a clean and safe laboratory environment, following good laboratory practices (GLP) and standard operating procedures (SOPs).

Computational Structural Biology

-AProficient in utilizing cutting-edge deep learning-based protein structure modeling software such as AlphaFold2, AlphaFill, ColabFold, Foldseek, OpenFold, IgFold, OmegaFold, and RoseTTAFold.

-Proficient in open source method for structure generation and protein design such RFDiffusion, ProteinMPNN, ProGen2, Rosetta

-Highly skilled in structure molecular modeling of various biomolecules, including nucleic acids (RNA/DNA), proteins, membranes, peptides, and small molecules using CHARMGUI, VMD, packmol

-Highly Skilled in analyzing protein-protein and small molecule interactions using DiffDock, AutodockGPU, EquiBind, Smina, GlideXP, CCDC Gold, HADDOCK, MOE and SwissDock.

-Proficient in protein homology modeling using Rosetta, Swiss model, HHpred, FoldX, Modeller, ModWeb, Phyre2

-Experienced in working with protein structure databases such as AlphaFold-DB, RCSB, SCOP, Uniprot, CATH, and SWISS-MODEL Repository.

-Proficient in data visualization and analysis using tools such as Gnuplot, ggplot, Matplotlib, Xmgrace, Stata, Prism, Origin, and MATLAB.

-Experienced in image analysis using software such as ImageJ, Bio-Blender, and Icy.

-Skilled in journal manuscript preparation using typeset, LaTeX, Overleaf, and Biorender.

-Proficient in programming, usage and installation of CUDA, high performance computing, Linux, R, NumPy, Biopython, PyTorch, Scikit-learn, Scipy, Docker conatiners, hugginface, Anaconda, and Jupyter Notebook.

CERTIFICATIONS/AWARDS

[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
[26 May 2022] **Introduction to the Certified Peer Reviewer Course -** Elsevier
[26 May 2022] **ACS Reviewer Lab -** American Chemical Society

PRESENTATIONS/WORKSHOPS/WEBINARS

[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] **RSC CICAG workshop series ChimeraX**
[10 Dec 2020] **Uncovering protein function with UniProt -** EMBL EBI Webinar

PROFESSIONAL SOCIETIES

[31 Dec 2020 – Current] **Royal Microscopical Society (RMS) Oxford UK**
[31 Oct 2021 – Current] **Alzheimer's Association International Society to Advance Alzheimer's Research and Treatment (ISTAART)**

REFERENCES

[01] **Prof. Dr. Sa**jid Rashid
Professor

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

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

[02] 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