SAMEE ULLAH

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Researchgate https://www.researchgate.net/profile/Ullah-Samee
Google Scholar https://scholar.google.com/citations?user=wtuV29QAAAAJ&hl=en
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EDUCATION

[September 2019] (02 Years) **MPhil Bioinformatics** ***National Center for Bioinformatics, Quaid-i-Azam University***, Islamabad

[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***

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

Main activities and responsibilities:

- Implemented deep learning techniques and algorithms for protein structure prediction and characterization in the laboratory (e.g., AlphaFold2, AlphaFill, AlphaFold Multimer, ColabFold, Foldseek and Rosetta)
- Screened the viral and bacterial proteins 3D-structures using the illumina sequences for the mutation and structural biology studies
- Established a computational structural biology unit for the simulations of proteins and nucleic acids complexes using the molecular dynamics simulation package Desmond.
- Trained staff and supervised undergraduates in 8-weeks short projects on "*SARS-CoV-2* structure based drug design using computational structural biology tools and techniques"

[1 Aug 2016 – 1 Jul 2017] **(01 Year)** **Research Assistant (Internship)** ***Quaid-i-Azam University***

Main activities and responsibilities:

- Executed independent research and identified the carbapenem resistant *E.coli* genes CTX-M15 under supervision
- 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, cell culturing, Gel preparation, PCR, microscopy, biosafety cabinets and GLPs)
- 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 ***6.6 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

[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 ***20.6 IF***
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] **Reshuffling of p-hydroxy benzoic acid ligand in Escherichia coli HosA transcription factor structure reveals unique chemical scavenging by flexible amino terminus**
https://pdbj.org/search/status?pdbid=8aga&lang=ko
Arpita Goswami*, **Samee Ullah**, S. Madan Kumar

[03] **De novo design: COVID-19 anti-variant vaccine construct with T-cell memory**
https://www.biorxiv.org/content/10.1101/2022.10.20.513049v1.full
Arpita Goswami1*, S. Madan Kumar, **Samee Ullah**, Milind M. Gore

RESEARCH SKILLS

Laboratory & molecular biology

Scanning Electron Microscopy (SEM) | Nuclear magnetic resonance spectroscopy(NMR) | light microscopy, DNA and Plasmid extraction | PCR | Gel electrophoresis | Centrifugation | Bacterial cell culturing | & media preparation | Western blot | Sterilization | General lab maintenance and safety compliance | Good laboratory practices (GLP)

Computational Structural Biology

Deep learning based protein structures modelling; AlphaFold2, AlphaFill, AlphaFold Multimer, ColabFold, Foldseek, OpenFold, IgFold, OmegaFold and RoseTTAFold

Protein homology modelling; prime Schrodinger, Robetta, Swiss model, HHpred, FoldX, Modeller, ModWeb, Phyre2, Galaxy

Protein-Protein and small mol. interactions; HADDOCK, GlideXP, Gold, Autodock, SwissDock

Protein structure databases; AlphaFold-DB, RCSB, SCOP, Uniprot, CATH, SWISS-MODEL Repository

Molecular modelling; Nucleic acids(RNA/DNA), Proteins, Membranes, Peptides, small molecules

Biomolecular simulations; Desmond, Amber, VMD, CHARMGUI, Siremol, OpenMM,

Data visualizations; Gnuplot, ggplot, Matplotlib, Xmgrace, Stata, Prism, Origin and MATLAB

Image analysis; ImageJ, Bio-Blender, Icy

Journals Manuscript preparation; Typeset, Latex, Overleaf, Biorender

Programming; Linux, R, NumPy, Biopython, PyTorch, NVIDIA Docker, Anaconda, Jupyter Notebook

CryoEM data analysis & tools: 2D preprocessing, Geometrical particlepicking, Initial modelgeneration, Particle pose optimisation, Subtomogram averaging, Multi-particle refinement, cryoDRGN, cryoSPARC, cisTEM, Coot, UCSF ChimeraX, Phenix, MotionCor2, CTFFIND4,

CERTIFICATIONS

[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**
[4 Sep 2021] **Essentials of Writing and Reviewing Scientific Abstracts a field epidemiology focus - ECDC**
[26 May 2022] **Introduction to the Certified Peer Reviewer Course - Elsevier**
[26 May 2022] **ACS Reviewer Lab - American Chemical Society**

WORKSHOPS / SYMPOSIUMS / 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)**