

## EDUCATION

- 2020-2022 King Abdul Aziz University, Saudi Arabia**  
MSc in Biological Science (Microbiology); CGPA: 4.95/5.00  
Thesis Title: Viral and Host Protein-Targeted Identification of Potential Natural Antiviral Drug Candidates Against MERS-CoV and SARS-CoV-2
- 2013-2018 Jessore University of Science & Technology, Bangladesh**  
BSc in Genetic Engineering & Biotechnology; CGPA: 3.10/4.00  
Thesis Title: Isolation and Characterization of *Lactic Acid* Bacteria from Arsenic-Contaminated Soil and Milk in Jashore for Environmental Detoxification and Microbial Bioremediation

## RESEARCH EXPERIENCE

- 2023-2025 Hamad Bin Khalifa University (HBKU), Qatar**  
Position: Research Assistant  
Project Title: A Precision Medicine Initiative To Target Paediatric Cerebral Palsy, A Movement Disorder (NPRP14S-0319-210075)
- Collected samples, PBMC isolation, and gDNA extraction from 110 families.
  - Conducted whole-exome, RNA sequencing, and downstream analysis.
  - Conducted Sanger sequencing for mutation validation and variant confirmation.
  - Performed epigenomic (DNA methylation) and scRNA-seq data analysis
  - Supported the development of AI-driven tools for biomarker discovery and precision diagnosis in cerebral palsy.
- 2021-2022 Center for Artificial Intelligence in Precision Medicine (KAU), Saudi Arabia**  
Position: Research Assistant
- Contributed to the development of ML/AI-driven pipelines for target identification
  - Participated in virtual large-scale drug screening for candidate molecule identification against prioritized targets.
  - Targeted viral proteins from SARS-CoV-2 and MERS-CoV for structure- and ligand-based drug discovery.
  - In-vitro validation of screened compounds against the target protein
- 2019-2020 International Islamic University Malaysia, Malaysia**  
Position: Research Assistant  
Project: Interrogating Novel Compounds for Improved Anti-dengue Therapies via Inhibition of Host's Glycolytic Pathway(FRGS/1/2016/STG04/UIAM/02/1/)
- Conducted molecular cloning, expression, and purification of the human Hexokinase 2 (**HK2**) enzyme.
  - Performed inhibition assays on virtual-screened compounds
  - Contributed to the validation of anti-dengue therapeutic candidates using enzyme activity-based profiling.
- 2017-2018 Central Laboratory of Biotechnology, Bangladesh**  
Position: Research assistant
- Isolated and screened LAB strains for arsenic resistance probiotic.
  - Characterized potential for environmental detoxification and microbial bioremediation.
  - Evaluated functional probiotic traits (acid/bile tolerance, antimicrobial activity).

## **TRAINING & WORKSHOP ATTENDED**

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| <b>2024, Sep</b> | <b>Variant Effect Prediction Training Course 2024</b><br>Organized by: Human Genome Organization (HUGO), Italy                                     |
| <b>2024, Apr</b> | <b>Hands-on training in the Next Generation Sequencing Technology</b><br>Organized by: Qatar Biomedical Research Institute (QBRI), Qatar           |
| <b>2019, Feb</b> | <b>Training on Molecular cloning, expression, and purification</b><br>Organized by: National Institutes of Biotechnology Malaysia, Four (4) months |
| <b>2017, Apr</b> | <b>Overview &amp; safe use of laboratory ventilation equipment</b><br>Organized by: ESCO Life Sciences Bangladesh Pvt. Ltd                         |
| <b>2016, May</b> | <b>Workshop on Human Genome Project</b><br>Organized by: Military Institute of Science & Technology  |

## **AWARDS & ACHIEVEMENTS**

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|------------------|---|
| <b>2024, Sep</b> | <b>Travel Grant Award – VEPTEC Conference 2024</b><br>Host Organization: Human Genome Organization (HUGO), Italy<br>Award Type: International Travel Grant                                  |
| <b>2021, Nov</b> | <b>Student Exchange Award – Artificial Intelligence and Drug Discoveries</b><br>Host Institutions: Oxford University and King Abdul Aziz University<br>Award Type: Student Exchange Program |
| <b>2020-2022</b> | <b>Graduate Scholarship – King Abdul Aziz University</b><br>Degree: MSc in Biological Sciences<br>Funding: Fully Funded   |
| <b>2013-2018</b> | <b>Undergraduate Scholarship – Bangladesh Army Welfare Trust</b><br>Degree: BSc in Genetic Engineering & Biotechnology<br>Funding: Fully Funded   |

## **EDUCATIONAL OUTREACH & TRAINING LEADERSHIP**

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| <b>2024, May</b> | <b>Genome-wide Microarray data analysis and genetic effects on disease</b><br>Host Organization: BioSol Centre<br>Session Type: Training                     |
| <b>2021, Aug</b> | <b>Computer-Aided Antiviral Peptide Identification and Design</b><br>Host Organization: BioSol Centre<br>Session Type: Training & Project (04) Months        |
| <b>2021, Jan</b> | <b>Discovery of Bioactive Compounds against Human Virus and Bacteria</b><br>Host Organization: BioSol Centre<br>Session Type: Training & Project (04) Months |
| <b>2020, Nov</b> | <b>Bioinformatics for Beginners</b><br>Host Organization: BioSol Centre<br>Session Type: Training  |
| <b>2020, Aug</b> | <b>Identifications of Novel Compounds by CADD Approaches</b><br>Host Organization: BioSol Centre<br>Session Type: Training                                   |
| <b>2020, Jan</b> | <b>Computer-aided drug design and research methodology</b><br>Host Organization: Jessore University of Science & Technology (JUST)<br>Session Type: Seminar  |

## PEER-REVIEWED PUBLICATIONS

- 2025, Feb** Molecular docking, QSAR, and simulation analyses of EGFR-targeting phytochemicals in non-small cell lung cancer  
Published: Journal of Molecular Structure (IF: 4.00)  
DOI: [10.1016/j.molstruc.2024.139924](https://doi.org/10.1016/j.molstruc.2024.139924)
- 2025, Jan** Investigating new drugs from marine seaweed metabolites for cervical cancer therapy by molecular dynamic modeling approach  
Published: Scientific Reports (IF: 3.80)  
DOI: [s41598-024-82043-0](https://doi.org/10.1016/j.sci.2024.82043-0)
- 2024, Dec** *In-vitro* and *in-silico* evaluation of rue herb for SARS-CoV-2 treatment  
Published: International Immunopharmacology (IF: 4.80)  
DOI: [10.1016/j.intimp.2024.113318](https://doi.org/10.1016/j.intimp.2024.113318)
- 2024, Jul** Cheminformatics-based identification of phosphorylated RET tyrosine kinase inhibitors for human cancer  
Published: Frontiers in Chemistry (IF: 3.80)  
DOI: [10.3389/fchem.2024.1407331](https://doi.org/10.3389/fchem.2024.1407331)
- 2023, Oct** Natural defense against multi-drug resistant *Pseudomonas aeruginosa*: Cassia occidentalis L. *in vitro* and *in silico* antibacterial activity  
Published: RSC Advances (IF: 3.900)  
DOI: [10.1039/D3RA03923D](https://doi.org/10.1039/D3RA03923D)
- 2023, Jul** The ortholog of human ssDNA-binding protein SSBP3 influences neurodevelopment and autism-like behaviors in *Drosophila melanogaster*  
Published: PLoS Biology (IF: 9.800)  
DOI: [10.1371/journal.pbio.3002210](https://doi.org/10.1371/journal.pbio.3002210)
- 2023, Jun** Computational formulation of a multiepitope vaccine unveils an exceptional prophylactic candidate against Merkel cell polyomavirus  
Published: Frontiers in Immunology (IF: 8.786)  
DOI: [10.3389/fimmu.2023.1160260](https://doi.org/10.3389/fimmu.2023.1160260)
- 2023, Feb** In-silico formulation of a next-generation multiepitope vaccine for use as a prophylactic candidate against Crimean-Congo hemorrhagic fever  
Published: BMC Medicine (IF: 11.150)  
DOI: [10.1186/s12916-023-02750-9](https://doi.org/10.1186/s12916-023-02750-9)
- 2022, Dec** GC-MS analysis of phytoconstituents from *Ruellia prostrata* and *Senna tora* and identification of potential antiviral activity against SARS-CoV-2  
Published: RSC Advances (IF: 4.036)  
DOI: [10.1039/D1RA06842C](https://doi.org/10.1039/D1RA06842C)
- 2022, Jun** Application of Mathematical Modeling and Computational Tools in the Modern Drug Design and Development Process  
Published: Molecules (IF: 4.927)  
DOI: [10.3390/molecules27134169](https://doi.org/10.3390/molecules27134169)
- 2021, Sep** Evaluation of *in vitro* and *in silico* anti-inflammatory potential of some selected medicinal plants of Bangladesh against cyclooxygenase-II enzyme  
Published: Journal of Ethnopharmacology (IF: 4.360)  
DOI: [10.1016/j.jep.2021.114900](https://doi.org/10.1016/j.jep.2021.114900)
- 2021, Sep** A systematic analysis of ATPase Cation transporting 13A2 (ATP13A2) transcriptional expression and prognostic value in human brain cancer  
Published: Biomedical Signal Processing and Control (IF: 5.076)  
DOI: [10.1016/j.bspc.2021.103183](https://doi.org/10.1016/j.bspc.2021.103183)

- 2021, Sep** Spike protein recognizer receptor ACE2 targeted identification of potential natural antiviral drug candidates against SARS-CoV-2  
Published: International Journal of Biological Macromolecules (IF: 8.025)  
DOI: [10.1016/j.ijbiomac.2021.09.146](https://doi.org/10.1016/j.ijbiomac.2021.09.146)
- 2021, Aug** Pharmacophore-Based Virtual Screening, Quantum Mechanics Calculations, and Molecular Dynamics Simulation Approaches Identified Potential Natural Antiviral Drug Candidates against MERS-CoV S1-NTD  
Published: Molecules (IF: 4.927)  
DOI: [10.3390/MOLECULES26164961](https://doi.org/10.3390/MOLECULES26164961)
- 2021, Apr** Pharmacoinformatics and molecular dynamics simulation-based phytochemical screening of neem plant (*Azadiractha indica*) against human cancer by targeting MCM7 protein  
Published: Briefings in Bioinformatics (IF: 13.994)  
DOI: [10.1093/BIB/BBAB098](https://doi.org/10.1093/BIB/BBAB098)
- 2021, Feb** Structure-based pharmacophore modeling, virtual screening, molecular docking and ADMET approaches for identification of natural anti-cancer agents targeting XIAP protein  
Published: Scientific Reports (IF: 4.996)  
DOI: [10.1038/S41598-021-83626-X](https://doi.org/10.1038/S41598-021-83626-X)
- 2020, Dec** High expression of bone morphogenetic protein 1 (BMP1) is associated with a poor survival rate in human gastric cancer, a dataset approach  
Published: Genomics (IF: 5.736)  
DOI: [10.1016/J.YGENO.2020.11.012](https://doi.org/10.1016/J.YGENO.2020.11.012)
- 2020, Oct** Computational assessment of MCM2 transcriptional expression and identification of the prognostic biomarker for human breast cancer  
Published: Heliyon (IF: 3.776)  
DOI: [10.1016/J.HELIYON.2020.E05087](https://doi.org/10.1016/J.HELIYON.2020.E05087)
- 2020, Jul** Designing a multi-epitope vaccine against SARS-CoV-2: an immunoinformatics approach  
Published: Biomolecular Structure and Dynamics (IF: 5.235)  
DOI: [10.1080/07391102.2020.1792347](https://doi.org/10.1080/07391102.2020.1792347)
- 2019, Sep** Contemporary Strategies and Current Trends in Designing Antiviral Drugs against Dengue Fever via Targeting Host-Based Approaches  
Published: Microorganisms (IF: 4.926)  
DOI: [10.3390/MICROORGANISMS7090296](https://doi.org/10.3390/MICROORGANISMS7090296)
- 2019, Apr** Anti-inflammatory, antinociceptive and antidiarrhoeal activities of methanol and ethyl acetate extract of *Hemigraphis alternata* leaves in mice  
Published: Clinical Phytoscience  
DOI: [10.3390/MD19050253](https://doi.org/10.3390/MD19050253)

#### UNDER REVIEW

- 2025, Feb** Machine Learning Driven Modeling of Synergistic Perinatal Risk Profiles in Early Onset Pediatric Cerebral Palsy  
Published: BMC Medical Informatics and Decision Making (IF:3.80)  
Manuscript Number: [f1fe7e87-5cd9-4bc0-9c70-826005c543fa](https://doi.org/10.1186/s12911-025-0543-fa)

#### UNDER PREPARATION

- 2025, Aug** AutoML-Guided Discovery of Hub Genes in Cerebral Palsy Reveals Shared Pediatric Disease Mechanisms

## PRESENTATIONS & CONFERENCES

- 8th Variant Effect Prediction Training Course (VEPTC) -2024, Oral Presentation, Palermo, Italy (Pathogenic disease-causing mutations in BRG1 domain of SMARCA4 destabilize the SWI/SNF complex and lead to neurodevelopmental disorders)

## RESEARCH INTERESTS

- Artificial intelligence-driven target and biomarker discovery across multi-omics datasets
- Computational drug and peptide discovery and design (Pharmacophore modeling, MD simulation)
- Machine learning-based precision medicine models and large-scale drug screening
- Whole-exome sequencing (WES), DNA methylation, and single-cell omics data analysis
- Network pharmacology and systems biology modeling of disease mechanisms
- Integration of spatial transcriptomics and single-cell RNA-seq for cellular heterogeneity
- Translational applications in virology, oncology, and neurodevelopmental disorders

## SKILLS

- Computational Biology & Multi-omics Analysis: WES, RNA-seq, DNA methylation, scRNA-seq
- Molecular Modeling: Pharmacophore modeling, Docking, MD Simulation, QSAR, ADMET
- Artificial Intelligence: ML/DL-based Biomarker, Drug Target Discovery, and Virtual Screening
- Bioinformatics Tools: GSEA, Enrichr, Cytoscape, Bioconductor (R), Seurat
- Programming: Python, R, Shell scripting
- Operating system: Linux, Windows
- Molecular Biology: Proficient in PCR, gel electrophoresis, cloning, expression, purification (IMAC, HPLC), qPCR, DNA/RNA extraction, and Sanger sequencing.
- Data Science: Feature selection, SHAP, UMAP, PCA, scikit-learn
- Clinical Genomics: Variant Annotation, Gene Prioritization, Disease Risk Modeling
- Data Visualization: ggplot2, seaborn, matplotlib, UCSF ChimeraX, PyMOL, Biorender, plotly

## LEADERSHIP & SERVICE

- Founder & CEO, Biological Solution Centre (BioSol Centre): Leading computational biology and bioinformatics research projects, collaborations, and training initiatives.
- Peer Reviewer: Reviewed 70+ manuscripts for journals including Scientific Reports, Briefings in Bioinformatics, and NPJ Breast Cancer.
- Event Organizer: Coordinated academic seminars, workshops, and community outreach in biotechnology and computational biology.

## ACADEMIC REFERENCES

**Dr. Ishtiaq Qadri.** Professor (Thesis Supervisor / Master's)  
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