

# ASHFAQ AHMAD, *Ph.D., PostDoc*

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Date of Birth & Nationality: April 10, 1984, Pakistan

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## RESEARCH INTERESTS

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I possess a diverse skill set as a hybrid researcher, capable of conducting experiments in both wet and dry lab environments. My expertise extends from de novo protein design to novel drug discovery and design employing RFDiffusion, Deep Learning, Machine Learning and QSAR models. I am interested in exploring HER+ cancers, and neurological disorders from the lens of Gut-Brain Axis using Metformin.

## TEACHING AND RESEARCH EXPERIENCE

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**Including PhD = 12 Years; Post-PhD = 09 Years**

**Assistant Professor in Bioinformatics -**

November 13, 2020- To date

Department of Bioinformatics, Hazara University, Mansehra.

<https://www.hu.edu.pk/faculty/detail/458>

**Assistant Professor (adjunct) in Bioinformatics –**

February 2020 – November 2020

Department of Bioinformatics, Hazara University, Mansehra.

**Assistant Professor (IPFP) in Bioinformatics-**

February 2019 - February 2020

Department of Bioinformatics, Hazara University, Mansehra.

**Post-doctorate in Structure Biology and Bioinformatics –**

June 2016 - August 2018

Southern University of Science and Technology, Shenzhen, Guangdong Province, China

## EDUCATION

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**Xiamen University**

**China**

Ph.D. Biochemistry and Molecular Biology, (Supervisor Dr. Han Aidong) Sep. 2011 - Jul.

2015Dissertation: Molecular dynamics and Co-evolutionary study of the RegX3 response regulator from the *Mycobacterium tuberculosis*.

- Protein Structure, Function & Signaling (X-ray diffraction, Computational tools, Molecular Dynamics). Targeted system was Bacterial two-component system. The structure of Histidine Kinase from Bacterial two-component system was solved in active and inactive states. Molecular and Essential dynamics simulation (ENM, NMA, PCA, CNA) were applied for functional states detection and conformational changes. (Completed).
- 2nd Project, Conformational dynamics were analyzed of RegX3 response regulators for 150 nanoseconds of SenX3-RegX3 two-component system *Mycobacterium tuberculosis*. (Completed).
- 3rd Project, Detection of Dynamic network of HAMP signaling system from

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Streptococcus mutant Two-component system. (completed).

**University of Peshawar**

M.Phil/Master. Biotechnology, (Supervisor: Dr. Ghousia Lutfullah)  
Master's Thesis: Homology Modeling and Evolutionary Study of Streptolysin O: Prediction of Important Residues and their Functional Analysis.

**Pakistan**

Aug. 2007 – Jul. 2011

**University of Peshawar**

BSc (Hons). Biotechnology, Courses studied of 140 Credit Hours

**Pakistan**

Mar. 2003 – Jul. 2006

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**AUTHORED BOOK**

**Accelerating Drug Discovery: A Tutorial-Based Approach with Machine Learning**

ISBN-10: 1636486584, ISBN-13: 978-1636486581, Publication date: August 04, 2023. Eliva Press.

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**PROFESSIONAL CERTIFICATIONS**

- i. AI for Everyone (Coursera)
- ii. Visualization with BioPython (Coursera)

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**BIOCHEMICAL AND COMPUTATIONAL SKILLS**

**Deep/Machine Learning in Drug Discovery**

*Scikit-Learn, RDKit, PaDEL, Seaborn, Lazypredict, Pickle, Streamlit, Programming languages: R, Python*

**Protein Design**

*RFdiffusion, MPNN, Binder*

**Protein Structure and Ligand Docking**

*Deep Learning and AI: AlphaFold3, Boltz-1, Chai-1, TR-Rosetta, AutoDock, AutoDock Vina, and Schrodinger Glide*

**Evolutionary Networks**

*PopArt, DNASp6, Virus evolutionary network analysis system (VENAS)*

**Molecular Dynamics Simulation**

*NAMD, OpenMM, Gromacs*

**Dataset Analysis**

*PROMO, GEO2R, R*

**Visualization**

*Plotly, ggplot2, Plotnine, PyMOL, Chimera, VMD*

**Protein Interaction Interface Detection**

*DCA, Gremlin, ANN and SVM*

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## **Protein Expression**

*DNA Extraction, Cloning and PCR Amplification, Protein Expression and Purification, Gel Filtration, Protein-Protein Interaction: Pull-Down Assays  
Protein-Ligand Interaction: Iso-thermal Calorimetry  
Protein Crystallization by X-ray diffraction*

## **Cloud Computing Personal Space**

*<https://github.com/Ash100/>  
Jupyter Notebooks*

## **RECENT TRAINING PROVIDED THE COMMUNITY**

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“**Colaboratory, A Gateway for Bioinformatics and Innovation**” training workshop delivered on November 22, 2024, in iCOBLET2024 at **University of Doha for Science and Technology**, Qatar.

“**Applications of AI in Drug Discovery**” training workshop delivered on November 1, 2024, at **Muhammad Ali Jinnah University**, Karachi, Pakistan.

## **EDITORIAL BOARD MEMBER**

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Academic Editor: PlosONE

## **PROFESSIONAL MEMBERSHIPS**

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Outreach member of the American Society of Microbiology (ASM)

## **STUDENT SUPERVISION**

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Supervised 12 Graduates and Post-graduates students in Bioinformatics

## **SCIENTIFIC OPENIONS IN NATIONAL AND INTERNATIONAL NEWS PAPERS**

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The technological revolution we must lead Published in ***Pakistan Today***. July 27, 2025  
<https://www.pakistantoday.com.pk/2025/07/27/the-technological-revolution-we-must-lead/>

## **BIOINFORMATICS TEACHING FOR THE COMMUNITY VIA YOUTUBE**

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Name: Bioinformatics Insights URL: [www.youtube.com/@Bioinformaticsinsights](http://www.youtube.com/@Bioinformaticsinsights)

## **INTERNATIONAL ACHIEVMENTS**

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Included in the list of 2% productive scientist in the year of 2023, released by Elsevier and Stanford.

### **ADDRESS**

Department of Bioinformatics, Hazara University, Dhodhyal Manshra, Pakistan 21300.

## RESEARCH PUBLICATIONS

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### **Submitted**

Reporting of Four Novel PARP1 Inhibitors using Artificial Neural Networks and 3D-QSAR Models – Under Review to **Chinese Herbal Medicine**.

**(First Author)**

Reporting of Novel de novo protein designs against Salmonella PagC. Submitted to **Translational Medicine**. **(Corresponding Author and in progress)**

Discovering novel LXXLL motifs proteins as a possible co-activator of nuclear receptors through ESM-2 protein language model. Submitted to **Nature Communication**. **(First Author)**

### **Already Published and Online**

**Ashfaq Ahmad\***, Sidra Majaz, Aamir Saeed, Shumaila Noreen, Muhammad Abbas, Bilal Khan, Hamid Ur Rahman, Faisal Nouroz, Yingqiu Xie, Abdur Rashid, Atta Ur Rehman\*. Microevolution and Phylogenomic Study of Respiratory Syncytial Virus Type A. (2025). **Plos ONE**. <https://doi.org/10.1371/journal.pone.0319437>

(Impact Factor: **3.2**) (First author)

Tayyaba Saeed, Nousheen Bibi, **Ashfaq Ahmad**, Saadullah Khan, Muhammad Ansar, Naveed Wasif, Umm-e- Kalsoom. A novel biallelic variant in IHH gene causing Acrocapitofemoral dysplasia in a Pakistani family. (2025). **Molecular Genetics & Genomic Medicine**.

<https://doi.org/10.1002/mgg3.70085>

Guldan Nazarbek, Chenglin Mu, Ainur Shaimoldina, Zhuldyz Omarova, Nurlan Toktarov, Lianxiang Wang, **Ashfaq Ahmad**, Didar Zeitkazyeva, Haiyan Fan, Lei Shi, Zhenbang Chen, Yingqiu Xie. (2024). Deer antler extract-nanoparticles exhibit co-nanozyme activity and targeting of prostate cancer cells. **Journal of Functional Foods**. <https://doi.org/10.1016/j.jff.2024.106089>

(Impact Factor: **5.6**) (Co-author)

Asad Munir, Inam Ullah Khan, Abdur Rashid, Ijaz Anwar, Sabawoon Shah, Sergey Oreshkov, Mukhtar Ullah, Haider Ali Khan, Ubaid Ullah, **Ashfaq Ahmad**, Muhammad Ansar, and Atta Ur Rehman. (2024). A novel homozygous missense variant in POC1B causes cone dystrophy in a consanguineous Pakistani family. **Ophthalmic Genetics**.

<https://doi.org/10.1080/13816810.2024.2430700>

Impact Factor: **2.4** (Co-author)

**Ashfaq Ahmad**, Aliya Orassay, Sidra Majaz, Aamir Saeed, Darya Sadvokassova, Alan Berdigaliyev, Salar Ahmad, and Yingqiu Xie. (2023). Computational Analysis of Target Genes in

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Department of Bioinformatics, Hazara University, Dhodhyal Mansehra, Pakistan 21300.

Monkeypox Virus Infection and Potential Therapeutic Precursors. **Expert Review of Anti-Infective Therapy**. <http://doi.org/10.1080/14787210.2023.2259614>. (Impact Factor: **5.9**) (First author)

Haseeb Nisar, Bilal Wajid, Faria Anwar, **Ashfaq Ahmad**, Anum Javaid, Syed Awais Attique, Wardah Nisar, Amir Saeed, Samiah Shahid, and Saima Sadaf. (2023). Bioinformatics and systems biology analysis revealed PMID26394986-Compound-10 as potential repurposable drug against covid-19. **Journal of Biomolecular structure and dynamics**. <https://doi.org/10.1080/07391102.2023.2242500>. (Impact Factor: **5.235**) (Co-author)

Dongsheng Liu, Aamir Saeed, Sidra Majaz, Bashrat Ahmad, **Ashfaq Ahmad**<sup>✉</sup>, and Yingqiu Xie<sup>✉</sup>. (2023). Targeting severe symptoms of early 2023 new outbreak of COVID-19 by classical drug dexamethasone: a potential fatality reducing agent. **Journal of Translational Medicine**. <https://doi.org/10.1186/s12967-023-04186-4>. (Impact Factor: **8.4**) (Corresponding)

**Ashfaq Ahmad**<sup>#</sup>, Zhandaulet Makhmutova<sup>#</sup>, Wenwen Cao, Sidra Majaz and Yingqiu Xie. (2023). Androgen receptor, a possible anti-infective therapy target and a potent immune respondent in SARS-CoV-2 spike binding: a computational approach. **Expert Review of Anti-Infective Therapy** <https://doi.org/10.1080/14787210.2023.2179035>. (Impact Factor: **5.9**). (First author)

Hamid Ur Rahman, Sobia Attaullah, Tariq Mahmood, and **Ashfaq Ahmad**. (2023). Distribution, Morphometrics and DNA barcoding of *Archotermopsis wroughtoni* Desneux (Termopsidae: Blattodea) in District Mansehra, Pakistan. *Proceedings of the Pakistan Academy of Sciences:B*, 60(2)-257-266. [http://doi.org/10.53560/PPASB\(60-2\)888](http://doi.org/10.53560/PPASB(60-2)888). (Impact Factor. **0.4**) (Co-author)

Bexultan Kazybay, **Ashfaq Ahmad** and Yingqiu Xie<sup>✉</sup>. (2022). Urgency of COVID-19 vaccination in adolescents: androgen and estrogen receptors view. **Travel Medicine and Infectious Diseases**. <https://doi.org/10.1016/j.tmaid.2022.102306>. (Impact Factor. **20.441**) (Co-author)

Aamir Saeed, Basharat Ahmad, Sidra Majaz, Faisal Nouroz, **Ashfaq Ahmad**<sup>✉</sup> and Yingqiu Xie<sup>✉</sup>. (2022). Targeting Omicron and other reported SARS-CoV-2 lineages by Potent inhibitors of Main Protease 3CL Mpro: Molecular Simulation Analysis. **Journal of Infection**. <https://doi.org/10.1016/j.jinf.2022.02.012>. (Impact Factor. **38.637**) (Corresponding)

Bexultan Kazybay<sup>†</sup>, **Ashfaq Ahmad**<sup>†</sup>, Chenglin Mu, Diana Mengdesh and Yingqiu Xie. (2021). Omicron N501Y mutation among SARS-CoV-2 lineages: In-silico analysis of potent binding to tyrosine kinase and hypothetical repurposed medicine. **Travel Medicine and Infectious Diseases**. <https://doi.org/10.1016/j.tmaid.2021.102242>.

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Department of Bioinformatics, Hazara University, Dhodhyal Mansehra, Pakistan 21300.

(Impact Factor. **20.441**) (Co-first author)

Xin Wang, Jiwen Pan, Liqing Chen, Roushan Li, Yu Han, Zihao Di, Bo Ling, **Ashfaq Ahmad**, Nuo Yang, Lixia Fan, Qian Li, Jifeng Zeng, Guiying Guo, Jiping Zheng. (2022). Prevalence, virulence-related genes and antimicrobial resistance of *Aeromonas* spp. from loach *Misgurnus anguillicaudatus* with skin ulcer and healthy controls in Southern China. **Aquaculture**. <https://doi.org/10.1016/j.aquaculture.2022.738040>.

(Impact Factor. **5.135**) (co-author)

Guixing Ma, Sanshan Wang, Kebin Wu, Weizhe Zhang, **Ashfaq Ahmad**, Quan Hao, Xiaoguang Lei, Hongmin Zhang. (2020). Structure-guided optimization of D-captopril for discovery of potent NDM-1 inhibitors. **Bioorganic & Medicinal Chemistry**. <https://doi.org/10.1016/j.bmc.2020.115902>.

(Impact Factor: **3.641**) (co-author)

Zain Ul Abideen†, **Ashfaq Ahmad**✉, Muhammad Usman, Sidra Majaz, Waqar Ali, Shumaila Noreen, Tariq Mahmood and Faisal Nouroz. (2020). Dynamics and conformational propensities of Staphylococcal CntA. **Journal of Biomolecular Structure and Dynamics**. <https://doi:10.1080/07391102.2020.1782263>. (Impact Factor. **3.392**)

**Ashfaq Ahmad**✉, Sidra Majaz and Faisal Nouroz. (2019). Two-component systems regulate ABC transporters in antimicrobial peptides production, immunity and resistance. **Microbiology**. <https://dx.doi.org/10.1099/mic.0.000823> (Impact Factor. **2.7**) (First author)

Hongmin Zhang, Guixing Ma, Yifan Zhu, Lingxiao Zeng, **Ashfaq Ahmad**, Changzhi Wang, Bo Pang, Huiyan Fang, Liqing Zhao, Quan Hao. (2018). Active Site Conformational Fluctuations Promote the Enzymatic Activity of NDM-1. **Antimicrob Agents and Chemotherapy**. <https://doi.org/10.1128/AAC.01579-18>.

(Impact Factor. **5.191**) (Co-author)

Yongfei Cai, Minyang Su, **Ashfaq Ahmad**, Xiaojie Hu, Lingyuan Kong, Xingqiang Chen, Chen Wang, Jianwei Shuai, Aidong Han (2017). Conformational dynamics of the essential sensor histidine kinase Walk. **Acta Crystallography D Struct Biol**. Oct 27;73(Pt 10):793-803. <https://doi:10.1107/S2059798317013043>. (Impact Factor. **7.652**) (Co-author)

Guixing Ma, Yifan Zhu, Zhicheng Yu, **Ashfaq Ahmad**, Zhang hongmin (2016). High resolution crystal structure of the catalytic domain of MCR-1. **Scientific Reports**. <https://doi:10.1038/srep39540>. (Impact Factor. **4.996**) (Co-author)

**Ashfaq Ahmad**, Yongfei Cai, Xingqing Chen, Jianwei Shuai, Aidong Han. (2015) Conformational dynamics of response regulator RegX3 from *Mycobacterium tuberculosis*. **PLoS ONE** 10(7). <https://doi:10.1371/journal.pone.0133389>.

(Impact Factor. **3.24**) (First author)

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Department of Bioinformatics, Hazara University, Dhodhyal Mansehra, Pakistan 21300.

Fawad Khan†, **Ashfaq Ahmad**✉, Abid Ali, Syed Shujait Ali, Tayyab ur Rehman (2017). Conformational Hotspots of Dengue Virus NS5 RdRp. **Current Bioinformatics**. 12. <https://doi.org/10.2174/1574893612666161214124827>. (Impact Factor. **3.543**) (Co-first author)

**Ashfaq Ahmad**✉, Ghosia Lutfullah, Roshan Ali (2011). Structure and Functional features of Streptolysin O. **Int J Bioinform Research and Applications**. 7(4):427-44. [https://doi: 10.1504/IJBRA.2011.043772](https://doi.org/10.1504/IJBRA.2011.043772). (Impact Factor. **0.366**) (First author)

Roshan Ali, Ghosia Lutfullah\*, Zahid Khan, and **Ashfaq Ahmad** (2011). Homology Modeling of Ring Necked Pheasant (Phasianus Colchicus, Galliformes) Minor Hemoglobin Component. **Int. J. Chem.Soc.Pak**. 33(3) 379-388. (Impact Factor. **0.536**) (Co-author)

Roshan Ali\*, Ghosia Lutfullah, Zahid Khan, and **Ashfaq Ahmad** (2011). Homology Modeling of Ring Necked Pheasant (Phasianus colchicus, Galliformes) major Hemoglobin component (HbA). **Int. J. Chem.Soc.Pak**. 33(4) 539-544. (Impact Factor. **0.536**) (Co-author)

Ajab Khan, Salman Akbar Malik, Abid Ali Khan, **Ashfaq Ahmad** and Roshan Ali\* (2011). Effects of Tobacco (Smoking and Snuffing) in Type 2 diabetic patients. **Int. J. Food Safety, Nut. and Pub. Health**. 4(2/3/4) 196-204. (Co-author)

Azra amjad, Farhat Amin, Ghosia lutfullah, **Ashfaq Ahmad** (2011). Homology Modeling of Bovine Kappa-Casein. **Int. J. Chem.Soc.Pak**. 33(3) 433. (Impact Factor. **0.536**) (Co-author)

## REFERENCES

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Dr. Aidong Han  
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University, China.  
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