Rashid Hussain, Ph.D.

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SUMMARY

I am a computational scientist with a Ph.D. in Chemistry, specializing in computational chemistry and cheminformatics. My expertise includes developing and applying advanced computational techniques such as molecular dynamics simulations, AI-based methods, and Python programming to analyze and interpret complex biological data. I am skilled in developing and customizing software tools, conducting data analysis, and visualizing results. My background in bioinformatics and experience with protein sequence analysis and molecular modeling align well with the focus on integrating and analyzing multi-omics data. I am highly motivated to contribute to cutting-edge research and collaborate with multidisciplinary teams to advance scientific understanding and innovation.

Go to: [Publications Research Experience] **Profiles Links**: [Google Scholar LinkedIn GitHub YouTube]

EDUCATION

01/2022 – 06/2022	**Visiting Research Student Program – The University of Manchester, UK** Areas: Structural Biology, Drug Design/Development
08/2017 – 03/2023	**Ph.D. in Chemistry – Forman Christian College, A Chartered University, Pakistan** Areas: Computational Chemistry, Bioinformatics Award: Magna Cum Laude [Award: Higher Honors]
09/2011 – 06/2013	**M.S. in Bioinformatics – COMSATS University Islamabad, Pakistan** Areas: Bioinformatics, Computer-Aided Drug Design (CADD)
09/2006 – 07/2010	**B.S. in Bioinformatics – COMSATS University Islamabad, Pakistan** Areas: Bioinformatics, Phylogenetic analysis

SKILLS

Bioinformatics Applications, Programming Experience – Python, Bash Scripting, MATLAB

- Developed and deployed VSpipe, a Python-based virtual screening tool, across Mac, Linux, and Windows in Prof. Tabernero's lab at the University of Manchester. Published in the International Journal of Molecular Sciences. [**Paper Link**] [**GitHub Link**] [**Demo Video**]
- Contributed to the development and validation of 'SPECTRUM' on MATLAB by implementing advanced bioinformatics techniques. Published in: *Scientific Reports – Nature*. [**Paper Link**] [**GitHub Link**] [**Video Tutorials**]
- Contributed to automating the Fibromyalgia (F420) Pipeline at Ayass BioScience by optimizing code and enhancing the user-interactive interface.
- Developed a PyMOL plugin at Deep Waters to analyze water thermodynamics using Grid Inhomogeneous Solvation Theory (GIST) via AMBER.

Data Science and Machine Learning Proficiency

- Developed and deployed a QSAR model for predicting bioactivity against Receptor Tyrosine Kinase, demonstrating machine learning expertise in anticancer drug prediction. [**GitHub Link**] [**Demo Video**]
- Completed a comprehensive 27-hour course covering key topics in data science and machine learning, including statistics, data cleaning, regression, classification, clustering, ensemble learning, and deep learning. [**GitHub Link**]

Expertise in structure-based drug design, molecular dynamics simulations, molecular modeling

- Advanced drug design by applying structure-based drug design, homology modeling, and MD simulations, resulting in the successful synthesis and assay of novel HCV NS3 protease inhibitors, with achievements published in RSC Advances. [**Paper Link**]
- Designed potent ligands and pharmacophores using structure- and ligand-based drug design approaches during Ph.D. research at Forman Christian College and as a Research Associate at Lahore University of Management Sciences.

Umbrella Sampling Simulations

- Performed simulations to study Alzheimer's Abeta(1-42) fibrils using PMF and ΔGbind calculations. Skilled in generating configurations, sampling space, and reconstructing PMF curves.

Solid background of Cheminformatics and Medicinal Chemistry

- Led interdisciplinary research to synthesize innovative HCV NS3 protease inhibitors, combining computational chemistry, medicinal chemistry, MD simulations, and biological assays for comprehensive insights. Published in: *RSC advances* [**Paper Link**]; *Pure and Applied* Chemistry [**Paper Link**]; *J. Comput. Biophys. Chem* [**Paper Link**]

Leadership Skills and Teamwork

- Led a team to achieve Good Manufacturing Practice certification at A.Z. Pharmaceuticals, demonstrating strong leadership in ensuring quality compliance.
- Organized and actively participated in a two-day workshop on Computational Tools for Drug Design and Discovery, hosted by Forman Christian College, ACS Punjab Chapter, and ORIC. [**Link**]

Voluntary Work

- Trained postgraduate students and faculty on using Mendeley for automatic citations and bibliography management through a conducted webinar. [**Webinar Link**] [**Homology Modeling**] [**Learn to perform docking**]
- Led a team to train teachers in online education at The Educators during the COVID-19 pandemic.
- Volunteered as a teaching assistant for a "High-Performance Computing" course with The Carpentries, a non-profit organization, providing remote support. [**Certificate**]

RESEARCH EXPERIENCE

07/2023 – Present **Bioinformatician – Ayass BioScience LLC, TX, USA (Remote)**

- Optimized code and enhanced the user interface of the Fibromyalgia (F420) Pipeline supporting the goal of utilizing transcriptome AI for disease characterization and treatment options.
- Applied bioinformatics and ML techniques to perform transcriptome analysis.

11/2021 – 04/2022 **Software Developer (Contractor) – Deep Waters, LLC, NY, USA (Remote)**

- Successfully developed a PyMOL plugin for analyzing water thermodynamics using Grid Inhomogeneous Solvation Theory (GIST) through AMBER.

01/2022 – 06/2022 **Visiting Postgraduate Researcher – The University of Manchester (UoM), UK (On-site)**

- Successfully developed an open-source Python-based virtual screening toolkit with a cross-platform user-interactive GUI interface.

02/2016 – 12/2019 **Research Assistant – A.Z. Pharmaceuticals Company Limited, PK**

- Finalized a structure-based drug design pipeline and modeled pharmacophores using ligand-based approaches, supporting research groups under the Higher Education Commission of Pakistan's joint venture initiative.
- Secured cGMP certification from the drug regulatory authority, showcasing leadership in compliance.
- Collaborated with universities to advance industry-university partnerships, enhancing R&D efforts.

02/2015 – 01/2016 **Research Associate – Biomedical Informatics Research Laboratory, LUMS, PK**

- Designed the complete GUI for the MATLAB-based SPECTRUM toolbox and contributed to the intact mass tuner algorithm for protein identification from databases.
- Developed a ligand-based pharmacophore for HCV, enhancing drug discovery.
- Managed lab operations and compiled annual reports as Lab Chief, ensuring efficient workflow and accurate documentation.
- Played a key role in paper manuscript preparation, facilitating successful publication.

06/2014 – 01/2015 **Research Intern – National Center of Bioinformatics, Quaid-e-Azam University, PK**

- Gained hands-on experience with experimental techniques, enhancing practical research skills.
- Applied bioinformatics tools to identify conserved regions in Zebrafish, advancing genomic analysis.

1) **Hussain, R.**, Hackett, A.S., Álvarez-Carretero, S., Tabernero, L. (2024). "VSpipe-GUI, An Interactive Graphical User Interface for Virtual Screening and Hit Selection." *International Journal of Molecular Sciences*. Vol. 25, No. 04, pp. 2002. DOI: 10.3390/ijms25042002. [Link] [GitHub Link]

2) **Hussain, R.**, Haider, Z., Khalid, H., Fatmi, M. Q., Carradori, S., Cataldi, A., Zara, S. (2023). "Computational medicinal chemistry applications to target Asian-prevalent strain of hepatitis C virus." *RSC advances*. Vol. 13, No.43, pp. 30052-30070. DOI: 10.1039/D3RA04622B. [Link]

3) **Hussain, R.**, Khalid, H., Fatmi, M. Q. (2022). "HCV genotype-specific drug discovery through structure-based virtual screening." *Pure and Applied* Chemistry. DOI: 10.1515/pac-2021-1104. [Link]

4) **Hussain, R.**, Khalid, H., Fatmi, M. Q. (2021). "Molecular modelling approach of Serine Protease NS3-4A genotype 3a as a potential drug target of Hepatitis C Virus: Homology Modelling and Virtual Screening Study." *J. Comput. Biophys. Chem.,* Vol. 20, No. 06, pp. 631-639. [Link]

5) Khalid, H., **Hussain, R.**, & Hafeez, A. (2020). "Virtual screening of piperidine-based small molecules against COVID-19". *Lab-in-Silico*, Vol. 01, No. 02, pp. 50-55. DOI: 10.22034/lins20012050. [Link]

6) Basharat, A. R., Iman, K., Bibi, Z., **Hussain, R.,** Kabir, H. G., Shahid, A., Humayun, M., Hayat, H. A., Mustafa, M., Shoaib, M. A., Ullah, Z., Zarina, S., Ahmed, S., Uddin, E., Hamera, S., Ahmad, F., & Chaudhary, S. U. (2019). " SPECTRUM – A MATLAB toolbox for proteoform identification from top-down proteomics data." *Scientific Reports - Nature*, Vol. 09, Issue 01, pp. 1 -14. DOI: 10.1038/s41598-019-47724-1. [Link] [GitHub Link]

7) Ashraf, M. U., Iman, K., Khalid, M. F., Shafi, T., Salman, H. M., Rafi, M., Javaid, N., **Hussain**, **R.**, Ahmad, F., Shahzad-ul-Hussan, S., Mirza, S., Shafiq, M., Afzal, S., Idrees, M., Hamera, S., Anwar, S., Qazi, R. Qureshi, S. A., Chaudhary, S. U. (2019). " Evolution of efficacious pangenotypic Hepatitis C Virus therapies." *Medicinal Research Reviews*, Vol. 39, No. 03, pp. 1091-1136. DOI: 10.1002/med.21554. [Link]

8) Arfan, M., Siddiqui, S.Z., Abbasi, M.A., ur Rehman, A., Shah, S.A.A., Ashraf, M., Rehman, J., Saleem, R. S. Z., Khalid, H., **Hussain, R.**, Khan, U. (2018). "Synthesis, in vitro and silico studies of S-alkylated 5-(4-methoxyphenyl)-4-phenyl-4H-1, 2, 4-triazole-3-thiols as cholinesterase inhibitors." *Pak. J. Pharm. Sci*, Vol. 31, No. 6, pp. 2697-2708. [Link]

9) Khalid, H., Abbasi, M. A., **Hussain, R.,** Malik, A., Ashraf, M., & Fatmi, M. Q. (2017). "Synthesis, spectral analysis and biological evaluation of 5-Substituted 1,3,4-oxadiazole-2-yl-4-(piperidin-1-ylsulfonyl)benzyl sulfide." *Emerging Trends in Chemical Sciences*, Chapter-14 in Springer books, pp. 221-238. DOI: 10.1007/978-3-319-60408-4_14. [Link]

10) Abubakar, M., Bibi, A., **Hussain, R.**, Bibi, Z., Gul, A., Bashir, Z., Arshad, S.N., Uppal, S.U., Chaudhary, S. U. (2016). "Towards Providing Full Spectrum Antenatal Health Care in Low and Middle Income Countries." Proceedings of 9th International Joint Conference on Biomedical Engineering Systems and Technologies (BIOSTEC 2016), Vol 5 (HEALTHINF), pp. 478-483, 2016, Rome, Italy. [Link]

11) Mumtaz, S., **Hussain, R.,** Rauf, A., Fatmi, M. Q., Bokhari, H., Oelgemöller, M., & Qureshi, A. M. (2014). "Synthesis, molecular docking studies, and in vitro screening of barbiturates/thiobarbiturates as antibacterial and cholinesterase inhibitors." *Medicinal Chemistry Research*. Vol. 23, No. 06, pp. 2715-2726. DOI: 10.1007/s00044-013-0847-2. [Link]

12) Khalid, H., Rehman, A. U., Abbasi, M. A., **Hussain, R.,** Khan, K. M., Ashraf, M., Ejaz, S.A., & Fatmi, M. Q. (2014). "Synthesis, biological evaluation, and molecular docking of N'-(Aryl/alkylsulfonyl)-1-(phenylsulfonyl) piperidine-4-carbohydrazide derivatives." *Turkish Journal of Chemistry*. Vol. 38, No. 02, pp. 189-201. DOI: 10.3906/kim-1303-89. [Link]

HONORS AND AWARDS

03/2023	**Magna cum Laude,** by FCCU, for getting distinction in Ph.D.
02/2022	**Best Poster Award,** by FCCU, for winning the poster presentation competition
01/2021	**International Research Support Initiative Program (IRSIP),** by Higher Education Commission of Pakistan
07/2015	**Best Poster Award**, by Institute of Space Technology, Pakistan
02/2015	**Marathon Race Winner**, Lahore University of Management Science (LUMS), Pakistan

INTELLECTUAL PROPERTY

Copyright filed with Intellectual Property Organisation of Pakistan:

04/2023	**GROMACS Molecular Dynamic Simulator**	Application no. 1153/2023	in-process
07/2023	**BIOPREDICT – Insilico Bioactivity Predictor**	Application no. 2183/2023	in-process

PEER REVIEWER

10/2023 – Present	**Royal Society of Chemistry – RSC Advances**	ISSN: 2046-2069
05/2022 – Present	**Molecular Diversity – Springer Nature**	ISSN: 1381-1991
07/2023 – Present	**International journal of biological macromolecules**	ISSN: 0141-8130

MEMBERSHIPS

10/2023 – Present	**Royal Society of Chemistry**	ID: 755587	Affiliate
05/2022 – Present	**American Chemical Society**	ID: 33206538	Standard
01/2024 – Present	**ACS Computers in Chemistry Division**		

CERTIFICATIONS

10/2022	**Certified Carpentries Instructor**	Carpentries, USA	[**Certificate**]
07/2022	**The Unix Workbench**	Johns Hopkins University, USA	[**Certificate**]
07/2022	**What is Data Science?**	IBM	[**Certificate**]
01/2020	**Molecular Modeling in Drug Discovery**	Schrödinger	[**Certificate**]
03/2021	**Python**	Online course, 1100 minutes	
06/2019	**Computer-Aided Drug Design**	NPTEL India online course, 900 minutes	

TEACHING EXPERIENCE

08/2021 – 03/2022	**Voluntary Teaching Assistant**	**The Carpentries, California, USA. Remote**
	High-Performance Computing: Provided teaching assistance and help in practical exercises	
03/2019 – 02/2020	**Visiting Faculty**	**Minhaj University, PK**
	Bioinformatics: Delivered 30 lectures, conducted 16 labs of the course, wrote and graded exams	
02/2015 – 01/2016	**Teaching Assistant**	**Lahore University of Management Sciences, PK**
	Computational Biology: Conducted 16 labs, wrote and graded lab exams, graded lab assignments	
	Protein Informatics: Conducted 12 labs, wrote and graded lab exams, graded lab assignments	

CONFERENCES (Selected)

- *Workshop*: Khalid, H. Fatmi, M. Q., **Hussain, R.** (Oct 17-18, 2023). "Two Days Workshop on Computational Tools for Drug Design and Discovery". Forman Christian College (A Charted University), Pakistan.
- *Webinar*: **Hussain, R.**, Khalid, H. (Sep 28, 2020). "References made easy using Mendeley". Forman Christian College (A Charted University), Pakistan.
- *Talk*: Basharat, A.R., Bibi, Z., **Hussain, R.**, Kabir, H. G., Shahid, A., Humayun, M., Hayat, H. A., Mustafa, M., Shoaib, M. A., Ullah, Z., Zarina, S., Ahmed, S., Uddin, E., Hamera, S., Ahmad, F., Chaudhary, S. U. (2017)." SPECTRUM: A MATLAB Toolbox for Identifying Proteins from Top-down Proteomics Data."16th Annual Human Proteome Organization World Congress (HUPO), Dublin, Ireland.
- *Talk*: Abubakar, M., Bibi, A., **Hussain, R.**, Bibi, Z., Gul, A., Bashir, Z., Arshad, S. N., Uppal, M. A., Chaudhary, S. U. (2016). "Towards Providing Full Spectrum Antenatal Health Care in Low and Middle-Income Countries." 9th International Joint Conference on Biomedical Engineering Systems and Technologies (BIOSTEC 2016), Vol 5 (HEALTHINF), pp.478-483, 2016, Rome, Italy.
- *Poster*: **Hussain, R.**, Khalid, H., Fatmi, M.Q., (2022)." Computer-aided drug design and synthesis of HCV NS3 protease inhibitors. "American Chemical Society Fall Meeting IL Chicago, USA.
- *Poster*: **Hussain, R.**, Khalid, H., Fatmi, M.Q., (2022)." Computer-aided drug design and synthesis of HCV NS3 protease inhibitors. " Forman Christian College (A Charted University), Pakistan. (3rd prize).
- *Poster*: **Hussain, R.**, Kabir, G. H., Chaudhary, S. U. (2015). "Towards an Accurate Measurement of Intact Protein Mass in High-Resolution Mass Spectrometry." 3rd National Computational Science Conference (NCSC), Islamabad, Pakistan. (2nd prize in project presentation competition).