Rashid Hussain, Ph.D.

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SUMMARY

I am a computational chemist with a Ph.D. in Chemistry, specializing in bioinformatics and computer-aided drug design. My expertise includes structure-based and fragment-based design, ligand-based design with ML and QSAR models, SAR analysis, and ADME/Tox property calculation. I am proficient in Python scripting, data pipelining tools, molecular modeling, and virtual screening using protein X-ray structures and ligand-based methods. With experience in protein sequence analysis and homology modeling across various protein classes, I have contributed to diverse research projects and developed computational tools. Highly motivated and committed to advancing the scientific community, I bring a strong foundation in drug discovery from both academic and industrial settings.

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

EDUCATION

Jan 2022 – Jun 2022	**Visiting Research Student Program, The University of Manchester, UK**	
	Research Focus:	Structural Biology, Drug Design/Development
2017 – 2022	**Ph.D. Chemistry**	**Forman Christian College, A Chartered University (FCCU), Pakistan**
	Research Focus:	Computational Chemistry, Bioinformatics Award: Magna Cum Laude [Award: Higher Honors]
2011 – 2013	**MS Bioinformatics**	**COMSATS University Islamabad, Pakistan**
	Research Focus:	Bioinformatics, Computer-Aided Drug Design (CADD)
2006 – 2010	**BS Bioinformatics**	**COMSATS University Islamabad, Pakistan**
	Research Focus:	Bioinformatics, Phylogenetic analysis

SKILLS

Bioinformatics Applications, Programming Experience – Python, Bash Scripting, MATLAB, C++s

- Successfully developed VSpipe, a cross-platform, Python-based application for virtual screening and hit selection at Prof. Tabernero's lab, University of Manchester. Deployed on Mac, Linux and Windows within Tabernero's lab. Published in: *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**]
- Applied advanced bioinformatics skills as a Bioinformatician at Ayass BioScience, LLC, leading the development of a Python-based GUI interface for the Fibromyalgia (F420) Pipeline.
- Demonstrated expertise as a Software Developer at Deep Waters, LLC, by creating a PyMOL plugin for analyzing water thermodynamics using Grid Inhomogeneous Solvation Theory (GIST) through AMBER. GIST is implemented in AmberTools. [**Ref**]

Machine Learning

- Designed and deployed a successful QSAR model, a Machine learning-based prediction app for predicting bioactivity against the target Receptor Tyrosine Kinase involved in cancer, showcasing expertise in machine learning for accurate anticancer drug activity prediction. [**GitHub Link**] [**Demo Video**]

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

- Conducted doctoral research on structure-based drug design, homology modeling, MD simulations, and free energy calculations. Advanced drug design with MD simulations, leading to successful synthesis and assay of novel HCV NS3 protease inhibitors at Forman Christian College. Published in *RSC Advances*. [**Paper Link**]
- Applied molecular docking for designing potent ligands and pharmacophores, contributing to drug design progress during Ph.D. research at Forman Christian College and as a Research Associate at Lahore University of Management Sciences.

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**]

Dedicated Scientist

- I have contributed to 12 publications in prestigious peer-reviewed journals with 84 citations. [**Google Scholar**]

Cheminformatics

- Applied cheminformatics techniques, including ligand-based drug design and pharmacophore modeling, leading to significant advancements in the structure-based drug design pipeline during the tenure as a Research Assistant at A.Z. Pharmaceuticals Company Limited.

Leadership Skills and Teamwork

- Facilitated Good Manufacturing Practice certification by playing an active role with a group of professionals at A.Z. Pharmaceuticals, showcasing leadership in quality compliance.
- Collaborated with a group of scientists for writing review on Hepatitis C Virus. Published in: *Medicinal Research Reviews* [**Paper Link**]
- Played an active role in a 2-days workshop on Computational Tools for Drug Design and Discovery organized by Forman Christian College Department of Chemistry in collaboration with the American Chemical Society (ACS) Punjab Chapter and the Office of Research, Innovation, and Commercialization (ORIC). [**Link**]

Voluntary Work

- Conducted a webinar to train postgraduate students and faculty members on how to use Mendeley for automatic citations and bibliography management. [**YouTube Link**]
- Recorded tutorials on YouTube for homology modeling and learning to perform docking. [**Homology Modeling**] [**Learn to perform docking**]
- Led a team to train teachers in online education during the COVID-19 pandemic at a local school, The Educators.
- Provided voluntary assistance as a teaching assistant for a course titled "High-Performance Computing" through the non-profit organization platform, The Carpentries, based in California, USA, conducted remotely. [**Certificate**]

WORK EXPERIENCE

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

- Developed a Python-based GUI interface for Fibromyalgia pipeline.
- Involved in projects of transcriptome analysis

Nov 2021 – Apr 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.

Jan 2022 – Jun 2022 **Visiting Postgraduate Researcher – The University of Manchester (UoM), UK**

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

Aug 2021 – Mar 2022 **Voluntary Teaching Assistant – The Carpentries, California, USA. Remote**

- *High-Performance Computing***:** Voluntary helper to mentor the learners and answer their questions

Mar 2019 – Feb 2020 **Visiting Faculty – Minhaj University, PK**[1]

- *Bioinformatics*: Delivered 30 lectures, conducted 16 labs of the course, wrote and graded exams

Jul 2016 – Dec 2019 **Research Assistant – A.Z. Pharmaceuticals Company Limited, PK**

- Completed Structure-based drug design pipeline
- Modeled pharmacophore through Ligand-based drug design
- Provided facilitation for academia-industry research collaboration
- Played key role in cGMP certificate award by drug regulatory authority

[1] PK: Pakistan

Feb 2015 – Jan 2016 **Research Associate – Biomedical Informatics Research Laboratory, LUMS, PK**

- Designed complete GUI of MATLAB-based toolbox, SPECTRUM
- Successfully designed ligand-based pharmacophore of HCV
- Lab management and compiling of annual lab reports as a lab chief
- Key role in paper manuscript preparation

Feb 2015 – Jan 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

Jun 2014 – Jan 2015 **Research Intern – National Center of Bioinformatics, Quaid-e-Azam University, PK**

- Acquired hands-on experience in experimental techniques
- Used bioinformatics tools to find conserved regions in Zebrafish

Jul 2013 – Mar 2014 **Subject Specialist / Tutor – Keys College, PK**

- Acquired hands-on experience in experimental techniques
- Used bioinformatics tools to find conserved regions in Zebrafish

PUBLICATIONS *Number: 12* *Citations: 85*

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

13) 2023 **Magna cum Laude,** by FCCU[2], for getting distinction in Ph.D.
14) 2022 **Best Poster Award,** by FCCU, for winning the poster presentation competition
15) 2021 **International Research Support Initiative Program (IRSIP),** by Higher Education Commission of Pakistan
16) 2015 **Best Poster Award**, by Institute of Space Technology, Pakistan
17) 2015 **Marathon Race Winner**, Lahore University of Management Science (LUMS), Pakistan

INTELLECTUAL PROPERTY

Copyright filed with Intellectual Property Organisation of Pakistan:

1) GMDS - GROMACS Molecular Dynamic Simulator. Apr 2023. Application no. 1153/2023 *in process*
2) BIOPREDICT – Insilico Bioactivity Predictor. Jul 2023. Application no. 2183/2023 *in process*

PEER REVIEWER

Oct 2023 – Present	**Royal Society of Chemistry – RSC Advances**	ISSN: 2046-2069
May 2022 – Present	**Molecular Diversity – Springer Nature**	ISSN: 1381-1991

MEMBERSHIPS

Oct 2023 – Present	**Royal Society of Chemistry**	ID: 755587	Affiliate
May 2022 – Present	**American Chemical Society**	ID: 33206538	Standard
Jan 2024 – Present	**ACS Computers in Chemistry Division**		

CERTIFICATIONS

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

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.

[2] FCCU: Forman Christian College, A Chartered University

(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).

LIST OF REFEREES

1) **Dr. Hira Khalid**, Associate Professor, Medicinal Chemistry
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Email: hirakhalid@fccollege.edu.pk

2) **Dr. M. Qaiser Fatmi**, Professor, Bioinformatics & Computational Chemistry
Relationship: MS research supervisor
Address: Bio Sciences Department, COMSATS University Islamabad, Islamabad 45550, Pakistan.
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Email: qaiser.fatmi@comsats.edu.pk

3) **Professor Lydia Tabernero**, Professor of Structural Biology & Drug Discovery,
Relationship: Supervisor during research fellowship (IRSIP)
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Tel: +44 (0) 161 275 7794
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