Rashid Hussain

Ph.D. (Chemistry)

Male, 36 years old

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Interests

- Bioinformatics & Cheminformatics
- Machine Learning & Deep Learning
- Artificial Intelligence
- Cloud Computing
- Computer-aided drug design
- MD Simulations

Skills

Programming:

- C, Python ●●●●●
- Bash Scripting ●●●●●
- MATLAB, SQL, R ●●●●○
- Linux ●●●●●
- GitHub, LaTeX ●●●●●
- C++, JAVA ●●●○○

CAAD Tools:

- Autodock Vina, DOCK6 ●●●●●
- GROMACS, AMBER ●●●●●
- MOE, PyMOL ●●●●○
- Schrödinger Suite ●●●●○
- RDKit ●●●○○

Machine Learning:

- Pandas, NumPy ●●●○○
- Scikit-learn ●●●○○
- KNIME, Streamlit ●●○○○

Research Experience

Jul 2023 – Present
Bioinformatician (Contractor) — **Ayass BioScience LLC, TX, USA**
Remote, Part time
Project: GUI of Fibromyalgia (F420) Pipeline for Transcriptome analysis.
Responsibilities: Developed a Python-based GUI interface for Fibromyalgia pipeline.

Nov 2022 – May 2023
Software Developer (Contractor) — **Deep Waters, LLC, NY, USA**
Remote, Part time
Project: GUI interface for Deep Waters GIST
Responsibilities: Successfully developed a PyMOL plugin for analyzing water thermodynamics using Grid Inhomogeneous Solvation Theory (GIST) through AMBER.

Jan 2022 – Jun 2022
Visiting Postgraduate Researcher — **University of Manchester, UK**
In campus: Jan 2022 - Apr 2022; Remote: Apr 2022 - Jun 2022
Project: VSpipe, an Integrated Resource for Virtual Screening and Hit Selection.
Responsibilities: Successfully developed an open-source Python-based virtual screening toolkit with a cross-platform user-interactive GUI interface.

Jul 2016 – Dec 2019
Research Assistant — **A.Z. Pharmaceuticals Company Limited, PK**
Focus: Research and management tasks.
Responsibilities:
- 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 authority

Feb 2015 – Jan 2016
Research Associate — **Lahore University of Management Sciences, PK**
Projects: 1) Higher Education Commission funded project on Hepatitis C Virus drug design. 2) MATLAB-based toolbox for top-down proteomics data.
Responsibilities:
- 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

Jun 2014 – Jan 2015
Research Intern — **Center of Bioinformatics, Quaid-e-Azam University, PK**
Project: Computational methods to detect conserved non-genic elements in zebrafish.
Responsibilities:
- Performed in-vivo testing on Zebrafish
- Acquired hands-on experience in experimental techniques
- Used bioinformatics tools to find conserved regions in Zebrafish

Education

2017 – 2022
Ph.D. in Chemistry — **Forman Christian College (A Chartered University), PK**
Title: Computer-aided drug design and synthesis of HCV NS3 protease inhibitors.
Supervisors: Dr. Hira Khalid and Prof. M. Qaiser Fatmi.
Computational Chemistry | MD Simulations | Cheminformatics

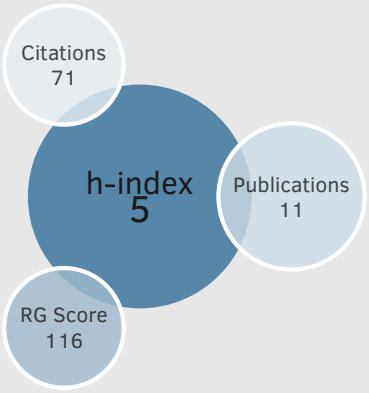
2011 – 2013
M.S. in Bioinformatics — **COMSATS University Islamabad, PK**
Title: Rationalizing ligand-protein interactions and identifying cholinesterase inhibitors using computational methods.
Supervisor: Prof. M. Qaiser Fatmi
Structure-based drug design | Molecular docking

2006 – 2010
B.S. in Bioinformatics — **COMSATS University Islamabad, PK**
Title:Phylogenetic analysis of major protein-coding genes of *Geminiviridae*: A single-stranded DNA virus family.
Supervisor: Dr. Muhammad Zeeshan Hyder
phylogenetic tree | Bioinformatics tools

Short Bio

I'm a passionate Computational Chemist with a Ph.D. in Chemistry, specializing in structure-based drug design, molecular modeling, MD simulations, and virtual screening. Proficient in Python, Linux, and Bash scripting, I've successfully bridged scientific innovation with practical applications in both academia and industry. I'm committed to advancing Medicinal Chemistry and am eager to collaborate on projects that push the boundaries of drug discovery and computational chemistry. Let's connect and work together to make a positive impact on healthcare.

Metrics



Profiles

Languages

Urdu (Mother Tongue)

English (IELTS:7.0, 2017)

German (Intro. course, 2011)

Peer Reviewer

Oct 2023 - Present — Royal Society of Chemistry – RSC Advances. ISSN: 2046-2069

May 2022 - Present — Molecular Diversity – Springer Nature. ISSN: 1381-1991

Teaching Experience

Carpentries, USA, Remote — **High-Performance Computing (HPC)** Fall'21, Spring'22
Teaching Assistant: Voluntary helper to mentor the learners and answer their questions. Provided technical support to the students.

Minhaj Univ., PK — **BIO 603: Bioinformatics** Spring'19, Fall'19
Visiting Faculty: Designed/presented 30 lectures and conducted 8 labs to B.S. students at Biochemistry department.

BIO 610: Bioinformatics Spring'19, Fall'19
Visiting Faculty: Designed/presented 30 lectures and conducted 8 labs to M.Sc. students at Biochemistry department.

LUMS Univ., PK — **CS 330/BIO 331: Computational Biology II** Spring'15, Fall'15
Teaching Assistant: Conducted 16 labs, wrote, graded lab exams and class assignments.

BIO 435: Protein Informatics Spring'15, Fall'15
Teaching Assistant: Conducted 12 labs, wrote, graded lab exams and class assignments.

YouTube — **How to model protein using Modeller** Since May 26, 2020
Learn to perform Molecular Docking, CADD Since May 24, 2020

Academic Supervision

2015–2016 — Supervised and trained four summer interns on using computer aided drug design applications. B.S.

2018–2022 — Supervised students in doctoral supervisor's lab and applied computational chemistry approaches in their medicinal chemistry projects. Also helped them in academic writing. B.S., M.S.

Honours and Awards

Mar 2023 — **Magna cum Laude** Distinction in Ph.D.
FCCU, PK

Nov 2022 — **Best Poster Award** CADD and synthesis of HCV NS3 protease inhibitors
FCCU, PK

Oct 2021 — **International Research Support Initiative Program** Research fellowship (9800 USD), Higher Education Commission, PK

May 2015 — **Best Poster Award** Accurate Measurement of Intact Protein Mass in HRMS
Institute of Space Technology, PK

Invited Talks

May 2021 — **Virtual Conference on Chemistry & its App.** University of Mauritius, MA
Talk on molecular modelling approach of serine protease NS3-4A genotype 3a as a potential drug target of Hepatitis C Virus.

Sep 2020 — **References made easy using Mendeley** Webinar, Int.
Introductory and practical demonstration of using Mendeley to manage references and bibliography in academic writing.

Dec 2018 — **6th Int. Drug Design Congress** Bahcesehir Univ., TR
Talk on HCV genotype-Specific drug discovery through structure and ligand-based virtual screening.

Structure-based Drug Design

Molecular Modeling

Molecular Docking

MD Simulations

Bioinformatics

Cheminformatics

Machine Learning

Python

MATLAB

Publications

Published

1. **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. [Open]

2. **Hussain, R.**, Khalid, H., Fatmi, M. Q. (2022). "HCV genotype-specific drug discovery through structure-based virtual screening." *Pure and Applied Chemistry*. Vol. 94, No. 7, pp. 809-818. DOI: 10.1515/pac-2021-1104. [Open]

3. **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. DOI: 10.1142/s273741652150037x. [Open]

4. 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. [Open]

5. 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, p. 11267. DOI: 10.1038/s41598-019-47724-1. [Open]

6. 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. [Open]

7. 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. PMID: 30587482. [Open]

8. Khalid, H., Abbasi, M. A., **Hussain, R.**, Malik, A., Ashraf, M., Fatmi, M. Q. (2018). "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. [Open]

9. 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. [Open]

10. 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. [Open]

11. 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. [Open]

In Prep

1. **Hussain, R.**, Hackett, A., Khalid, H., Álvarez-Carretero, S., Tabernero, L. "Vspipe 2.0, an integrated resource for virtual screening and hit selection with a graphical user interface."

Software

1. 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. SPECTRUM: A MATLAB Toolbox for Identifying Proteins from Top-down Proteomics Data. [GitHub Link]

2. **Hussain, R.** COVID-19 predictor - A machine learning-based QSAR model for COVID19 Replicase Polyprotein to predict pIC50 of a given compound – Successfully developed and deployed. [GitHub Link]

Conferences

Talks

1. 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.
2. 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." Trends and Prospects in Molecular Biosciences, Punjab University, 2017, Lahore, Pakistan.
3. 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.
4. Bibi, Z., Basharat, A.R., **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. (2016). "LUMSProT: A MATLAB Toolbox for Identifying Proteins from Top-down Proteomics Data." Biosymposium, Lahore University of Management Sciences, Lahore, Pakistan.

Posters

1. **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.
2. **Hussain, R.**, Khalid, H., Fatmi, M.Q., (2022)." Computer-aided drug design and synthesis of HCV NS3 protease inhibitors. "Forman Christian College University, Pakistan. *(3rd prize in project presentation competition)*
3. **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)*.
4. **Hussain, R.**, Fatmi, M. Q. (2013). "Identification of Prospective Cholinesterase Inhibitors using Structure-Based Virtual Screening Approach." Poster presented at Chemistry Department, COMSATS Institute of Information Technology, Abbottabad, Pakistan.
5. **Hussain, R.**, Hyder, M.Z. (2010). "Phylogenetic analysis of major proteins coding genes of Geminiviridae: A single-stranded DNA virus family." Poster presented at Industrial Exhibition. COMSATS University Islamabad, Islamabad, Pakistan.

Professional Societies

2023	**Royal Society of Chemistry** (Member ID: 755587)	Affiliate member
2022	**American Chemical Society** (Member ID: 33206538)	Student member

Certifications

2022	**Certified Carpentries Instructor** Certificate	The Carpentries, USA
2022	**The Unix Workbench** Certificate	Johns Hopkins University
2022	**What is Data Science?** Certificate	IBM
2020	**Introduction to Molecular Modeling in Drug Discovery** Certificate	Schrödinger

Online Courses

2022	**Machine Learning**	DataCamp
2021	**Python**	YouTube Course
2019	**Computer-Aided Drug Design**	NPTEL India online course