Rashid Hussain

Software Developer at Deep Waters NYC, LLC, USA

Male, 35 years old

Lahore, Punjab, Pakistan

(92)3155235956

rashid.bioinfo@gmail.com

rashid-bioinfo.github.io

0000-0002-6586-7241

Interests

- Structure based drug design
- MD Simulations
- Cloud Computing
- Machine Learning and AI
- Cheminformatics

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

Nov 2022 – Present — **Software Developer** — **Deep Waters NYC, LLC, USA**
Remote, Part time
Project: GUI interface for Deep Waters GIST
Responsibilities: To develop a PyMOL plugin for analyzing water thermodynamics using Grid Inhomogeneous Solvation Theory through AMBER.

Jan 2022 – Dec 2022 — **Visiting Postgraduate Researcher** — **University of Manchester, UK**
In campus: Jan 2022 - Apr 2022; Remote: Apr 2022 - Dec 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

Postgraduate Studies

2017 – ongoing — **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

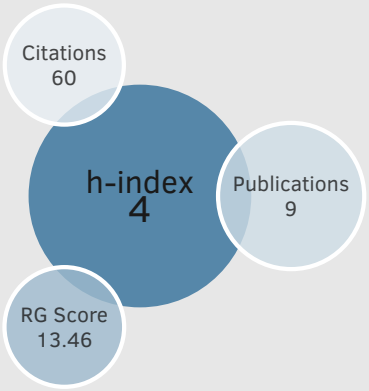
Undergraduate Study

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 am a software developer at Deep Waters NYC, USA. I am developing a PyMOL plugin for analyzing water thermodynamics using Grid Inhomogeneous Solvation Theory through AMBER. Previously, I have successfully developed a graphical user interface of a pipeline, VSpipe, an integrated resource for virtual screening and hit selection. I am a passionate researcher in computational medicinal chemistry. I have rich experience working in computational chemistry and bioinformatics domains. My career aspiration is to play my role in improving healthcare through extension and innovations in IT.

Metrics



Profiles

Languages

Urdu (Mother Tongue)

English (IELTS:7.0, 2017)

German (Intro. course, 2011)

Personal

I am a proud father of two kids, Zohan and Azaan. Zohan is three and half years old and Azaan's first birthday is in October 2022. I consider myself lucky to have a supportive and loving partner. She is an ultrasound specialist and doing her master's. My life philosophy is to contribute regardless of what capacity you are in, be it in science or society.

Peer Reviewer

Journal	Molecular Diversity – Springer Nature. ISSN: 1381-1991

Teaching Experience

Carpentries, USA, Remote	**High-Performance Computing (HPC)** *Teaching Assistant*: Voluntary helper to mentor the learners and answer their questions. Provided technical support to the students.	Fall'21, Spring'22
Minhaj Univ., PK	**BIO 603: Bioinformatics** *Visiting Faculty*: Designed/presented 30 lectures and conducted 8 labs to B.S. students at Biochemistry department.	Spring'19, Fall'19
	BIO 610: Bioinformatics *Visiting Faculty*: Designed/presented 30 lectures and conducted 8 labs to M.Sc. students at Biochemistry department.	Spring'19, Fall'19
LUMS Univ., PK	**CS 330/BIO 331: Computational Biology II** *Teaching Assistant*: Conducted 16 labs, wrote, graded lab exams and class assignments.	Spring'15, Fall'15
	BIO 435: Protein Informatics *Teaching Assistant*: Conducted 12 labs, wrote, graded lab exams and class assignments.	Spring'15, Fall'15
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

Nov 2022	Best Poster Award	FCCU, PK
Oct 2021	International Research Support Initiative Program (9800 USD)	Higher Education Commission, PK
May 2015	Best Poster Award	Institute of Space Technology, PK
Feb 2015	Marathon Race Winner	LUMS Univ., PK

Invited Talks

May 2021	**Virtual Conference on Chemistry & its App.** Talk on Molecular Modelling Approach of Serine Protease NS3-4A Genotype 3a as a Potential Drug Target of Hepatitis C Virus.	University of Mauritius, MA
Sep 2020	**References made easy using Mendeley** Introductory and practical demonstration of using Mendeley to manage references and bibliography in academic writing.	Webinar, Int.
Dec 2018	**6th Int. Drug Design Congress** Talk on HCV Genotype-Specific Drug Discovery through Structure and Ligand based Virtual Screening.	Bahcesehir Univ., TR

References

Ref. 1	**Prof. Lydia Tabernero** Lydia.Tabernero@manchester.ac.uk	University of Manchester, UK
Ref. 2	**Prof. M. Qaiser Fatmi** qaiser.fatmi@comsats.edu.pk	COMSATS Univ., PK
Ref. 3	**Dr. Hira Khalid** hirakhalid@fccollege.edu.pk	FCCU Univ., PK

Structure-based Drug Design
Molecular Modeling
Molecular Docking
MD Simulations
Bioinformatics
Cheminformatics
Machine Learning
Python
MATLAB

Publications

Published

1. **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. [Open]
2. **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]
3. 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]
4. 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. [Open]
5. 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]
6. 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]
7. 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. [Open]
8. 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]
9. 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. (2022). "Vspipe 2.0, an integrated resource for virtual screening and hit selection with a graphical user interface."
2. **Hussain, R.**, Khalid, H., Fatmi, M. Q. (2022). "Computer-aided drug design and synthesis of HCV NS3 protease inhibitors".

Published 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

American Chemical Society (ACS Member Number - 33206538)

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