# Rashid Hussain

Male, 35 years old, Pakistani national.



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BS & MS, Bioinformatics

Ph.D. Computational Chemistry

Research Experience

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

**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, Pakistan**

**Focus**: Research and management tasks

**Responsibilities**: Structure-based drug design of HCV NS3 protease genotype 3a

Ligand-based pharmacophore modeling

Coordination with universities for research facilitation

Monitoring of cGMP compliance and training of technical staff

Feb 2015 – Jan 2016 **Research Associate – Biomedical Informatics Research Laboratory, Lahore University of Management Sciences (LUMS), Pakistan**

**Projects**: Higher Education Commission funded project on Hepatitis C Virus drug design

MATLAB-based toolbox for top-down proteomics data

**Responsibilities**: Ligand-based drug design

Designing GUI of top-down proteomics toolbox

Lab management and compiling annual lab reports

Paper manuscript preparation

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

**Responsibilities**: In-vivo testing on Zebrafish and hands-on experimental techniques

Use bioinformatics tools to find conserved regions in Zebrafish

Education

2017 – Present **Ph.D. Chemistry –** **Forman Christian College (A Chartered University), Pakistan**

Thesis Title: Computer-aided drug design and synthesis of HCV NS3 protease inhibitors.

Supervisors: Dr. Hira Khalid and Dr. M. Qaiser Fatmi

2011 – 2013 **MS Bioinformatics – COMSATS University Islamabad, Pakistan**

Majors: Computer-Aided Drug Design (CADD)

Thesis Title: Rationalizing ligand-protein interactions and identifying cholinesterase

inhibitors using computational methods

Supervisor: Dr. M. Qaiser Fatmi

2006 – 2010 **BS Bioinformatics – COMSATS University Islamabad, Pakistan**

Majors: Phylogenetic analysis

Thesis Title: Phylogenetic analysis of major protein-coding genes of Geminiviridae:

A single-stranded DNA virus family

Supervisor: Dr. Muhammad Zeeshan Hyder

Publications

1. **Hussain, R.**, Khalid, H., Fatmi, M. Q. (2022). "HCV genotype-specific Drug Discovery through structure-based virtual screening.” *Pure and Applied Chemistry.* [[**Link**](https://www.degruyter.com/document/doi/10.1515/pac-2021-1104/html)]
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. [[**Link**](https://www.worldscientific.com/doi/abs/10.1142/S273741652150037X)]
3. Khalid, H., **Hussain, R.**, & Hafeez, A. (2020). "Virtual screening of piperidine-based small molecules against COVID-19". *Lab-in-Silico*, 1(2), 50-55. [[**Link**](https://www.researchgate.net/profile/Hk-Haris/publication/348370221_Lab-in-Silico_Virtual_Screening_of_Piperidine_Based_Small_Molecules_Against_COVID-19/links/5ffb14c292851c13fe02d327/Lab-in-Silico-Virtual-Screening-of-Piperidine-Based-Small-Molecules-Against-COVID-19.pdf)]
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 Identifying Proteins from Top-down Proteomics Data." *Scientific Reports - Nature*, Vol. 9, Issue 1, pp. 1 -14. [DOI: 10.1038/s41598-019-47724-1](https://doi.org/10.1038/s41598-019-47724-1). **[**[**Link**](http://www.nature.com/articles/s41598-019-47724-1)]
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, Issue 3, pp. 1091-1136. DOI: 10.1002/med.21554. [[**Link**](https://onlinelibrary.wiley.com/doi/10.1002/med.21554)**]**
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. [[**Link**](https://pdfs.semanticscholar.org/24cd/2875385b10a0c56904f6c30e3f30f5848568.pdf)]
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. [[**Link**](https://link.springer.com/chapter/10.1007/978-3-319-60408-4_14)]
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. 6, pp. 2715-2726. [DOI: 10.1007/s00044-013-0847-2](https://link.springer.com/article/10.1007/s00044-013-0847-2). [[**Link**](https://link.springer.com/article/10.1007/s00044-013-0847-2)]
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*. 38.2: 189-201. [DOI:10.3906/kim-1303-89](http://journals.tubitak.gov.tr/chem/abstract.htm?id=14590). [[**Link**](http://journals.tubitak.gov.tr/chem/abstract.htm?id=14590)]

Manuscripts in Preparation

1. **Hussain, R.**, Hackett, A., Álvarez-Carretero, S., Khalid, H., 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,** [[**Link**](https://github.com/BIRL/SPECTRUM)]

Conferences Webinar/Talks/Posters

1. **Hussain, R.**, Khalid, H. (2020). "References made easy using Mendeley”. Forman Christian College (A Charted University), Pakistan – Webinar.
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". Virtual Conference on Chemistry and its Applications. The University of Mauritius. Mauritius – Talk.
3. **Hussain, R.**, Khalid, H. (2018). "HCV genotype-specific drug discovery through Structure and Ligand-based Virtual Screening." 6th International Bau Drug Design Congress. Bahcesehir University School of Medicine, Istanbul, Turkey – Talk.
4. Khalid, H., ur Rehman, A., Ahmad, I., Arshad, S., Nadeem, M.H., **Hussain, R**. (2018). Synthesis of Potential Antibacterial Agents Derived from 5-[1-(Phenylsulfonyl) piperidin-4-yl]-1,3,4-oxadiazol-2-thiol. "International Conference on Chemical and Pharmaceutical Sciences." Forman Christian College (A Charted University), Lahore, Pakistan – Talk.
5. 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.
6. 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 – Talk.
7. **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) – Poster.
8. **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 – Poster.

Projects

1. **Machine Learning QSAR model for COVID19 Replicase Polyprotein to predict pIC50 of a given compound – Successfully developed and deployed.** <https://github.com/rashid-bioinfo/DS-ML_COVID_pIC50_Predictor>

Professional Skills

***Computer Programing:*** Python, Bash Scripting, GitHub (for version control) – Expert level

R, MATLAB, SQL – Proficient

C++, JAVA, LaTeX, Django, Bootstrap – Intermediate level

***Operating System:*** Linux, Mac, Windows

***Computational Chemistry:*** Docking – AD4, Autodock Vina, UCSF DOCK6

MD Simulations – GROMACS

Modeling – MODELLER, SWISS-MODEL

Visualization/Interactions – PyMOL, MOE, VMD, UCSF Chimera, BIOVIA DS

Other – Schrödinger Suite

***Data Science &:*** Scikit-learn, Pandas, NumPy, KNIME, Streamlit, RDKit (Cheminformatics)

***Machine Learning***

Honors and Awards

2021 – 22 **International Research Support Initiative Program (IRSIP)**, $9800 for six months

by Higher Education Commission of Pakistan

2015 **Best Poster Award**, by Institute of Space Technology, Pakistan

2015 **Marathon Race Winner**, Lahore University of Management Science (LUMS), Pakistan

Teaching Experience

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

**Course**: High-Performance Computing (HPC) **Level**: Undergraduate

**Responsibilities**: Voluntary helper to mentor the learners and answer their questions

Mar 2019 – Feb 2020 **Visiting Faculty – Minhaj University, Pakistan**

**Course**: Bioinformatics **Level**: Undergraduate

**Responsibilities**: Designed and presented 30 lectures each to different batches

Conducted 16 labs of the course

Wrote and graded exams

Feb 2015 – Jan 2016 **Teaching Assistant – Lahore University of Management Sciences (LUMS), Pakistan**

**Courses**: Computational Biology and Protein Informatics **Level**: Undergraduate

**Responsibilities**: Conducted 16 labs, wrote and graded lab exams – Comp. Biology

Conducted 12 labs, wrote and graded lab exams – Protein Informatics

Graded class assignments for both courses

Supervisory and Mentoring Experience

Supervised four undergraduate summer intern students

Mentoring undergraduate/graduate research students in these writeup/presentations

Voluntary Academic Service

As a team lead, trained teachers, students, and parents for taking online classes using Google

Classroom, Google Meet, Zoom, etc. during COVID19

Recorded online tutorials on YouTube Channel, Eduwareness on computer-aided drug design

and for general public awareness, like traffic signs and rules

Memberships

American Chemical Society (ACS) – Punjab, Pakistan

Journal Reviewer

Springer – Molecular Diversity

Professional Courses and Certifications

2022 **Machine Learning**, Datacamp – In progress

2022 **Data Science**, Online course – Completed

2021 **Python**, Online course, 1100 minutes – Completed

2020 **Introduction to Molecular Modeling in Drug Discovery**, Schrödinger online course, 1 month

2019 **Computer-Aided Drug Design**, NPTEL India online course, 900 minutes

2017 **IELTS**, British Council, Band 7.0