**Rashid Hussain**
BS & MS, Bioinformatics
Ph.D. Computational Chemistry

Male, 35 years old, Pakistani national.
(92) 3155235956
rashid.bioinfo@gmail.com
https://rashid-bioinfo.github.io/

***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. DOI: 10.1515/pac-2021-1104. [**Link**]
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**]
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. [**Link**]
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. [**Link**]
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. [**Link**]
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**]
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. [**Link**]
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. [**Link**]
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. [**Link**]

***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**]

***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/BioPredict

***Professional Skills***

| | |
|---|---|
| ***Computer Programing:*** | Python, Bash Scripting, GitHub (for version control) – Expert level<br>R, MATLAB, SQL – Proficient<br>C++, JAVA, LaTeX, Django, Bootstrap – Intermediate level |
| ***Operating System:*** | Linux, Mac, Windows |
| ***Computational Chemistry:*** | Docking – AD4, Autodock Vina, UCSF DOCK6<br>MD Simulations – GROMACS |

Modeling – MODELLER, SWISS-MODEL
Visualization/Interactions – PyMOL, MOE, VMD, UCSF Chimera, BIOVIA DS
Other – Schrödinger Suite

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

***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 Member Number - 33206538)

***Journal Reviewer***

Springer – Molecular Diversity

***Professional Courses and Certifications***

| | |
|---|---|
| 2022 | The Unix Workbench, Johns Hopkins University – Completed |
| 2022 | What is Data Science, IBM – Completed |
| 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 |