Dr Hafiz Saqib Ali

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Personal

An enthusiastic, adaptive and fast-learning person with a broad and acute interest in the field of computational chemistry, chemical biology, and medicine. I possess a versatile and fast learning abilities, and an avid interest in the development and implementation of algorithms within the realm of natural sciences. My expertise lies in the field of quantum mechanics, molecular dynamics, machine learning, hybrid quantum mechanics/molecular mechanics and bioinformtics. Not only do I excel in these areas but am also passionate for advancing methodologies and working collaboratively with scientists from diverse fields to accomplish project objectives.

Profesional Experience

University of Oxford *2022 – Present*
Postdoctoral Research Associate, Drug Modelling and Design for Antimicrobial Resistant (AMR) enzymes with the INEOS Oxford Institute
***Supervisors*:** Profs. Christopher Schofield and Fernanda Duarte
***Project*:** Development and Implementation of Computational Strategies to Identify New Active Molecules and Study Their Mechanism by Means of the State-of-Art Computational Techniques

The University of Edinburgh *2021 – 2022*
Postdoctoral Research Associate, Modelling and Design of Novel Artifical Metalloenzymes
***Supervisor*:** Dr. Amanda Jarvis
Project: Molecular Modelling of Artificial Metalloenzymes in Order to Optimise Their Activities and Design of Novel Artificial Metalloenzymes

Education

The University of Manchester *2018 – 2021*
PhD student, Computational and Theoritical Chemistry
Recipient of Chief Minister Merit Scholarship (CMMS)
***Supervisors*:** Dr. Richard Henchman and Prof. Samuel de Visser
***Thesis Title*:** Development and Implementation of Algorithms to Determine the Reaction Kinetics and Stability of Biomolecules

Govt. College University Faisalabad *2015 – 2017*
M.Phil. Chemistry
Recipient of Punjab Educational Endowment Fund (PEEF) Scholarship
***Supervisors*:** Prof. Asim Mansha
***CGPA*:** 3.89/4.00 (3rd position)
***Thesis Title*:** A Quantum Mechanical Study of Nitrile-based Dyes as Photosensitizers for Photodynamic Therapy Applications

Govt. College University Faisalabad *2011 – 2015*
BS (hons), Chemistry
Recipient of Higher Education Commision (HEC) Merit Scholarship
CGPA: 3.34/4.00

Honors and Awards

Chief Minister Merit Scholarship *2017 – 2021*
A PhD foreign scholarship from the Government of Pakistan that covered all expenses related to studying abroad for a period of 3-4 years. This scholarship included 100% coverage of tuition fees, boarding and lodging expenses, health insurance, and airfare.

The Punjab Educational Endowment Fund (PEEF) *2015 – 2017*
The Government of Punjab, Pakistan, offered a Masters level PEEF scholarship for a period of two years, which covered all education-related expenses including tuition fees and living expenses.

Higher Education Commision (HEC) Scholarship *2011 – 2015*
The Government of Pakistan, offered an undergraduate degree scholarship that covered the entire four-year duration of the program.

Grants

CCPBioSim Software Project Funding *July 2023 – Present*

Funding from CCPBioSim (EPRSC grant **EP/T026308/1**) in collaboration with the Scientific and Technology Facilities Council (STFC) to generalise the software "*CodeEntropy: Generalising Multiscale Cell Correlation to Molecular Mixtures and Complexes*" to biomolecular systems

Computing Time *March 2023 – Present*

Application for Computing time of 47,520 GPU hrs on the supercomputer BEDE was acceped by HECBioSim

CCPBioSim Software Project Funding *February – July 2022*

Funding from CCPBioSim (EPRSC grant **EP/T026308/1)** in collaboration with STFC for "*Multiscale Entropy and Structure Quantification from Molecular Dynamics Simulation*" to combine the CodeEntropy software with the POSEIDON software to enable the calculation of the entropy of aqueous proteins

Teaching & Supervision

CCPBioSim Workshop *January 2023*

The CodeEntropy Hackathon hosted at the University of Leeds, UK, provided training to participants on utilizing CodeEntropy for the calculation of entropy in biomolecular systems, including water, ions and solutes.

DPhil Student Supervisor *March 2022 – Present*

- Day-to-day supervision of DPhil and master students in the Profs. C.J. Schofield and F. Duarte groups

PhD Student Supervisor *September* 2021 – *March* 2022

- Day-to-day supervision of PhD and master students in the Dr. A. Jarvis group

PhD & Master Student Supervisor *February* 2018 – *September* 2020

- Day-to-day supervision of PhD students in the Profs. R.H. Henchman and S.P. de Visser groups

Graduate Teaching Assistance, Department of Chemistry, University of Manchester *2018 – 2020*

- Advanced Practical Training (**CHEM30620**) *January – April 2020*
- Molecular Modelling & Simulation (**CHEN40232 & 60232**) *February 2020*
- Computational Studies of Structure and Reactivity, (**CHEM30620**) *December 2019*
- Reaction of Cu Coordinated Compounds, (**CHEM30620**) *September – December 2019*
- Molecular Modelling & Simulation, (**CHEN40232 & 60232**) March – *2019*
- Computational Lab mini-Project, (**CHEM30600**) *September 2018 – April 2019*
- Modelling Nanoporous Crystal Growth: Fotran programing (**CHEM30600**) *September – December 2018*

Scientific Computing Skills

Computing Platforms

- High Performance Computing (HPC) Cluster (Aleph) and Advance Research Computing (ARC), University of Oxford *March 2022 – Present*
- Edinburgh Compute and Data Facility (ECDF), University of Edinburgh *2021 – 2022*
- High Performance Computing Shared Facility (CSF3), University of Manchester *2018 – 2022*

Computing Softwares

- AMBER, GROMACS, CP2K, Schrödinger, Gaussian, ORCA, OLEX2, Mercury, GaussView, ChemCraft, Hyper-Chem, Chem-3D, Avogadro, End Note and Notepad++

Programming

- Python, Bash, Matlab, Fortran, Git, C++, PyTorch, TensorFlow, and Machine Learning

Attended Conferences & Workshops

- Medicinal Chemistry Workshop series from Blue Burgundy and Ineos Oxford Institute for AMR *March 2023*
- 5th RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry, University of Cambridge *September 2022*
- Inorganic Reaction Mechanisms International Conference, RSC (*talk*) *July 2020*
- Inorganic Reaction Mechanisms & Inorganic Biochemistry Discussion Group Meeting at Manchester Institute of Biotechnology, Manchester, UK *April 2019*
- Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and Beyond. CECAM-HQ-EPFL, Lausanne, Switzerland (*poster*) *April 2019*
- DL_Software's Training Workshop, The University of Manchester (*poster*) *December 2018*
- 6th Annual CCPBioSim Meeting, University of Oxford, UK (*poster*) *September 2018*
- CCP5 Summer School, University of Lancaster, UK *July 2018*
- 3rd Conference on Multiscale Modelling of Condensed Phase and Biological Systems-CCPBioSim and CCP5, The University of Manchester (*poster*) *May 2018*
- CCPBioSim Training Week, University of Bristol, UK *April 2018*

Profesional Affilications

Associate Member of The Royal Society of Chemistry (**725043**) *July 2022 – Present*

References

For references, please enquire to:

Prof. Christropher Schofield, University of Oxford (christopher.schofield@chem.ox.ac.uk)
Prof. Fernanda Duarte, University of Oxford (fernanda.duartegonzalez@chem.ox.ac.uk)
Prof. Samuel de Visser, The University of Manchester (sam.devisser@manchester.ac.uk)
Dr. Richard Henchman, The University of Sydney (rhen7213@uni.sydney.edu.au)
Dr. Amanda Jarvis, The University of Edinburgh (amanda.jarvis@ed.ac.uk)

Peer-reviwed Publications

Outputs: 40 **per-reviwed** publications, including *JACS* (1), *ACS Catal* (1) *Acc Chem Res*(1), *Int. J. Biol. Macromol.* (1) *Chem Eur J* (5) etc. 14 as a first author. *: Coresponding author. **ORCID**: *0000-0001-5770-5376*
Full list of publications: **i10-index:**19 **h-index:** 13 ***Citations:*** 448 ***Impact Factor*** *=>250*
https://scholar.google.com/citations?user=qEVrdecAAAAJ&hl=en

1. E. Klemencic, R.C. Brewster, **H.S. Ali**, J.M. Richardson and A.G. Jarvis, Using BpyAla to generate Copper Artificial Metalloenzymes: a catalytic and structural study. *ChemRxiv.* (https://doi.org/10.26434/chemrxiv-2023-9f4xc)
2. **H.S. Ali*,** Emerging perception of activity cliffs: A barief review, *UCP J. Sci. Technol.* **2023** (*accepted*).
3. S. Zaib, N. Ranaa, **H.S. Ali**, M. Rehmana, N. S. Awwadd, H. A. Ibrahiume, I. Khan, Identification of potential inhibitors targeting yellow fever virus helicase through ligand and structure-based computational studies. *J. Biomol. Struct. Dyn.* **2023**, (*accepted*)
4. **H.S. Ali*** and R.H. Henchman, Energy-entropy method with multiscale cell correlation to predict toluene-water logP in SAMPL9 challenge. *Phys. Chem. Chem. Phys.* **2023**, 25, 27524.
5. S. Zaib, N. Rana, **H.S. Ali,** N. Hussain, Areeba, H.A. Ogaly, F. Al-Zahrani and I Khan, Discovery of druggable potent inhibitors of serine proteases and farnesoid X receptor by ligand-based virtual screening to obstruct SARS-CoV-2*, Int. J. Biol. Macromol.* **2023**, 253, 127379.
6. W. Hussain, M.S. Iqbal, M. R. Bashir, M.A. Khan and **H.S. Ali**, The computational study of supramolecular interactions between perylene diimide derivatives and nucleotides for electronic properties. *Int. J. Quantum Chem.,* **2023**, 124, e27223.
7. S. Zaib, M.T Younas, I. Khan, **H.S. Ali,** J. McAdam, J.M. White, F. Jaber, N.S. Awwad, H.A. Ibrahium, Pyrimidine-morpholine hybrids as potent druggable therapeutics for Alzheimer's disease: Synthesis, biochemical and in silico analyses. *Bioorg. Chem.* **2023**, 141, 106868.
8. **H.S. Ali,** J. Warwicker and S.P. de Visser, How does the non-heme iron enzyme NapI react through l-arginine desaturation rather than hydroxylation? A quantum mechanics/molecular mechanics study. *ACS Catal.* **2023**, 13, 10705-10721.
9. **H.S. Ali,** A.A. Hussein and M. Obies, Impact of counteranions on n-heterocyclic carbene gold(I)-catalyzed cyclization of propargylic amide. *RSC Adv*., **2023**, 13, 2896-2902.
10. S. A. Ejaz, A. Farid, S. Zargar, P. A. Channar, M. Aziz, T. A. Wani, H. M. Attaullah, R. Ujhan, A. Tehzeeb, A. Saeed, **H. S. Ali** and M. F. Erben, Computational and theoretical chemistry of newly synthesized and characterized 2,2'-(5,5'-(1,4-phenylene) bis(1H-tetrazole-5,1-diyl))bis-N-acetamide. *BMC Chem.,* **2023**, 17:97.
11. M. Ali, M. Usman, A. Shah, A. Rehman, **H.S. Ali,** Spectroscopic and conductometric investigaton of mixed micellar-assisten solubilization of nile blue sulfate. *J. Mol. Liq.*, **2023**, 386, 122507.
12. M.Q.E. Mubarak, **H.S. Ali,** J. Zhou, C. Li, J. Xiao and S.P. de Visser, Dehydrogenative α-oxygenation of cyclic ethers by a high-valent manganese(IV)-oxo species. *Eur. J. Inorg. Chem.* **2023**, 26, e202200621, 1-11.
13. S. Aslam, **H.S. Ali*,** M. Ahmad, A. Mansha, N. Ali, S. Khan, S.A.R. Naqvi, Z. Khalid, S. Asim, M. Parvez and M. Khalid, A combined experimental and theoretical study of alkyl 2-(3-benzoyl-4-hydroxy-1,1-dioxido-2H-benzo[e][1,2]thiazin-2-yl)acetates: Synthesis, x-ray crystallography and DFT. *J. Mol. Struct.* **2022**,1258, 132671.
14. **H.S. Ali** and S.P. de Visser, Electrostatic perturbations in the substrate-binding pocket of taurine/α-ketoglutarate dioxygenase determine its selectivity. *Chem. Eur. J.* **2022**, 28, e202104167. (**VIP**)
15. Y. Ma Y., **H.S. Ali** and A.A. Hussein, A mechanistic study on gold(I)-catalyzed cyclization of propargylic amide: revealing the impact of expanded-ring n-heterocyclic carbenes. *Catal. Sci. Technol.* **2022**, 12, 674-685.
16. Y.T. Lin, **H.S. Ali** and S.P. de Visser, Biodegradation of herbicides by a plant non-heme iron dioxygenase: mechanism and selectivity of substrate analogues. *Chem. Eur. J.* **2022**, 28, e202103982.

17. S.P. de Visser, G. Mukherjee, **H.S. Ali** and C.V. Sastri, Local charge distributions, electric dipole moments, and local electric fields influence reactivity patterns and guide regioselectivities in α-ketoglutarate-dependent non-heme iron dioxygenases. *Acc. Chem. Res.* **2022**, 55, 65-74.
18. **H.S. Ali,** S. Ghafoor and S.P. de Visser, Density functional theory study into the reaction mechanism of isonitrile biosynthesis by the non-heme iron enzyme ScoE. *Top. Catal.* **2022**, 65, 528-543.
19. **H.S. Ali,** A. Chakravorty, J. Kalayan, S.P. de Visser and R.H. Henchman, Energy–entropy method using multiscale cell correlation to calculate binding free energies in the SAMPL8 host–guest challenge. *J. Comput. Aided Mol. Des.* **2021**, 35, 911-921.
20. **H.S. Ali,** R.H. Henchman and S.P. de Visser, Mechanism of oxidative ring-closure as part of the hygromycin biosynthesis step by a non-heme iron dioxygenase. *ChemCatChem*, **2021**, 13, 3053-3066.
21. Y.T. Lin, **H.S. Ali** and S.P. de Visser, Electrostatic perturbations from the protein affect C−H bond strengths of the substrate and enable negative catalysis in the TmpA biosynthesis enzyme. *Chem. Eur. J.* 2021, 27,8851-8864. (**VIP**).
22. M.M. Bacha, H. Nadeem, S. Rahman, S. Sarwar, A. Imran, S. Zaib, **H.S. Ali,** M. Arif and J. Iqbal, Rhodanine-3-acetamide derivatives as aldose and aldehyde reductase inhibitors to treat diabetic complications: synthesis, biological evaluation, molecular docking and simulation studies. *BMC Chem.* **2021**, 15, 28.
23. S.B. Han, **H.S. Ali** and S.P. de Visser, Glutarate hydroxylation by the carbon starvation-induced protein D: A computational study into the stereo- and regioselectivities of the reaction. *Inorg. Chem.* **2021**, 60, 4800-4815.
24. S.P. de Visser, Y.T. Lin, **H.S. Ali,** U.K. Bagha, G. Mukherjee and C.V. Sastri, Negative catalysis/non-Bell-Evans-Polanyi reactivity by metalloenzymes: Examples from mononuclear heme and non-heme iron oxygenases. *Coord. Chem. Rev.* **2021**, 439, 213914.
25. **H.S. Ali,** R.H. Henchman, J. Warwicker and S.P. de Visser, How do electrostatic perturbations of the protein affect the bifurcation pathways of substrate hydroxylation versus desaturation in the non-heme iron-dependent viomycin biosynthesis enzyme? *J. Phys. Chem. A,* **2021**, 125, 1720-1737.
26. **H.S. Ali,** R.H. Henchman and S.P. de Visser, What determines the selectivity of arginine dihydroxylation by the non-heme iron enzyme OrfP? *Chem. Eur. J.* **2021**, 27, 1795-1809.
27. H. Andleeb, L. Danish, S. Munawar, M.N. Ahmad, I. Khan, **H.S. Ali,** M.N. Tahir, J. Simpson and S. Hameed, Theoretical and computational insight into the supramolecular assemblies of Schiff bases involving hydrogen bonding and C-H…π interactions: Synthesis, X-ray characterization, Hirshfeld surface analysis, anticancer activity and molecular docking analysis. *J. Mol. Struct.* **2021**, 1235, 130223.
28. A.S. Chowdhury, **H.S. Ali,** A.S. Faponle and S.P. de Visser, How external perturbations affect the chemoselectivity of substrate activation by cytochrome P450 OleTJE. *Phys. Chem. Chem. Phys.* **2020**, 22, 27178-27190.
29. **H.S. Ali,** R.H. Henchman and S.P. de Visser, Lignin biodegradation by a cytochrome P450 enzyme: A computational study into syringol activation by GcoA. *Chem. Eur. J.* **2020**, 26, 13093-13102.
30. S. Louka, S.M. Barry, D.J. Heyes, M.Q.E. Mubarak, **H.S. Ali,** L.M. Alkhalaf, A.W. Munro, N.S. Scrutton, G.L. Challis and S.P. de Visser, The catalytic mechanism of aromatic nitration by cytochrome P450 TxtE: Involvement of a ferric-peroxynitrite intermediate. *J. Am. Chem. Soc.* **2020**, 142, 15764-15779.
31. **H.S. Ali,** J. Higham, S.P. de Visser and R.H. Henchman, Comparison of free-energy methods to calculate the barriers for the nucleophilic substitution of alkyl halides by hydroxide. *J. Phys. Chem. B*, **2020**, 124, 6835-6842.
32. **H.S. Ali,** R.H. Henchman and S.P. de Visser, Cross-linking of aromatic phenolate groups by cytochrome P450 enzymes: A model for the biosynthesis of vancomycin by OxyB. *Org. Biomol. Chem.* **2020**, 18, 4610-4618.
33. A.A. Hussein and **H.S. Ali,** Revealing mechanism and origin of reactivity of Au(I)-catalyzed functionalized indenone formation of cyclic and acyclic acetals of alkynylaldehydes. *J. Org. Chem.* **2020**, 85, 12682-12691.
34. S. Rahman, **H.S. Ali,** B. Jafari, S. Zaib, A. Hameed, P. Langer and J. Iqbal, Structure-based virtual screening of dipeptidyl peptidase-4 inhibitors and their in vitro analysis. *Comput. Biol. Chem.* **2020**, 107326.
35. N. Akram, A. Mansha, R. Premkumar, A.M.F. Benial, S. Asim, S.Z. Iqbal and **H.S Ali,** Spectroscopic, quantum chemical and molecular docking studies on 2,4-dimethoxy- 1,3,5-triazine: A potent inhibitor of protein kinase CK2 for the development of breast cancer drug. *Mol. Sim.* **2020**, 46, 1340-1353.
36. **H.S. Ali,** J. Higham and R.H. Henchman, Entropy of simulated liquids using multiscale cell correlation. *Entropy*, **2020**, 21, 750.
37. S. Ghafoor, A. Mansha, S. Asim, M. Usman, A.F. Zahoor and **H.S. Ali,** The structural, spectral, frontier molecular orbital and thermodynamic analysis of 2-hydroxy 2-methyl propiophenone by MP2 and B3LYP methods. *J. Theor. Comput. Chem.* **2020**, 19, 2050020.

38. N. Ali, A. Mansha, S. Asim, **H.S. Ali** and M. Usman, Insight into the molecular characterization and spectral properties of 2-methoxy-1,4-naphthoquinone: A computational approach. *J. Struct. Chem.* **2020**, 61, 182-196.
39. M. Kazmi, A. Ibrar, **H.S. Ali,** M. Ghufran, A. Wadood, U. Flörke, J. Simpson, A. Saeed, A. Frontera and I. Khan, A combined experimental and theoretical analysis of the solid-state supramolecular self-assembly of N-(2,4-dichlorophenyl)-1-naphthamide: Synthesis, anticholinesterase potential and molecular docking analysis. *J. Mol. Struct.* **2019**, 1197, 458.
40. A. P. Channar , N. Arshad, A.F. Larik , S.I. Farooqi, A. Saeed, T. Hökelek, B. Batool, R. Ujan, **H.S. Ali** and U. Flörke, 4-(4-Bromophenyl)thiazol-2-amine: Crystal structure determination, DFT calculations, visualizing intermolecular interactions using Hirshfeld surface analysis, and DNA binding studies. *J. Phys. Org. Chem.* **2019**, 32, e3968.

Publications Submitted / In Preparation

1. **H.S. Ali**, F. Duarte and C. J. Schofield, A deep learning approach for the discovery of Metallo-β-Lactamase inhibitors (in-preparation).
2. M. J. Beech, E. Toma, A. Farley, **H.S. Ali**, H. Smith, Z. Butt, R. Demel, V. Goel, T. R. Walsh and C. J. Schofield, A fluorescence polarisation binding assay for the discovery of Tet(X) inhibitors. (in-preparation)
3. **H.S. Ali*** and S.P. de Visser, Revealing new perspective on the catalytic mechanism and structures of l-arginine hydroxylating enzymes. *Front. Chem.* (*submitted*)
4. **H.S. Ali*** and S.P. de Visser, QM/MM study into the mechanism of oxidative C=C double bond cleavage by lignostilbene-α,β-dioxygenase. *Chem. Sci.* (*submitted)*
5. R, Munir, I. Khan, L. Siddiqui, N. Javid, M. Zia-ur-Rehman, **H.S. Ali**, M. Saeed, S. Zaib, N. S. Awwad, H. A. Ibrahim, C. H. S. Yeow, J. M. White and A. A. Dera. Regioselective metal-free synthesis of sulfostyril-quinoline hybrid framework: Experimental and computational mechanistic insights. *J. Mol. Struct. (submitted)*.