Dr Hafiz Saqib Ali

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Peer-reviewed publications > 54 | **h-index** = 18 | **i10-index** = 32 | **Citations** = 1011 | **Impact Factor** = >350

Research Experience

Postdoctoral Research Associate, Department of Pure & Applied Chemistry, University of Strathclyde and GSK *2026 – present*

***Project*:** Data-driven approaches to design next-generation therapeutic modalities beyond Lipinski space.

- Investigate reaction profiles of oligonucleotides synthesis in different solvents with DFT integrated with AI/ML
- Develop physics-informed AI/ML models to predict solubility in organic solvents for efficient synthesis of ONs
- Develop QSAR model governing cellular uptake and efficacy of ONs through MD simulations and AI/ML

Postdoctoral Research Associate, The Ineos Oxford Institute for Antimicrobial Research, University of Oxford *2022 – 2026*

***Project 1*:** Designing next-gen antibiotics with advanced computational methods.

- Developed a robust structure-based virtual screening workflow for chemical exploration (e.g., Enamine Real).
- Used MD simulations and free energy perturbation (FEP) methods to optimize and select potent compounds.
- Created the first potent inhibitors of TetX and LpxC, showcasing the success of the computational methods.

***Project 2*:** Advancing drug design with machine learning and deep learning.

- Developed and validated ML and DL models for predicting bioactive molecule properties.
- Applied ML/AI models to design and optimize inhibitors for metallo-beta lactamases.
- Utilized MD simulations with enhanced sampling (e.g., umbrella sampling, metadynamics) for inhibitors against serine beta-lactamases (SBLs) and penicillin-binding proteins (PBPs).
- Used DFT and QM/MM calculations to elucidate the binding mechanisms of boronates with SBLs and PBPs.

***Project 3*:** Engineering oxygenases for enhanced antibiotic production.

- Developed *in silico* mutation protocol to engineer IPNS mutants with enhance antibiotic production.
- Used DFT, MD and QM/MM studies to understand the reaction mechanism of IPNS.

***Project 4*:** Unravelling Codanin-1 and CDIN-1: *In silico* insights into disease mechanisms, and patient mutations in congenital dyserythropoietic anemia type I.

- Predicted proteins and protein-substrate (DNA/RNA) complex structures using AlphaFold 3.
- Developed computational model to explore disease mechanisms and key binding interactions.
- Analyzed *in silico* mutation effects to understand function enhancement and disease mutation impact.

Postdoctoral Research Associate, School of Chemistry, The University of Edinburgh *2021 – 2022*

Project: Engineering copper-based artificial metalloenzymes for optimized activity

- Utilized MD simulations and large QM-cluster models with DFT calculations to study the Friedel-Crafts alkylation mechanism of copper-based artificial metalloenzymes (ArMs).
- Applied *in silico* mutations to design and enhance both the activity and high stereoselectivity of ArMs.

PhD Researcher, Manchester Institute of Biotechnology, The University of Manchester *2018 – 2021*

Project 1: Development of Multiscale Cell Correlations (MCC) theory for molecular quantification & entropy calculations.

- Developed MCC method to calculate the entropy for the ranged of industrial liquids.
- Integrated MCC with DFT method in QM/MM formulism to understand SN2 reaction kinetics in explicit solvents.
- Developed energy-entropy method based on MCC (EE-MCC) to calculate the binding free energies of drugs with CB8 host system and partition coefficient $\log P_{tol/wat}$ of drugs between toluene and water.

Project 2: Engineering highly reactive enzymes with regio- and stereoselectivity using multiscale modelling.

- Utilized MD and large QM-cluster models to explore substrate activation by non-heme and heme iron enzymes.
- Employed QM/MM calculations to engineer iron-based metalloenzymes for small molecule production.
- Integrated machine learning methods with MD simulations for protein conformation analysis.
- Employed DFT and *ab initio* calculations to derive new reactivity models and guide synthetic effort.

MPhil Researcher, Department of Chemistry, Government College University Faisalabad, Pakistan *2016 – 2017*

Project: Quantum mechanical modelling of nitrile-based photosensitizers for photodynamic therapy (PDT) applications.

- Applied DFT and time-dependent-DFT to design and evaluate nitrile-based dyes for PDT.
- Validated designed small molecules using FTIR and UV-visible spectroscopic techniques.

Education

Preparation for Learning and Teaching at Oxford' (PLTO) course *December 2022*

PLTO course in the Department of Chemistry, University of Oxford.

PhD Computational and Theoretical Chemistry, The University of Manchester, UK *2018 – 2021*

Funding: 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 kinetics and stability of biomolecules

M.Phil. Physical Chemistry, Government College University Faisalabad, Pakistan *2015 – 2017*
Funding: Recipient of Punjab Educational Endowment Fund (PEEF) Scholarship
Supervisor: Prof. Asim Mansha
Thesis Title: A QM model for designing nitrile-based dyes as photosensitizers in photodynamic therapy applications.

BS (hons), Chemistry, Government College University Faisalabad, Pakistan *2011 – 2015*
*Funding***:** Recipient of Higher Education Commission (HEC) Merit Scholarship

Funding

CCPBioSim Software Project Funding (*co-PI*) *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 (*co-PI*) *March 2023 – Present*
Application for Computing time of 47,520 GPU hrs on the supercomputer BEDE was accepted by HECBioSim.

CCPBioSim Software Project Funding (*co-PI*) *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.

Chief Minister Merit Scholarship (CMMS) (*PhD studentship*) *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) (*Master's studentship*) *2015 – 2017*
The Government of Punjab, Pakistan, offered a master's level PEEF scholarship for a period of two years, which covered all education-related expenses including tuition fees and living expenses.

Higher Education Commission (HEC) Scholarship (*Bachelor's studentship*) *2011 – 2015*
The Government of Pakistan offered an undergraduate degree scholarship that covered the entire four-year.

Teaching & Supervision

Tutor Fellow, Immerse Education, Oxford *July 2025 – Present*
Designed and delivered an advanced chemistry course for high-achieving students.

Tutorial Fellow, Stanford House, University of Oxford *January 2025 – Present*
Tutorial fellow in Biochemistry and Computational Modelling for molecular design and enzyme engineering

Ambassador, Bug Fight an Outreach Initiative *July 2023 – September 2024*
Delivered interactive workshops to high school students on antibiotic resistance.

CCPBioSim Workshop *January 2023*
The CodeEntropy Hackathon at the University of Leeds, trained 20 participants to compute biomolecular entropy.

Student Supervision *August 2016 – Present*
Co-supervised 5 PhD and 2 visiting PhD, 3 rotation and 8 master students on their respective thesis projects.

Graduate Teaching Assistance, Department of Chemistry, University of Manchester *2018 – 2020*
- Advanced Practical Training *January – April 2020*
- Molecular Modelling & Simulation *February 2020*
- Computational Studies of Structure and Reactivity *December 2019*
- Reaction of Cu Coordinated Compounds *September – December 2019*
- Molecular Modelling & Simulation March – *2019*
- Computational Lab mini-Project *September 2018 – April 2019*
- Modelling Nano-porous Crystal Growth: Fortran programing *September – December 2018*

Lecturer of Science *2014 – 2017*
- Taught O-Level Chemistry and Biology at Moon Light School Systems, Pakistan.
- Delivered A-Level Chemistry courses at Superior Group of Colleges, Pakistan.
- Designed lessons, practical demonstrations, and assessments to strengthen student learning and performance.

Scientific Computing Skills

Computing Platforms
- High Performance Computing Cluster Aleph, BEDE and ARC, University of Oxford. *March 2022 – Present*
- High Performance Computing Shared Facility (CSF3), University of Manchester *2018 – 2022*

Programming and Research Tools
- **Languages/Frameworks:** Python, Bash, Git, C++, Pearl, PyTorch, Pytorch Geometric, TensorFlow, NumPy, Pandas, scikit-learn, Data Analysis, MATLAB, RDKit, Matplotlib & Jupiter-notebook
- **Computing Software's:** AMBER, GROMACS, Schrödinger, Gaussian, ORCA, ChemShell, OpenMM & Ash

Technical Knowledge & Research Expertise

- **Cheminformatics:** QSAR/QSPR modelling, cheminformatics databases (e.g. ChEMBL, PubChem), Molecular descriptor engineering, chemical data curation & analysis, compound clustering and diversity analysis.
- **Computational Chemistry & Biology:** Molecular docking, virtual screening, molecular dynamics (classical & enhanced sampling e.g. Umbrella Sampling, Metadynamics), free energy perturbation (FEP), DFT and *ab initio*.
- **Multiscale Modelling:** MCC theory (entropy & binding free energy), hybrid QM/MM workflows, ADMET, large QM-cluster models, statistical modelling and cheminformatics pipelines.
- **Enzyme & Protein Engineering:** *In silico* mutagenesis, RoseTTAFold, AlphaFold3 protein/DNA-RNA structure prediction, mechanistic modelling & disease mechanisms.
- **Core Machine Learning:** Supervised/unsupervised/self-supervised learning (QSAR, feature engineering), model evaluation & prediction**.**
- **Deep Learning:** Generative models (VAEs, diffusion/flow matching), graph neural networks, geometric deep learning, transformers & large language models.

Professional Affiliations

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

References

For references, please enquire to:

Prof. Christopher 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)

Output

Peer-reviewed Publications

Outputs: >54 **peer-reviewed** publications, including *Nat Comm (1) JACS* (1), *ACS Catal* (2) *Chem Sci* (1), *Int J Biol Macromol* (3) *Chem Eur J* (6) etc. ¶: Equal Contribution *: Corresponding author. 6 **ORCID**: *0000-0001-5770-5376*
i10*-index:**31 ***h*-index:** 18 ***Citations: 1003 https://scholar.google.com/citations?user=qEVrdecAAAAJ&hl=en

Key selected publications:

1. S. Brolih, **H.S. Ali¶,** C. Scott, A-A, Olijnik, H. Aitkenhead, G. Moir-Meyer, A.E. Gavard, Y. Yosaatmadja, D.R. Higgs, V. Veronica, V. Buckle, N. Roy, O. Gileadi, J.A. Newman, F. Duarte, C. Babbs and P.J. McHugh. The CDIN1-Codanin-1 complex, defective in Congenital Dyserythropoietic Anaemia Type I, is an RNA nuclease, *Nat. Comm.* **2026***,* (*accepted/in-press*).

Brief Synopsis. In this study, we demonstrate for the first time that *CDIN1* and Codanin-1 form a functional complex with intrinsic RNA nuclease activity. Using an integrative approach combining machine learning models i.e. AlphaFold3, biochemical assays, biophysical analysis, and MD simulations, we reveal the structural basis for this novel enzymatic activity and how disease-causing mutations disrupt its function. This work establishes a direct link between defective RNA processing and CDA-I, offering a new framework for therapeutic intervention.

2. M.J. Beech, E.C. Toma, H.G. Smith, M. Trush, **H.S. Ali**, Z. Butt, V. Goel, M.D. Allen, F. Duarte, A.J.M Farley, T. R. Walsh and C.J. Schofield, Binding assays enable discovery of Tet(X) inhibitors that combat tetracycline destructase resistance, *Chem. Sci.* **2025**, 16, 9691-9704.

Brief Synopsis. In this project, we have developed a new screening method to tackle bacterial resistance to the tetracycline class of antibiotics, identifying novel Tet(X) inhibitors from a bioactive library. Our work provides 1st non-tetracycline scaffolds for development of potent Tet(X) inhibitors and highlight the need to evaluate the impact of non-antibiotics on antimicrobial resistance. This work has stimulated my interest in antibiotic discovery targeting bacterial ribosomes as described in my research proposal.

3. A. Ravi, S. Zaib, I. Khan, **H.S. Ali**, M.I. El-Gamal, H.S. Anbar, Synthesis, *in vitro* and *in vivo* evaluation, and computational modelling analysis of thioxothiazolidine derivatives as highly potent and selective α-amylase inhibitors. *Eur. J. Med. Chem.* **2025**, 291, 117584.

Brief Synopsis. In this study we introduced novel thioxothiazolidine derivatives as selective α-amylase inhibitors for diabetes management. Compound **5r** showed exceptional inhibitory activity (IC50 = 0.71 ± 0.01 μM), outperforming acarbose. *In vivo*, **5r** reduced blood glucose and protected vital organs, with mechanistic studies revealing mixed-type inhibition, supporting its potential as a promising antidiabetic agent.

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.

Brief Synopsis. I have developed the Energy-Entropy method based on Multiscale Cell Correlation theory (EE-MCC) to accurately calculate physical properties, like toluene–water logP, directly from MD simulations for drug molecules. This method uniquely provides thermodynamics from a single simulation, enhancing utility beyond experimental measures.

5. **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.

Brief Synopsis. NapI, a key enzyme in naphthyridinomycin biosynthesis, offers a sustainable solution to desaturation reactions, which is crucial for antibiotic production. Leading the computational study, I unveiled its substrate-binding mechanism, paving the way for eco-friendly enzymatic alternatives.

All other publications:

6. G. Khoder, E.M. Mustafa, S. Zaib, A. Ravi, A.I. Shahin, S.O. Zaraei, N. Rana, H.S. Anbar, **H.S. Ali**, S. Qumar, M. Sebastian, R.A. Zein, M.I. El-Gamal, Novel indole-based sulfonate and sulfamate derivatives as potent and selective urease inhibitors targeting Helicobacter pylori: A promising therapeutic strategy. *Gut Pathog.* **2026**, (*accepted*).
7. S. Zaib, I. Khan, A. Ibrar, **H.S. Ali**, N. Rana, R. Munir, S. Zahra, A.B. Al-Odayni, J. Mcadam, T.Hökelek, A. Frontera. Synergistic effect of hydrogen bonding and C–H…π interactions to modulate the supramolecular assemblies of isobenzofuranones: X-ray crystallography, DFT analysis and antihyperglycemic potential. *J. Mol. Struct.* **2025**, 1321, 140263.
8. **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. Eur. J.* **2024**, 30, e202304172.
9. S. Zaib, I. Khan, **H.S. Ali,** A. Ibrar, M.T. Younas, A.B. Al-Odayni, A. Frontera, Design and discovery of anthranilamide derivatives as a potential treatment for neurodegenerative disorders via targeting cholinesterases and monoamine oxidases. *Int. J. Biol. Macromol.* **2024**, 272, 132748.
10. S. Zaib, I. Khan, A. Ibrar, N. Rana, **H.S. Ali,** C.J. McAdam, R.M. Gomila, I.H. El Azab, M.H.H. Mahmoud, Z.M. El-Bahy, A. Frontera. Hydrogen bonding, halogen bonding and C–H...π interactions governing the supramolecular architecture of 1-(4-(4-bromophenyl)piperazin-1-yl)-2- chloroethan-1-one: insights from X-ray crystallography, DFT calculations and urease inhibitory assessment. *J. Mol. Struct.* **2024**, 1317, 139065.
11. **H.S. Ali*** and S.P. de Visser, Catalytic divergencies in the mechanism of L-arginine hydoxylating nonheme irom enzymes. *Front. Chem.* **2024**, 12, 1-14.
12. **H.S. Ali*,** Emerging perception of activity cliffs: A brief review, *UCP J. Sci. Technol.* **2024**, 1, 15-29.
13. F.J. Hardy, M. Ortmayer, M. G. Quesne, E. F. Gerard, J. Zhao, C. J. Taylor, **H.S. Ali**, J. W. Slater, C. W. Levy, D.J. Heyes, J.M. Bollinger, S.P. de Visser, A.P. Green, Probing ferryl reactivity in a nonheme iron oxygenase using an expanded genetic code. *ACS Cat.* **2024**, 14, 11584-11590.
14. 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. *Catal. Sci. Technol.* **2024**, 14, 1622-1632.
15. 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.* **2024**, 1315, 138894.
16. M. Riaz, E. Yasmeen, M. Liu, **H.S. Ali**, M. Lv, H. Shi, C. Du, T. Dong, Z. Liu, Q. Song, Q. Ma, K. Zuo, Mitochondrial oxidative phosphorylation (mtOXPHOS) serves as a sentinel to gauge fluctuations under heat stress in Arabidopsis thaliana elucidated by comparative transcriptomics. *Plant Stress*, **2024**, 14, 10061.
17. W. Hussain, **H.S. Ali**, M.S. Iqbal, M. R. Bashir, M.A. Khan, M. Hanif, Y. Sandali, H. Li, Exploring nonlinear optical properties of perylene diimide and biomolecules complexes: A computational supramolecular study. *Theor. Chem. Acc.* **2024**, 143, 1-23.
18. W.Hussain, M. Sulaman, Y. Sandali, C. Li, M.S. Iqbal, M.R. Bashir, M.A. Khan, **H.S. Ali**, A.Irfan, H. Li. Computational exploration of nonlinear optical properties in supramolecular naphthalene diimides and nucleotide complexes. *Mater. Sci. Eng. B*, **2024**, 305, 117429.
19. **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.
20. 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.
21. 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**, 253, 127379.
22. 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.
23. 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.
24. M. Ali, M. Usman, A. Shah, A. Rehman, **H.S. Ali**. Spectroscopic and conductometric investigation of mixed micellar-assisted solubilization of Nile blue sulfate. *J. Mol. Liq.* **2023**, 386, 122507.
25. W. Hussain, M.S. Iqbal, H. Li, M. Sulaman, H. Guo, C. Li, Y. Sandali, A. Irfan, **H.S. Ali**. A comprehensive analysis of electronic transitions in naphthalene and perylene diimide derivatives through computational methods. *Int. J. Quantum Chem.* **2023**, 124, e27223.

26. 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., 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-acetamides. *BMC Chem.* **2023**, 17, 97.

27. **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**)

28. **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.

29. 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.

30. 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.

31. 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.

32. 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.

33. **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.

34. **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.

35. **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.

36. **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.

37. 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**

38. 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.

39. 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.

40. 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.

41. H. Andleeb, L. Danish, S. Munawar, M.N. Ahmed, I. Khan, H.S. Ali, M.N. Tahir, J. Simpson, 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.

42. **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.

43. **H.S. Ali,** J. Higham and R.H. Henchman, Entropy of simulated liquids using multiscale cell correlation. *Entropy*, **2020**, 21, 750.

44. **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.

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51. S. Ghafoor, A. Mansha, S. Asim, M. Usman, A.F. Zahoor, **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.
52. N. Akram, A. Mansha, R. Premkumar, A.M.F. Benial, S. Asim, S. Z. Iqbal, **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. Simul.* **2020**, 46, 1340-1353.
53. M. Kazmi, A. Ibrar, **H.S. Ali**, M. Ghufran, A. Wadood, U. Flörke, J. Simpson, A. Saeed, A. Frontera, I. Khan. A combined experimental and theoretical analysis of the solid-state supramolecular self-assembly of N-(2,4-dichlorophrnyl)-1-naphthamide: synthesis, anticholinesterase potential and molecular docking analysis. *J. Mol. Struct.* **2019**, 1197, 458-470.
54. P.A. Channar, N. Arshad, F.A. Larik, S.I. Farooqi, A. Saeed, T. Hökelek, B. Batool, R. Ujan, **H.S. Ali**, 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. Phy. Org. Chem.* **2019**, 32, e3968.

Attended Conferences & Workshops

- UKQSAR Spring Meeting, The University of Edinburgh *April 2026*
- Early Career Researcher conference: Multidisciplinary Approaches to AMR, University of Oxford *March 2025*
- Early Career Researcher conference: Multidisciplinary Approaches to AMR, University of Oxford *March 2024*
- 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 *July 2020*
- Inorganic Biochemistry Discussion Group Meeting at Manchester Institute of Biotechnology (*oral*) *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*