



# Aqeel A. Hussein

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*Married: 3 Daughters, Nationality: Iraqi, Languages: Arabic & English (Both Fluent)*

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## PROFESSIONAL SUMMARY

I am a highly qualified university researcher with a PhD in Organic and Computational Chemistry, specializing in advancing synthetic methodologies at the intersection of experimental organic synthesis and computational investigations. My expertise lies in meticulously designing and executing projects with precision to discover new, efficient reactions, reagents, and catalysts. My goal is to drive innovation and make substantial contributions to the field.

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## WORK EXPERIENCE

- **March 2023 – Till Now:** Lecturer of Organic Chemistry at the Al-Qassim Green University
- **July 2022 – Till Now:** Visiting Scientist at the University of Malaya (Prof. Dr. Azhar Ariffin)
- **September 2021 – September 2023:** Lecturer of Organic Chemistry (I & II) and Biochemistry I at Komar University of Science and Technology
- **March 2019 – July 2021:** Academic Scientist and Lecturer of General Chemistry at the University of Al-Ameed
- **March 2019 – July 2021:** Head of Continuing Education Department at the University of Al-Ameed
- **February 2019 – February 2023:** Visiting Scientist at the University of Southampton (Prof. Dr. Richard Brown)
- **May 2016 – January 2019:** Part-Time Lab Teaching & Grading in Undergraduate Lab, and Supervision of Three Undergraduate Project Students at the University of Southampton/UK during my Doctorate Studies

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## EDUCATION

- **May 2015 – January 2019:** Doctor of Philosophy in Chemistry, University of Southampton/UK  
Supervised by Richard C. D. Brown (Professor of Organic Chemistry) and Chris-Kriton Skylaris (Professor of Computational Chemistry).
- **September 2009 – July 2012:** Master's Degree in Chemistry, University of Babylon/Iraq  
Supervised by Prof. Dr. Abbass Abid Ali Drea.
- **October 2005 – June 2009:** Bachelor's Degree in chemistry, University of Babylon/Iraq (5<sup>th</sup> out of 110 students)

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## RESEARCH & TEACHING INTERESTS

- Organcatalysis and organometallic reactions for asymmetric synthesis through the interface of experimental organic synthesis and computational chemistry
- Developing organic methodologies through computational investigations to predict and design of new efficient reactions, reagents, and catalysts
- Understanding and developing photochemical synthesis
- Realizing and rationalizing reaction mechanisms through high-level computational simulations

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## COURSES TAUGHT

- **Organic Chemistry I:** Structure and Bonding, Acids and Bases, Functional Groups of Organic Chemistry, Conformational Isomerism, Stereochemistry, Introduction to Reaction Mechanisms.
- **Organic Chemistry II:** Nucleophilic Substitution and Elimination, Nucleophilic Carbonyl Addition, Nucleophilic Acyl Substitution, Carbonyl  $\alpha$ -Substitution, Electrophilic Addition to Alkenes and Alkynes, Electrophilic Aromatic Substitution, Rearrangement, Pericyclic, and Metal-Catalyzed Cross Coupling Reactions
- **Biochemistry I:** Carbohydrates, Amino acids, Proteins, Enzymes, Lipids & Fatty Acids, and Nucleic acids
- **General Chemistry:** Acids & Bases & Salts, pH & Buffers, Solutions & Solubility & Concentration, introduction to organic chemistry, and introduction to biochemistry.

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## ACADEMIC SERVICES

- **February 2023 – September 2023:** Main Paper Reviewer for “The 3<sup>rd</sup> International Conference on Research Challenges and Recent Trends in Applied and Humanitarian Science”
- **October 2022 – July 2023:** Scientific Committee at Komar University of Science and Technology
- **February 2020 - July 2022:** Plagiarism Central Committee at the University of Al-Ameed
- **February 2020 - July 2022:** Scientific Committee for the University’s Website at the University of Al-Ameed
- **February 2020 - July 2022:** Central Scientific Committee for the University’s Ranking at the University of Al-Ameed
- **May 2019 - July 2022:** Head of Continuing Education Department at the University of Al-Ameed

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## RESEARCH SKILLS

- **Lab Skills:** Synthesis, column chromatography, crystallization, distillation, rotary evaporators, high-vacuum line pumps, and characterization of complex organic compounds using NMR spectroscopy analysis adapted with ACD lab program, high- and low-resolution mass spectroscopy, HPLC analysis, FTIR spectroscopy, Melting points, Polarimeter. Motivated to learn more analysis skills
- **Computational Chemistry Skills:** Proficient in using computational scripts and programs with Linux operating system for **Computational Chemistry Simulations** such as Gaussian, ORCA, NWChem and so on. Professional in rationalizing reaction mechanisms and determine their transition states and intermediates along potential energy surface, and professional in excited state simulations. Motivated to learn more analysis skills.

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## AWARDS

- Excellence Golden-Shield Award for Science **2020**/The Institution of Holy Abbassya Shrine
- Researcher of the Year Acknowledgment Letter **2020**/University of Al-Ameed
- Researcher of the Year Award **2020**/The University of Al-Ameed
- Eleven Recognizable Appreciation Awards for Research Achievements **2019-2020** /University of Al-Ameed
- PhD Scholarship of the Iraqi Prime Minister (HCED) **2013**
- MSc Scholarship from the University of Babylon **2009**

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## TALKS AND POSTERS

- NSCCS Applied Computational Chemistry Workshop for Synthetic Chemists, **5<sup>th</sup> and 6<sup>th</sup> July 2016**, Department of Chemistry Imperial College London, UK
- Oxford Synthesis Summer Conference 2016 OSSC, **11<sup>th</sup> & 12<sup>th</sup> August 2016**, University of Oxford/UK
- RSC Organic Division South-West Regional Meeting, **1<sup>st</sup> February 2017**, University of Bath/UK
- 32<sup>nd</sup> Annual Postgraduate Symposium, **20<sup>th</sup> September 2017**, Burlington House, London/UK
- University of Southampton, **15<sup>th</sup> September 2017**, University of Southampton/UK
- ChemCYS Chemistry Conference for Young Scientists, **21<sup>st</sup> - 23<sup>rd</sup> February 2018**, Blankenberge/Belgium

- SCI 29<sup>th</sup> Regional Postgraduate Symposia on Novel Organic Chemistry-UCL, **10<sup>th</sup> April 2018**, University College London/UK
- Oxford Synthesis Summer Conference 2018 OSSC, **25<sup>th</sup> & 26<sup>th</sup> June 2018**, University of Oxford/UK
- Postgraduate Chemistry Talks, **21<sup>st</sup> September 2018**, University of Southampton/UK
- RSC Physical Organic Chemistry Postgraduate Meeting 2018, **27<sup>th</sup> September 2018**, GSK Stevenage/UK.
- Continuing Educational Department Talk, **31<sup>st</sup> December 2019**, University of Al-Ameed/Iraq.
- Komar University of Science and Technology Talk, **December 2021**, Sulaymaniyah, Iraq.
- Scientific Meeting Talk, **25<sup>th</sup> September 2021**, Komar University of Science and Technology/Iraq

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## PROFESSIONAL MEMBERSHIP

- Associate Member of Royal Society of Chemistry/UK
- Associate Member of American Chemical Society/USA

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## COLLABORATORS

- Prof. Dr. Richard C. D. Brown / University of Southampton /United Kingdom
- Assoc. Prof. Dr. Sami Lakhdar / Université Toulouse 3 Paul Sabatier / France
- Prof. Dr. Azhar Ariffin / Universiti Malaya / Malaysia
- Dr. Hafiz Saqib Ali / University of Oxford / United Kingdom

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## PUBLICATIONS (GS, ORCID, RG)

### *Under Review*

- 1- Nor Shafiq Mohd Jamel, Levani Skhirtladze, **Aqeel A. Hussein\***, Kai Lin Woon, Muhammad Kumayl Abd Wahab, Juozas V. Grazulevicius, and Azhar Ariffin\*, Two-Fold Buchwald-Hartwig Amination Assisted by Microwave Irradiation for the Preparation of Donor-Acceptor-Donor TADF Compounds, **2023**, Under Review.

### *Published*

- 2- **Aqeel A. Hussein\*** and Azhar Ariffin, Remote Steric and Electronic Effects of NHC Ligands on Alkene Reactivity and Regioselectivity Towards Hydrocupration Reactions: Role of Expanded-Ring NHCs, *J. Org. Chem.*, **2023**, 88, 13009–13021 (SCIE=Q1, IF=4.198) [DOI](#)
- 3- Hassan Hammud, Mohamad Hammoud, Aqeel A. Hussein, Youssef Fawaz, Malai Hamid, Nadeem Sheikh\*, Removal of Malachite Green using Hydrochar from Palm Leaves, *Sustainability*, 2023, 15, 8939. (SCIE=Q2, IF=4.39) [DOI](#)
- 4- Valentin Magnéa, Corentin Bellangera, **Aqeel A. Hussein**, Nathalie Saffon-Merceron, Sami Lakhdar\*, Visible Light-Mediated Germanylation of Aryl Fluorides: Synthetic and Mechanistic Insights, *Synthesis*, **2023**, 55, A-H. (SCIE=Q2, IF=3.0) [DOI](#)
- 5- Yumiao Ma\* and **Aqeel A. Hussein\***, Partner Effect in Accelerating Pincer-Co Catalyzed Nitrile Hydroboration Reactions, *Phys. Chem. Chem. Phys.*, **2023**, 25, 3110–3120. (SCIE=Q1, IF=3.945) [DOI](#)

- 6- Hafiz Saqib Ali, **Aqeel A. Hussein\***, and Mohammed Obies, Impact of Counteranions on N-Heterocyclic Carbene Gold(I)-Catalyzed Cyclization of Propargylic Amide, *RSC Advances*, **2023**, 13, 2896–2902. (SCIE=Q2, IF=4.036) [DOI](#)
  
- 7- Yumiao Ma\* and **Aqeel A. Hussein\***, Formal Pericyclic-Coupled Electron Transfer: I. Stepwise Formal Diels-Alder Cycloaddition Enabled by Addition-Coupled Electron Transfer, *ChemistrySelect*, **2022**, 7, e202202354. (SCIE=Q2, IF=2.307) [DOI](#)
  
- 8- **Aqeel A. Hussein\*** and Yumaio Ma, Unveiling the Origin of Chemoselectivity of Bismacrocycles-Catalyzed C–H Arylation of Phenols: From Mechanism Concept to New Coupling Design, *Org. Chem. Front.*, **2022**, 9, 4890–4901. (SCIE=Q1, IF=5.456) [DOI](#)
  
- 9- Yumiao Ma and **Aqeel A. Hussein\***, The Potential Role of Addition Coupled Electron Transfer (ACET) in Single Atom Catalysis: The Hydrogen Transfer from Metalloporphyrin to Imine is an ACET, *ChemRxiv*, **2022**, DOI: 10.26434/chemrxiv-2022-p1p49. (Preprint) [DOI](#)
  
- 10- Mohammed Obies\* and **Aqeel A. Hussein\***, The Nature of Metal-Metal Bonding in Re-, Ru- and Os-Corrole Dimer, *RSC Adv.*, **2022**, 12, 18728–18735. (SCEI=Q2, IF=4.036) [DOI](#)
  
- 11- Yumiao Ma and **Aqeel A. Hussein\***, Formal Pericyclic-Coupled Electron Transfer: I. Stepwise Formal Diels-Alder Cycloaddition Enabled by Addition-Coupled Electron Transfer, *ChemRxiv*, **2022**, DOI:10.26434/chemrxiv-2022-zt155-v3. (Preprint) [DOI](#)
  
- 12- Mohammed Obies and **Aqeel A. Hussein\***, The Nature of Metal-Metal Bonding in Re- and Os-Corrole Dimer, *ChemRxiv*, **2022**, DOI: 10.26434/chemrxiv-2022-f7tc8. (Preprint) [DOI](#)
  
- 13- Yuri M. Shafran, **Aqeel A. Hussein**, Nikolai A. Belyaev, Vadim A. Shevyrin, Sergey Shityakov, Tetyana V. Beryozkina, and Vasilii A. Bakulev\*, Selective Synthesis of Azoloyl NH-1,2,3-Triazoles and Azoloyl Diazoketones: Experimental and Computational Insights, *ACS Omega*, **2022**, 7, 5008–5031. (SCIE=Q1, IF=4.132) [DOI](#)
  
- 14- **Aqeel A. Hussein\***, Yumiao Ma, and Gamal A. I. Moustafa, Predominance of the Second Cycle in the Homogeneous Os-Catalyzed Dihydroxylation: Nature of Os(VI)→Os(VIII) Reoxidation and Unprecedented Roles for the Amine-N-Oxide, *Catal. Sci. Technol.*, **2021**, 12, 880–893. (SCIE=Q1, IF=6.177) [DOI](#)
  
- 15- Yumiao Ma, Hafiz Saqib Ali, and **Aqeel 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. (SCIE=Q1, IF=6.177) [DOI](#)
  
- 16- Yumiao Ma, **Aqeel A. Hussein\***, and Zhaohong Wang, Boosting Palladium Catalyzed Aryl–Nitro Bond Activation Reaction by Understanding the Electronic, Electrostatic and Polarization Effect: A Computational Study from Basic Understanding to Ligand Design, *J. Org. Chem.*, **2022**, 87, 531–539. (SCIE=Q1, IF=4.198) [DOI](#)
  
- 17- Fatima Rammal, Di Gao, Sondes Boujnah, **Aqeel A. Hussein**, Jacques Lalevée, Annie–Claude Gaumont, Fabrice Morlet-Savary, and Sami Lakhdar, Photochemical C–H Silylation and Hydroxymethylation of Pyridines and Related Structures: Synthetic Scope and Mechanisms, *ACS Catal.*, **2020**, 10, 13710–13717. (SCIE=Q1, IF=13.7) [DOI](#)

- 18- **Aqeel A. Hussein\***, Yumiao Ma, and Ahmed A. Al-Yasari, Hypervalent Iodine-Mediated Styrene Hetero- and Homodimerizations Initiation Proceeds with Two-Electron Reductive Cleavage, *Eur. J. Org. Chem.*, **2020**, 2020, 7219–7228. (SCIE=Q1, IF=3.192) [DOI](#)
- 19- Fatma Rammal, Di Gao, Annie–Claude Gaumont, Jacques Lalevée, Fabrice Morlet-Savary, **Aqeel A. Hussein**, and Sami Lakhdar\*, Visible-Light-Mediated C–H Alkylation of Pyridine Derivatives, *Org. Lett.*, **2020**, 22, 7671–7675. (SCIE=Q1, IF=6.07) [DOI](#)
- 20- **Aqeel A. Hussein\*** and Hafiz S. Ali, Revealing the 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. (SCIE=Q1, IF=4.198) [DOI](#)
- 21- **Aqeel A. Hussein\*** and Hafiz S. Ali, Revealing the Mechanism and Origin of Reactivity of Au(I)-Catalyzed Functionalized Indenone Formation of Cyclic and Acyclic Acetals of Alkynylaldehydes, *ChemRxiv*, **2020**, DOI :10.26434/chemrxiv.12745529.v2. (Preprint) [DOI](#)
- 22- Sergey Shityakov, Anneli Fischer, Kuan-Pin Su, **Aqeel A. Hussein** and Jens Broscheit, A Novel Approach for Characterizing Propofol Binding Affinities to Serum Albumins from Different Species, *ACS Omega*, **2020**, 5, 25543–25551. (SCIE=Q1, IF=4.132) [DOI](#)
- 23- **Aqeel A. Hussein\***, Ru-Catalysed Oxidative Cyclisation of 1,5-Dienes: an Unprecedented Role for the Co-Oxidant, *RSC Advances*, **2020**, 10, 15228–15238. (SCIE=Q1, IF=4.036) [DOI](#)
- 24- D. Esmailpour, **Aqeel A. Hussein**, F. A. Almalki, Sergey. Shityakov, A. K. Bordbar, Probing Inclusion Complexes of 2-Hydroxypropyl- $\beta$ -Cyclodextrin with Mono-Amino Mono-Carboxylic Acids: Physicochemical Specification and Characterization and Molecular Modelling, *Heliyon*, **2020**, 6, e03360. (SCIE=Q1, IF=3.77) [DOI](#)
- 25- **Aqeel A. Hussein\***, Azzam A. M. Al-Hadedi, Alaa J. Mahrath, Gamal A. I. Moustafa, Faisal A. Almalki, Alaa Alqahtani, Sergey Shityakov, and Moaed E. Algazally, Mechanistic Investigations on Pinnick Oxidation: A Density Functional Theory Study, *R. Soc. Open Sci.*, **2020**, 7, 191568. (SCIE=Q1, IF=3.65) [DOI](#)
- 26- **Aqeel A. Hussein**, Maximillian J. S. Phipps, Chris-Kriton Skylaris, and Richard C. D. Brown\*, Mechanism of the Os-Catalyzed Oxidative Cyclization of 1,5-Dienes, *J. Org. Chem.*, **2019**, 84, 15173–15183. (SCIE=Q1, IF=4.198) [DOI](#)
- 27- **Aqeel A. Hussein\***, Faisal A. Almalki, Alaa M. Alqahtani, and Sergey Shityakov, Computational Assessments on Diastereoselective [4+2] Cycloaddition and 1,3-Borotopic Shift of Dearomatized Tertiary Boronic Ester Intermediate: Reactivities Explained Through Transition-State Distortion Energies, *RSC Adv.*, **2019**, 9, 23148–23155. (SCIE=Q1, IF=4.036) [DOI](#)
- 28- Sergey Shityakov, Ehsan Bigdelian, **Aqeel A. Hussein**, Muhammad Bilal Hussain, Yogesh Chndra Tripathi, Muhammad Usman Khan, Mohammad Ali Shariati, Phytochemical and Pharmacological Attributes of Piperine: A Bioactive Ingredient of Black Pepper, *Eur. J. Med. Chem*, **2019**, 176, 149-161. (SCIE=Q1, IF=7.088) [DOI](#)
- 29- **Aqeel A. Hussein**, Chris-Kriton Skylaris, and Richard C. D. Brown, Oxidative Cyclisation of 1,5-Dienes by Metal Oxo Agents: Synthetic and Computational Investigations, *University of Southampton*, **2018**. (Doctoral Thesis) [DOI](#)

30- **Aqeel A. Hussein**, Chris-Christon Skylaris, and Richard C. D. Brown\*, Permanganate-Mediated Oxidative Cyclization of 1,5-Dienes using a Chiral Phase Transfer Catalyst: Synthetic and Computational Investigations, *Oxford Synthesis Summer Conference OSSC*, 25<sup>th</sup>-26<sup>th</sup> June **2018**. (Conference)