

# Jamie A. Cadge

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## Professional Appointments

- 2025–present      **Lecturer (Assistant Professor) at the University of Bath, UK**  
Joint between the Department of Chemistry and Department of Chemical Engineering
- 2021–2025      **Postdoctoral Research Fellow at the University of Utah, USA**  
Advisor: Prof. Matthew S. Sigman  
Research: Data science-driven organometallic chemistry and catalysis  
Affiliated with the NSF CCI Center for Computer Assisted Synthesis (C-CAS)
- 2015      **Summer Research Placement at GlaxoSmithKline (GSK) Medicines Research Centre, Stevenage, UK**  
Research: Synthesis of novel drug candidates for respiratory medicine
- 2014      **Summer Research Placement at the University of Nottingham, UK**  
Advisor: Dr James Dowden  
Research: Synthesis of organic compounds for use in additive manufacturing

## Education

- 2016–2021      **University of Bristol, UK**  
PhD (part of the Bristol Chemical Synthesis Centre for Doctoral Training)  
Advisors: Prof. John F. Bower and Dr Christopher A. Russell  
Thesis title: New strategies for gold redox chemistry
- 2012–2016      **University of Nottingham, UK**  
MSci (Hons), 1<sup>st</sup> Class, Medicinal and Biological Chemistry  
Final year project advisor: Dr (now Prof.) Liam T. Ball  
Project: Methodology towards bismuth-catalyzed aromatic fluorinations

## Professional Affiliations

- 2023–present      Member of the American Chemical Society (ACS)  
2022–present      Member of the Royal Society of Chemistry (MRSC)  
2016–2022      Associate Member of the Royal Society of Chemistry (AMRSC)

## Publications

10. Jacob C. Turner-Dore, Joseph J. Bell-Tyrer, Hannah E. Askey, Darren L. Richards, Oleksandr Polishchuk, Oleksandr P. Datsenko, Jamie A. Cadge, Pavel K. Mykhailiuk, Maria Ciaccia, Alexander J. Cresswell, Scalable Photocatalytic Annulation of Primary Amines to  $\delta$ -Lactams: Access to Privileged (Spiro)Piperidine Space. *ChemRxiv* **2025**, DOI: 10.26434/chemrxiv-2025-2cx97. [Pre-print]
9. Lucas Mele, Philipp D. Engel, Jamie A. Cadge, Vytautas Peciukenas, Hoonchul Choi, Matthew S. Sigman, Josep Cornella, Ligand-Controlled Chemodivergent Bismuth Catalysis. *J. Am. Chem. Soc.* **2025**, *147*, 42415.
8. Jamie A. Cadge, Sierra D. Hart, Richard C. Walroth, Kyle A. Mack, Matthew S. Sigman, Bisphosphine Ligand Conformer Selection to Enhance Descriptor Database Representation: Improving Statistical Modelling Outcomes. *Chem. Sci.* **2025**, *16*, 20473.

7. Brock A. Stenfors, [Jamie A. Cadge](#), Santeri Aikonen, Guilian Luchini, Jessica Whahlers, Kevin Koh, Mikko Muuronen, Maximilian Menche, Mark Pfeifle, Angus Keto, Robert S. Paton, Matthew S. Sigman and Olaf Weist. Conformation Dependent Features of Bisphosphine Ligands. *J. Org. Chem.* **2025**, 90, 13874.
6. [Jamie A. Cadge](#), Cedric Lozano, Morgan T. Merriman, Paul Oblad, Matthew S. Sigman and Sarah E. Reisman. A Data Science-Guided Approach for the Development of Nickel-Catalyzed homo-Diels-Alder Reactions. *J. Am. Chem. Soc.* **2025**, 147, 31175.
5. Jonas Düker, Maximilian Philipp, Thomas Lentner, [Jamie A. Cadge](#), João E. A. Lavarda, Ruth M. Gschwind, Matthew S. Sigman, Indrajit Ghosh and Burkhard König. Cross-coupling reactions with nickel, visible light, and tert-butylamine as a bifunctional additive. *ACS. Catal.* **2024**, 15, 817.
4. Samuel C. Scott, [Jamie A. Cadge](#), Grace K. Boden, John F. Bower and Christopher A. Russell, A hemilabile NHC-complex and its application to the redox neutral 1,2-oxyarylation of feedstock alkenes. *Angew. Chem. Int. Ed.* **2023**, 62, e202301526. [Hot Paper]
3. [Jamie A. Cadge](#), Paul J. Gates, John F. Bower and Christopher A. Russell, Migratory insertion of CO into a Au-C bond. *J. Am. Chem. Soc.* **2022**, 144, 19719.
2. [Jamie A. Cadge](#), John F. Bower and Christopher A. Russell, A systematic study of the effects of complex structure on aryl iodide oxidative addition at bipyridyl-ligated gold(I) centers. *Angew. Chem. Int. Ed.* **2021**, 60, 24976.
1. [Jamie A. Cadge](#), Hazel A. Sparkes, John F. Bower and Christopher A. Russell, Oxidative addition of alkenyl and alkynyl iodides to a gold(I) complex. *Angew. Chem. Int. Ed.* **2020**, 59, 6617.

Manuscripts submitted / currently in preparation:

- [Jamie A. Cadge](#), Charlotte Lorton, John F. Bower and Christopher A. Russell, A base-free gold-catalyzed Suzuki-Miyaura cross-coupling.
- [Jamie A. Cadge](#), Neal W. Sach and Matthew S. Sigman, Learning from high-throughput experimentation datasets using the kraken monophosphine ligand library: A case study.

## Awards and Prizes

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6. Selected talk from posters at the Physical Organic Chemistry Gordon Research Conference (2025)
5. NSF Center for Computer Assisted Synthesis Professional Development Award (2025)
4. University of Bristol Faculty of Science Thesis Commendation (2022)
3. University of Bristol Doctoral Prize nomination for the Faculty of Science (2022)
2. Poster prize at the Mechanistic Processes in Organometallic Chemistry Faraday Discussion, University of York, UK (2019)
1. Poster prize at the Oxford Synthesis Summer Conference, University of Oxford, UK (2018)

## Research Presentations and Posters

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18. *Presentation*: UK Catalysis Hub joint workshop with the Physical Sciences Data-Science Infrastructure (PSDI), Rutherford Appleton Laboratory, Harwell Campus, Oxfordshire, UK, March 2026
17. *Workshop*: Cheminformatics, Automation and Machine Learning in Chemistry (CAMLC), Consejo Superior de Investigaciones Científicas (CSIC) Aragon, Zaragoza, Spain, September 2025
16. *Presentation*: (Selected talk from posters) Physical Organic Chemistry Gordon Research Conference, NH, USA, July 2025
15. *Poster*: Physical Organic Chemistry Gordon Research Conference, NH, USA, July 2025
14. *Presentation*: Seminar (invited), Genentech, San Francisco, CA, USA, June 2024
13. *Poster*: Computational Chemistry Gordon Research Conference, ME, USA, July 2024
12. *Presentation*: Seminar (invited), University of Wisconsin-Madison, WI, USA, October 2023
11. *Poster*: National Organic Symposium, University of Notre Dame, IN, USA, July 2023
10. *Poster*: Center for Computer Assisted Synthesis (C-CAS) Bi-Annual Meeting, University of Notre Dame, IN, USA, July 2023
9. *Presentation*: Dalton 2021 – Joint Interest Group Meeting (virtual), June 2021
8. *Presentation*: Inorganic Reaction Mechanisms Discussion Group Annual Meeting (virtual), July 2020
7. *Presentation*: Dalton Younger Members Event (DYME 2019), Cardiff University, UK, October 2019

6. *Poster: Mechanistic Processes in Organometallic Chemistry* Faraday Discussion, University of York, UK, October 2019
5. *Presentation: Bristol Chemical Synthesis CDT Summer Conference*, University of Bristol, UK, June 2019
4. *Poster: Syngenta Poster Competition*, University of Bristol, UK, April 2019
3. *Presentation: CDT in Catalysis Half-Day Seminar (invited)*, Cardiff University, UK, November 2018
2. *Poster: Gold 2018*, Sorbonne Université, Paris, France, July 2018
1. *Poster: Oxford Synthesis Summer Conference*, University of Oxford, UK, June 2018

## Teaching

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- **CH52072:** AI and Machine Learning for Sustainable Chemical Technologies (Unit Convenor) – *Part of the Centre for Doctoral Training in Sustainable Chemical Technologies*
- **AR52001:** AI and Sustainable Development – *Part of the MSc in Artificial Intelligence for Engineering and Design*
- **CH22008:** Fundamental Concepts of Chemistry (organic chemistry tutorials)

### Previous teaching experience:

6. Designed and delivered content on data science in physical organic chemistry for Prof. Shannon S. Stahl's Physical Organic Chemistry postgraduate course at the University of Wisconsin-Madison
5. Delivered guest lectures as part of Prof. Matthew S. Sigman's Organometallics postgraduate course at the University of Utah
4. Mentored an undergraduate student as part of the NSF Research Experiences for Undergraduates (REU) program in the Sigman group
3. Mentored three 4<sup>th</sup> year MSci project students (two of whom won prizes), one 3<sup>rd</sup> year BSc project student and six 1<sup>st</sup> year Bristol Chemical Synthesis CDT rotation students, all in the Russell group
2. Ran a yearly "NMR Spectroscopy in Inorganic Chemistry" problem class for 1<sup>st</sup> year postgraduate students as part of the Bristol Chemical Synthesis CDT
1. Laboratory demonstrator in the 2<sup>nd</sup> year synthetic chemistry teaching lab at the University of Bristol

## Skills and Expertise

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### In the laboratory

Design of syntheses of organometallic complexes and ligands towards the development of novel gold-catalysed and -mediated reactions. Use of organic synthesis for ligand framework/substrates and physical organic chemistry techniques (including studying reaction kinetics by <sup>1</sup>H/<sup>19</sup>F/<sup>31</sup>P NMR spectroscopy and ReactIR) to study new reactivity of gold complexes. Extensive use of inert atmosphere techniques (Schlenk line and glovebox) for handling and synthesis of organometallic complexes. Experience with column chromatography (including automated flash chromatography systems) and distillation for compound purification. Developing skills around the design and use of automated synthesis platforms.

### Analytical techniques

Experienced in the use of NMR spectroscopy (including heteronuclear NMR spectroscopy and a range of 2D experiments), FTIR spectroscopy, UV/Vis spectroscopy, GC-FID/MS and HPLC for analysis of pure compounds for structural assignment and reaction mixture analysis. Use of powder and single-crystal X-ray diffraction and solving structures using the Olex2 software package.

### Computational and data science techniques

Have experience of running density functional theory (DFT) calculations using the Gaussian, ORCA and Jaguar software packages – implemented on command-line based Linux clusters. Experience of using the xTB program for tight-binding semi-empirical calculations and running conformer searches using MacroModel, CREST and RDKit. Good working knowledge of Python for implementing data science/machine learning packages such as scikit-learn, PyTorch, BoTorch. With this, I have experience with plotting and data visualization packages such as matplotlib and seaborn. Also, a frequent user of Git and GitHub for code versioning and dissemination of code.