

Professional Experience

Colorado State University, Department of Chemistry

- 2023 – Marshall Fixman and Branka Ladanyi Professor of Chemistry
2021 – Full Professor of Chemistry
2018 – 2021 Associate Professor: Colorado State University

University of Oxford, Department of Chemistry

- 2014 – 2017 Associate Professor in Organic Chemistry
2010 – 2014 University Lecturer in Organic Chemistry
2010 – 2017 Tutorial Fellow in Organic Chemistry: St Hilda's College, Oxford

Education & Training

UCLA, Department of Chemistry and Biochemistry

- 2009 – 2010 Fulbright UK-US Distinguished Postdoctoral Research Fellow
Research Advisor: Prof. K. N. Houk

University of Cambridge

- 2008 – 2009 St Catharine's College, Cambridge
Junior Research Fellow in Chemistry
2005 – 2008 PhD studies in the Department of Chemistry
Research advisor Prof. Jonathan M. Goodman
"Computational Studies of Boron Mediated C-C Bond Formation"
2000 – 2004 Trinity Hall, Cambridge
MA MSci Natural Sciences (Chemistry and Mathematics)
1st class degree, ranked top in the University
University Rafael Prize in Organic Chemistry; Trinity Hall prize in Natural Sciences

Awards & Honors

- 2026-2028 Chair, IUPAC Conference on Physical Organic Chemistry
2025 Lu Jiaxi Lecturer, Xiamen University
2024 CSU Faculty Excellence in Graduate Mentoring Award
2024 *ChemComm* Pioneering Investigator
2023 Marshall Fixman and Branka Ladanyi Professor of Chemistry
2022 – 2024 Co-chair, Gordon Conference on Computational Chemistry
2019 Fellow of the Royal Society of Chemistry (FRSC)
2017 *Nature Journals* Outstanding Reviewer
2016 *Chem. Soc. Rev.* Emerging Investigator
2015 ACS COMP Division Outstanding Junior Faculty Award
2015 RSC Harrison-Meldola Memorial Medal
2015 Thieme Chemistry Journal Award
2014 Molecular Graphics and Modelling Society Silver Jubilee Award
2014 ACS Organic Division Young Academic Investigators Award
2009 – 2010 Distinguished Fulbright-AstraZeneca Research Scholarship
2009 – 2010 Royal Commission for the Exhibition of 1851 Science Research Fellowship
2008 UK Head Mentor, 40th International Chemistry Olympiad, Budapest, Hungary

Publications

217. Fundamental Study of Density Functional Theory Applied to Triplet State Reactivity: Introduction of the

- TRIP50 Dataset. Hughes, W. B.; Popescu, M. V.; Paton, R. S. *J. Chem. Theory Comput.* **2026**, DOI: 10.1021/acs.jctc.6c00144
- 216.** A radical–polar crossover approach to complex nitrogen heterocycles via the triplet state. Lockhart, Z.; Popescu, M. V.; Alegre-Requena, J. V.; Ahuja, J.; Paton, R. S.; Smith, M. D. *Chem* **2026**, 102904
- 215.** Synthesis and properties of allylic, benzylic, propargylic and allenyl oxonium ions. Chan, H. S. S.; Li, Y.; Sutro, J. L.; Brown, D. S.; Paton, R. S.; Burton, J. W. *Nat. Synth.* **2026**, DOI: 10.1038/s44160-025-00964-8
- 214.** Potassium Metabisulfite’s Role in Developing a Robust Platform for Enantioenriched N-Alkylpyridinium Salts as Piperidine Precursors. Selingo, J. D.; King, J. R.; Pio, B.; Neel, A. J.; Lam, Y.-h.; Paton, R. S.; Maddess, M. L.; McNally, A. J. *Am. Chem. Soc.* **2026**, *148*, 8621–8633
- 213.** Peptide Catalysts Conformationally Tuned for Fluoride Binding and Delivery. Poškaitė, G.; Schlatzer, T.; Chen, Z.; Popescu, M. V.; Paton, R. S.; Gouverneur, V. *J. Am. Chem. Soc.* **2026**, *148*, 9238–9243
- 212.** Deep learning for asymmetric catalysis. Paton, R. S.; Kim, S. *Nat. Comput. Sci.* **2026**, *6*, 115–116
- 211.** The Atroposelective Iodination of 2-Amino-6-arylpyridines Catalyzed by Chiral Disulfonimides Actually Proceeds via Brønsted Base Catalysis: A Combined Experimental, Computational, and Machine-Learning Study. Parmar, K. S.; Bawel, S.; Popescu, M. V.; Mai, B. K.; Timmerman, J. C.; Altundas, B.; Paton, R. S.; Denmark, S. E. *J. Am. Chem. Soc.* **2026**, *148*, 2175–2190
- 210.** Direct Aziridine Synthesis from Amines and Styrenes via a Base-Promoted Oxidative Cascade Reaction. Vásquez Tapia Vera, C.; Hughes, W. B.; Klaus, D. R.; Paton, R. S.; Bandar, J. S. *J. Am. Chem. Soc.* **2026**, *148*, 494–503
- 209.** Direct Analysis of Nickel Catalyst Speciation in Reductive Biaryl Synthesis Using Thin Layer Electrochemistry and a Microelectrode. Punchihewa, B. T.; Romero-Arenas, A.; Paton, R. S.; Weix, D. J.; Stahl, S. S.; Rafiee, M. J. *Am. Chem. Soc.* **2025**, *147*, 44667–44672
- 208.** Direct C–H Lactonization of Carboxylic Acids Enabled by LMCT Photoactivation. Weber, K. M.; Villanueva, R.; Popescu, M. V.; Lutovsky, G. A.; Gockel, S. N.; Paton, R. S.; Yoon, T. P. *Angew. Chem. Int. Ed.* **2025**, e15582
- 207.** A Fragment Based Approach Towards Curating, Comparing and Developing Machine Learning Models Applied in Photochemistry. Pérez-Soto, R.; Popescu, M. V.; Kumar, S.; Adao Gomes, L. Lee, C.; Shore, E.; Lopez, S. A.; Paton, R. S.; Kim, S. *Chem. Sci.* **2025**, *16*, 21874–21886
- 206.** Structure-Property-Performance Relationships of Tetra-alkylated Phenazine Photoredox Catalysts in Organocatalyzed Atom Transfer Radical Polymerization. Wolff, A. M.; Clark, T. R.; Gomes, L. A.; Sau, A.; Portela, B. S.; Puffer, K. O.; Lamb, Y. M. L.; Paton, R. S.; Lopez, S. A.; Damrauer, N. H.; Miyake, G. M. *Macromolecules* **2025**, *58*, 12241–12249
- 205.** Organocatalyzed Atom Transfer Radical Polymerization (O-ATRP) Using a Super-Reducing Photoredox Catalyst. Zhao, Y.; Portela, B. S.; Green, A. R.; Wolff, A. M.; Liu, X.; Puffer, K. O.; Sau, A.; Damrauer, N. H.; Paton, R. S.; Miyake, G. M. *Angew. Chem. Int. Ed.* **2025**, e202517641
- 204.** Reduction and Deuteration of N-Heteroarenes Using an Organic Photoredox Catalyst. Bains, A. K.; Sau, A.; Portela, B. S.; Paton, R. S.; Miyake, G. M.; Damrauer, N. H. *Chem* **2025**, *5*, 102822
- 203.** Ir-Catalyzed Allylation of Boranes via Enantioselective Petasis-Type 1,4-Migration. Wen, J.; Zhang, L.; He, C.; Song, S.-m.; Tyler, J.; Paton, R. S.; Aggarwal, V. K. *J. Am. Chem. Soc.* **2025**, *147*, 36940–36946.
- 202.** Conformation Dependent Features of Bisphosphine Ligands. Stenfors, B.; Cadge, J.; Aikonen, S.; Luchcini, G.; Wahlers, J.; Koh, K.; Muuronen, M.; Menche, M.; Pfeifle, M.; Keto, A.; Paton, R.; Sigman, M.; Wiest, O. *J. Org. Chem.* **2025**, *90*, 13874–13884.
- 201.** Photocatalysis as a mechanistic probe for the Staudinger β -lactam synthesis. Popescu, M. V.; Parker, N. A.; Jia, Z.; Solon, P.; Alegre-Requena, J. V.; Paton, R. S.; Smith, M. D. *Chem Catal.* **2025**, *5*, 101493
- 200.** Impact of oxygen and sulfur heteroatom core substitution on properties and performance of phenoxazine photocatalysts. Lathrop, J. L.; Portela, B. S.; Paton, R. S.; Miyake, G. M. *Chem. Eur. J.* **2025**, e202501179
- 199.** Development and Mechanistic Exploration of Rhodium-Catalyzed Biaxially Atroposelective Click Chemistry.

Zeng, L.; Li, J.; Huang, Y.; Haug, G.; Paton, R.; Zhang, F.; Cui, S. *ACS Catal.* **2025**, *15*, 15844–15856

198. Enantioconvergent Chan–Lam Coupling: Synthesis of Chiral Benzylic Amides via Cu-Catalyzed Deborylative Amidation. Vu, J.; Haug, G.; Head, J.; Paton, R. S.; Dong, Y. *J. Am. Chem. Soc.* **2025**, *147*, 25527–25535.

197. Efficient super-reducing organic photoredox catalysis with PCET- mitigated back electron transfer. Bains, A. K.; Sau, A.; Portela, B.; Kajal, Green, A. R. Wolff, A. M.; Patin, L. F.; Paton, R. S.; Damrauer, N. H.; Miyake, G. M. *Science* **2025**, *388*, 1294–1300

196. Ethyl Pinacol Boronates as Advantageous Precursors for Copper-Mediated Radiofluorination. Hadjipaschalis, N.; Ortalli, S.; Chen, Z.; Paton, R. S.; Ford, J.; Tredwell, M.; Gouverneur, V. *Org. Lett.* **2025**, *27*, 6545–6550

195. Boron-mediated modular assembly of tetrasubstituted alkenes. Wei, L.; Popescu, M. V.; Noble, A.; Paton, R. S.; Aggarwal, V. K. *Nature* **2025**, *643*, 975–982.

194. Reductively Induced Aryl Transmetalation: An Alternative Catalytically Relevant Ni-Catalyzed Biaryl Coupling Mechanism. Romero-Arenas, A.; Popescu, M. V.; Goetz, M. K.; Sanders, K. M.; Guzei, I. A.; Rafiee, M.; Weix, D. J.; Paton, R. S.; Stahl, S. S. *J. Am. Chem. Soc.* **2025**, *147*, 21697–21707

193. Substrate-Photocatalyst Reactivity Matching Enables Broad Aryl Halide Scope in Light-Driven, Reductive Cross-Electrophile Coupling Using ¹³C NMR as a Predictor. Chrisman, C. H.; Elder, W. J.; Haug, G. C.; Pérez-Soto, R.; Bains, A. K.; Jepsen, C.; Stewart, T. K.; Sherwood, T. C.; Kudisch, M.; Boston, D. J.; Lim, C.-H.; Simmons, E. M.; Kim, S.; Paton, R. S.; Miyake, G. M. *ACS Catal.* **2025**, *15*, 8103–8113

192. Investigating Reactivity and Selectivity in a Palladium-Catalyzed Heteroleptic Ligand System for Electrophilic Arene Fluorination. Deolka, S.; Samha, M. H.; Garcia Roca, A.; Haug, G. C.; Howard, J. R.; Sandres, J.; Vasylevskiy, S.; Vanderlinden, R. T.; Paton, R. S.; Sigman, M. S. *J. Am. Chem. Soc.* **2025**, *147*, 12878–12889

191. Phosphate-enabled mechanochemical PFAS destruction for fluoride reuse. Yang, L.; Chen, Z.; Goult, C. A.; Tan, J.; Schlatzer, T.; Paton, R. S.; Gouverneur, V. *Nature* **2025**, *640*, 100–106

190. Ligand-enabled override of the memory effect in Rh-catalyzed asymmetric Suzuki reactions. Liu, K.; Egea-Arrebola, D.; Ardkehan, R.; Cunningham, L.; Christensen, K. E.; Paton, R. S.; Fletcher, S. P. *Chem* **2025**, 102550

189. Influence of dihydrophenazine photoredox catalyst excited state character and reduction potentials on control in organocatalyzed atom transfer radical polymerization. Puffer, K. O.; Portela, B. S.; Olson-Gwin, A. J.; Chism, K. A.; Dworakowska, S.; Crace, E.; Paton, R. S.; Miyake, G. M. *ACS Catal.* **2025**, *15*, 5002–5013

188. Enantioconvergent Nucleophilic Substitution of Alkyl Halides with Potassium Fluoride via Synergistic Phase-Transfer Catalysis. Dooley, C.; Ibba, F.; Botlik, B.; Goult, C.; Gao, Y.; Lister, A.; Paton, R. S.; Lloyd-Jones, G. C.; Gouverneur, V. *Nat. Catal.* **2025**, *8*, 107–115

187. Photocatalytic C–F bond activation in small molecules and polyfluoroalkyl substances. Liu, X.; Sau, A.; Green, A. R.; Popescu, M. V.; Pompetti, N. R.; Li, Y.; Zhao, Y.; Paton, R. S.; Damrauer, N. H.; Miyake, G. M. *Nature* **2025**, *637*, 601–607

186. Computer-Aided Design of Stability Enhanced Nicotinamide Cofactor Biomimetics. Platt, A.; Klem, H.; Mallinson, S.; Bomble, Y.; Paton, R. S. *Green Chem.*, **2025**, *27*, 6831–6844

185. Photooxidation of Polyolefin to Produce Materials with In-chain Ketones. Liu, X.; Hu, Z.; Portela, B. S.; Rettner, E. M.; Pineda, A.; Miscall, J.; Rorrer, N. A.; Krummel, A. T.; Paton, R. S.; Miyake, G. M. *Angew. Chem. Int. Ed.* **2025**, *64*, e202418411

184. Rapid Prediction of Conformationally-Dependent DFT-Level Descriptors using Graph Neural Networks for Carboxylic Acids and Alkyl Amines. Haas, B. C.; Hardy, M. A.; Sowndarya S. V., S.; Adams, K.; Coley, C. W.; Paton, R. S.; Sigman, M. S. *Digit. Discov.* **2025**, *4*, 222–233

183. Selective Ni-Catalyzed Cross-Electrophile Coupling of Heteroaryl Chlorides and Aryl Bromides at 1:1 Substrate Ratio. Su, Z.-M.; Poole, D. L.; Rafiee, M.; Paton, R. S.; Weix, D. J.; Stahl, S. J. *J. Am. Chem. Soc.* **2024**, *147*, 353–361

182. Molecular Complexity-Inspired Synthetic Strategies Toward the Calyciphylline A-type Daphniphyllum Alkaloids Himalensine A and Daphenylline. Wright, B. A.; Okada, T.; Regni, A.; Luchini, G.; Sowndarya, S. V. S.;

Chaisan, N.; Kölbl, S.; Kim, S. F.; Paton, R. S.; Sarpong, R. *J. Am. Chem. Soc.* **2024**, *146*, 33130–33148

181. Enantioconvergent Cross-Nucleophile Coupling: Cu-Catalyzed Deborylative Cyanation. Vu, J.; Haug, G. C.; Zhao, C.; Chang, C. J.; Paton, R. S.; Dong, Y. *Angew. Chem. Int. Ed.* **2024**, *63*, e202408745

180. Modular synthesis of aryl amines from 3-alkynyl-2-pyrones. Gardner, K. E.; de Lescure, L.; Hardy, M. A.; Tan, J.; Sigman, M. S.; Paton, R. S.; Sarpong, R. S. *Chem. Sci.* **2024**, *15*, 15632–15638

179. Platinum-Catalyzed Regio- and Enantioselective Diboration of Unactivated Alkenes with (pin)B–B(dan). Fang, H.; Manoj, N.; Popescu, M. V.; Noble, A.; Paton, R. S.; Aggarwal, V. K. *Angew. Chem. Int. Ed.* **2024**, e202413504

178. Ligand-Controlled Orthogonal Selectivity between δ and γ Positions of Long-Chain Picolinamides. Sinha, S. K.; Goswami, N.; Li, Y.; Maji, S.; Raja, D.; Sarala, A. S.; Guin, S.; Paton, R. S.; Maiti, D. *ACS Catalysis* **2024**, *14*, 12681–12693

177. Organocatalyzed Carbonylation of Alkyl Halides Driven by Visible Light. Liu, X.; Portela, B. S.; Wiedenbeck, A.; Chrisman, C. H.; Paton, R. S.; Miyake, G. M. *Angew. Chem. Int. Ed.* **2024**, e202410928

176. Combined Synthetic, Spectroscopic, and Computational Insights into a General Method for Photosensitized Alkene Aziridination. Meyer, A. R.; Popescu, M. V.; Sau, A.; Damrauer, N. H.; Paton, R. S.; Yoon, T. P. *ACS Catal.* **2024**, *14*, 12310–12317

175. Dynamic Vertical Triplet Energies: A metric for predicting triplet energy transfer. Popescu, M. V.; Paton, R. S. *Chem* **2024**, *10*, 3428–3443

174. Late-Stage “Benzenoid-to-Troponoid” Skeletal Modification of the Cephalotanes: Total Synthesis of Harringtonolide and Computational Analysis. Wiesler, S.; Sennari, G.; Popescu, M. V.; Gardner, K. E.; Aida, K.; Paton, R. S.; Sarpong, R. *Nat. Commun.* **2024**, *15*, 4125

173. A Deconstruction-Reconstruction Strategy for Pyrimidine Diversification. Uhlenbruck, B. J. H.; Josephitis, C. M.; Lescure, L.; Paton, R. S.; McNally, A. *Nature* **2024**, *631*, 87–93.

172. Radical Chlorination of Non-Resonant Heterobenzylic C–H Bonds and High-Throughput Diversification of Heterocycles. Golden, D. L.; Flynn, K. M.; Aikonen, S.; Kalyani, D.; Krska, S. W.; Paton, R. S.; Stahl, S. S. *Chem.* **2024**, *10*, 1593-1605.

171. Predicting Lewis Acidity: Machine Learning the Fluoride Ion Affinity of p-Block Atom-based Molecules. Sigmund, L. M.; Sowndarya, S. S. V.; Albers, A.; Erdmann, P.; Paton, R. S.; Greb, L. *Angew. Chem. Int. Ed.* **2024**, *63*, e202401084.

170. Mechanistic Investigation Reveals a Perylene-like Closed Shell Super-Photoreductant. Sau, A.; Pompetti, N. F.; Green, A.; Popescu, M. V.; Paton, R. S.; Miyake, G. M.; Damrauer, N. H. *ACS Catal.* **2024**, *14*, 2252–2263.

169. Designing solvent systems in chemical processes using self-evolving solubility databases and graph neural networks. Kim, Y.; Jung, H.; Kumar, S.; Claiborne, A.; Paton, R. S.; Kim, S. *Chem. Sci.* **2024**, *15*, 923–939.

168. Bottom-up Atomistic Descriptions of Top-Down Macroscopic Measurements: Computational Benchmarks for Hammett Electronic Parameters. Luchini, G.; Paton, R. S. *ACS Phys. Chem. Au.* **2024**, *4*, 259-267.

167. The catalytic effects of active site conformational change in the allosteric activation of imidazole glycerol phosphate synthase. Klem, H.; Alegre-Requena, J. V.; Paton, R. S. *ACS Catal.* **2023**, *13*, 16249–16257.

166. Expansion of Bond Dissociation Prediction with Machine Learning to Medicinally and Environmentally Relevant Chemical Space. Sowndarya, S. S. V.; Kim, K.; Kim, S.; St. John, P. C.; Paton, R. S. *Digit. Discov.* **2023**, *2*, 1900–1910.

165. Electrochemical Modification of Polypeptides at Selenocysteine. Mackay, A. G.; Maxwell, J. W. C.; Bedding, M. J.; Kulkarni, S. S.; Byrne, S. A.; Kambanis, L.; Popescu, M. V.; Paton, R. S.; Malins, L.R.; Ashhurst, A. S.; Corcilius, L.; Payne, R. J. *Angew. Chem. Int. Ed.* **2023**, *62*, e202313037.

164. Fluorochemicals from fluorspar with a phosphate-enabled mechanochemical process bypassing HF. Patel, C.; André-Joyaux, E.; Leitch, J. A.; Martínez de Irujo-Labalde, J.; Ibba, F.; Struijs, J.; Ellwanger, M. A.; Paton, R. S.; Browne, D. L.; Pupo, G.; Aldridge, S.; Hayward, M. A.; Gouverneur, V. *Science* **2023**, *381*, 302–306.

- 163.** Harnessing triaryloxonium ions for aryne generation. Smith, O.; Hindson, M.; Sreenithya, A.; Tataru, V.; Paton, R. S.; Burton, J. W.; Smith, M. D. *Nat. Synth.* **2023**, *3*, 58–66.
- 162.** Iridium-Catalyzed Asymmetric Difunctionalization of C–C σ -Bonds Enabled by Ring Strained Boronate Complexes. Shen, H. C.; Popescu, M.V.; Wang, Z. S.; Lescure, L.; Noble, A.; Paton, R. S.; Aggarwal, V. K. *J. Am. Chem. Soc.* **2023**, *145*, 16508–16516.
- 161.** Exploring Cuneanes as Benzene Isosteres and Energetic Materials: Scope and Mechanistic Investigations into Regioselective Rear-rangements from Cubanes. Son, J.Y.; Aikonen, S.; Morgan, N.; Harmata, A. S.; Sabatini, J. J.; Sausa, R.C.; Byrd, E. F. C.; Ess, D. H.; Paton, R. S.; Stephenson, C. R. J. *J. Am. Chem. Soc.* **2023**, *145*, 16355–16364.
- 160.** Pd-Catalyzed Asymmetric Amination of Enamines: Expedient Synthesis of Structurally Diverse N–C Atropisomers. Zhang, P.; Guo, C. Q.; Yao, W.; Lu, C. J.; Li, Y.; Paton, R. S.; Liu, R. R. *ACS Catal.* **2023**, *13*, 7680–7690.
- 159.** Experimental and computational studies of the production of 1,3-butadiene from bio-2,3-butanediol using silica-supported H_3PO_4 derivatives. Alegre-Requena, J. V.; Hafenstine, G. R.; Huo, X.; Guan, Y.; Stunkel, J.; Baddour, F. G.; Unocic, K. A.; Klein, B. C.; Davis, R. E.; Paton, R. S.; Vardon, D. R.; Kim, S. *Chem. Eng. J.* **2023**, *466*, 143346.
- 158.** Regiodivergent Nucleophilic Fluorination under Hydrogen Bonding Catalysis: A Computational and Experimental Study. Horwitz, M. A.; Dürr, A. B.; Afratis, K.; Chen, Z.; Soika, J.; Christensen, K. E.; Fushimi, M.; Paton, R. S.; Gouverneur, V. *J. Am. Chem. Soc.* **2023**, *145*, 9708–9717.
- 157.** Metal-free arylation of benzothiophenes at C4 by activation as their benzothiophene S-oxides. Bisht, R.; Popescu, M. V.; He, Z.; Ibrahim, A. M.; Crisenza, G. E. M.; Paton, R. S.; Procter, D. J. *Angew. Chem Int. Ed.* **2023**, e202302418.
- 156.** AQME: Automated Quantum Mechanical Environments for Researchers and Educators. Alegre-Requena, J. V.; Sowndarya, S. S. V.; Alturaifi, T.; Pérez-Soto, R.; Paton, R. S. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2023**, e1663.
- 155.** Control of stereogenic oxygen in a helically chiral oxonium ion. Smith, O.; Popescu, M. V.; Hindson, M.; Paton, R. S.; Burton, J.; Smith, M. *Nature* **2023**, *615*, 430–435.
- 154.** Catalytic enantioselective 6π photocyclization of acrylanilides. Jones, B.; Solon, P.; Popescu, M. V.; Du, J.-Y.; Paton, R. S.; Smith, M. *J. Am. Chem. Soc.* **2023**, *145*, 171–178.
- 153.** Halogenation of the 3-position of pyridines through Zincke imine intermediates. Boyle, B. T.; Levy, J. N.; de Lescure, L.; Paton, R. S.; McNally, A. *Science* **2022**, *378*, 773–779.
- 152.** Site-Selective Photocatalytic Functionalization of Peptides and Proteins at Selenocysteine. Dowman, L. J.; Kulkarni, S. S.; Alegre-Requena, J. V.; Giltrap, A. M.; Norman, A. R.; Sharma, A.; Gallegos, L. C.; Welegedara, A. P.; Watson, E. E.; Van Raad, D.; Huhmann, S.; Proschogo, N.; Patel, K.; Larence, M.; Becker, C. F. W.; Mackay, J. P.; Lakhwani, G.; Huber, T.; Paton, R. S.; Payne, R. J. *Nat. Commun.* **2022**, *13*, 6885.
- 151.** Mechanistic Studies on (3 + 2) Cycloaddition Reactions of Azides to Nitroolefins: A Computational and Kinetic Study. Kawamura, M. Y.; Alegre-Requena, J. V.; Barbosa, T. M.; Tormena, C. F.; Paton, R. S.; Ferreira, M. A. B. *Chem. Eur. J.* **2022**, *28*, e202202294.
- 150.** Umpolung Synthesis of Pyridyl Ethers via Bi(V)-Mediated O-Arylation of Pyridones. Ruffell, K.; Gallegos, L. C.; Ling, K. B.; Paton, R. S.; Ball, L. T. *Angew. Chem. Int. Ed.* **2022**, *61*, e2022128.
- 149.** Multi-objective goal-directed optimization of de novo stable organic radicals for aqueous redox flow batteries. Sowndarya, S. S. V.; Law, J.; Tripp, C.; Duplyakin, D.; Skordilis, E.; Biagioni, D.; Paton, R. S.; St. John, P. C. *Nat. Mach. Intell.* **2022**, *7*, 720–730.
- 148.** Expanding chemical space by para-C–H arylation of arenes. Maiti, S.; Li, Y.; Sasmal, S.; Guin, S.; Bhattacharya, T.; Lahiri, G.K.; Paton, R. S.; Maiti, D. *Nat. Commun.* **2022**, *13*, 3963.
- 147.** Mechanistic Studies Yield Improved Protocols for Base-Catalyzed anti-Markovnikov Alcohol Addition Reactions. Luo, C.; Alegre-Requena, J. V.; Sujansky, S. J.; Pajk, S.; Gallegos, L. C.; Paton, R. S.; Bandar, J. S. *J.*

Am. Chem. Soc. **2022**, *144*, 9586–9596.

146. ¹⁸F-Difluorocarbene for Positron Emission Tomography. Sap, J. B. S.; Meyer, C. F.; Ford, J.; Straathof, N. J. W.; Dürr, A. B.; Lelos, M. J.; Paisey, S. J.; Mollner, T. A.; Hell, S. A.; Trabanco, A.; Genicot, C.; am Ende, C. W.; Paton, R. S.; Tredwell, M.; Gouverneur, V. *Nature* **2022**, *606*, 102–108.

145. Asymmetric Azidation under Hydrogen Bonding Phase-Transfer Catalysis: A Combined Experimental and Computational Study. Wang, J.; Horwitz, M.; Dürr, A.; Ibba, F.; Pupo, G.; Gao, Y.; Ricci, P.; Christensen, K.; Pathak, T.; Claridge, T. W.; Lloyd-Jones, G.; Paton, R. S.; Gouverneur, V. *J. Am. Chem. Soc.* **2022**, *144*, 4572–4584.

144. Reading and Erasing of the Phosphonium Analogue of Trimethyllysine by Epigenetic Proteins. Kamps, J. J. A. G.; Belle, R.; Poater, J.; Kumar, K.; Pieters, B. J. G. E.; Salah, E.; Brown, T.; Claridge, T. D. W.; Paton, R. S.; Bickelhaupt, F. M.; Kawamura, A.; Schofield, C. J.; Mecinović, J. *Commun. Chem.* **2022**, *5*, 27.

143. Modeling catalysis in allosteric enzymes: Capturing conformational consequences. Klem, H.; McCullagh, M.; Paton, R. S. *Top. Catal.* **2022**, *65*, 165–186.

142. Homologation of Electron-Rich Benzyl Bromide Derivatives via Diazo C–C Bond Insertion. Modak, A.; Alegre-Requena, J. V.; Lescure, L.; Rynders, K. J.; Paton, R. S.; Race, N. *J. Am. Chem. Soc.* **2021**, *144*, 86–92.

141. A Quantitative Metric for Organic Radical Persistence Using Thermodynamic and Kinetic Features. Sowndarya, S. S. V.; St. John, P. C.; Paton, R. S. *Chem. Sci.* **2021**, *12*, 13158–13166.

140. Reactions of NO₃ with Aromatic Aldehydes: Gas phase Kinetics and Insights into the Mechanism of the reaction. Ren, Y.; Zhou, L.; Mellouki, A.; Daele, V.; Idir, M.; Brown, S.; Rusic, B.; Paton, R. S.; Ravishankara, A. R. *Atmos. Chem. Phys.* **2021**, *21*, 13537–13551.

139. Real-time Prediction of ¹H and ¹³C Chemical Shifts with DFT accuracy using a 3D Graph Neural Network. Guan, Y.; Sowndarya, S. S. V.; Gallegos, L. C.; St. John, P. C.; Paton, R. S. *Chem. Sci.* **2021**, *12*, 12012–12026.

138. Controlling Intramolecular Interactions in the Design of Selective, High-Affinity, Ligands for the CREBBP Bromodomain. Brand, M.; Clayton, J.; Moroglu, M.; Schiedel, M.; Picaud, S.; Bluck, J. P.; Skwarska, A.; Chan, A. K. N.; Laurin, C. M. C.; Scolah, A. R.; See, L.; Rooney, T. P. C.; Fedorov, O.; Perell, G.; Cortopassi, W. A.; Christensen, K. E.; Cooper, R. I.; Paton, R. S.; Pomerantz, W. C. K.; Biggin, P. C.; Hammond, E. M.; Filippakopoulos, P.; Conway, S. J. *J. Med. Chem.* **2021**, *64*, 10102–10123.

137. Phosphorus-mediated sp²–sp³ couplings for C–H fluoroalkylation of azines. Zhang, X.; Nottingham, K. G.; Patel, C.; Alegre-Requena, J. V.; Levy, J. N.; Paton, R. S.; McNally, A. *Nature* **2021**, *594*, 217–222.

136. Asymmetric Total Synthesis and Determination of the Absolute Configuration of (+)-Srilankenyne via Sequence-sensitive Halogenations Guided by Conformational Analysis. Jang, H.; Kwak, S. Y.; Lee, D.; Alegre-Requena, J. V.; Kim, H.; Paton, R. S.; Kim, D. *Org. Lett.* **2021**, *23*, 1321–1326.

135. Mechanistic Investigation of Rh(I)-Catalyzed Asymmetric Suzuki-Miyaura Coupling with Racemic Allyl Halides. van Dijk, L.; Ardkhean, R.; Sidera, M.; Karabiyikoglu, S.; Sari, O.; Claridge, T. D. W.; Paton, R. S.; Fletcher, S. P. *Nat. Catal.* **2021**, *4*, 284–292.

134. Importance of Engineered and Learned Molecular Representations in Predicting Organic Reactivity, Selectivity, and Chemical Properties. Gallegos, L. C.; Luchini, G.; St. John, P. C.; Kim, S.; Paton, R. S. *Acc. Chem. Res.* **2021**, *54*, 827–836.

133. Visible light mediated heterocycle functionalization via a geometrically interrupted 2+2. cycloaddition. Popescu, M. V.; Mekereeya, A.; Alegre-Requena, J. V.; Paton, R. S.; Smith, M. D. *Angew Chem. Int. Ed.* **2020**, *59*, 23020–23024.

132. Stereoretention in styrene heterodimerisation promoted by one-electron oxidants. Zhang, X.; Paton, R. S. *Chem. Sci.* **2020**, *11*, 9309–9324.

131. Elucidating the chemical pathways responsible for the sooting tendency of 1 and 2- phenylethanol. Etz, B. D.; Fioroni, G. M.; Messerly, R. A.; Rahimi, M. J.; St. John, P. C.; Robichaud, D. J.; Christensen, E. D.; Beekley, B. P.; McEnally, C. S.; Pfefferle, L. D.; Xuan, Y.; Vyas, S.; Paton, R. S.; McCormick, R. L.; Kim, S. *Proc. Combust. Inst.* **2020**, *38*, 1327–1334.

- 130.** Quantum chemical calculations for over 200,000 organic radical species and 40,000 associated closed-shell molecules. St John, P. C.; Guan, Y.; Kim, Y.; Etz, B. D.; Kim, S.; Paton, R. S. *Scientific Data* **2020**, *7*, 244.
- 129.** GoodVibes: automated thermochemistry for heterogeneous computational chemistry data. Luchini, G.; Alegre-Requena, J. V.; Funes-Ardoiz, I.; Paton, R. S. *F1000Research* **2020**, *9*, 291.
- 128.** Hydrogen Bonding Phase-Transfer Catalysis with Ionic Reactants: Enantioselective Synthesis of γ -Fluoroamines. Roagna, G.; Ascough, D. M. H.; Ibba, F.; Fontana, A.; Christensen, K. E.; Misale, A.; Trabanco, A. A.; Paton, R. S.; Pupo, G.; Gouverneur, V. *J. Am. Chem. Soc.* **2020**, *142*, 14045–14051.
- 127.** BIMP Catalyzed 1,3-Prototropic Shift for the Highly Enantioselective Synthesis of Conjugated Cyclohexenones. Golec, J. C.; Carter, E. M.; Ward, J. W.; Whittingham, W. G.; Simón, L.; Paton, R. S.; Dixon, D. *J. Angew. Chem. Int. Ed.* **2020**, *59*, 17417–17422.
- 126.** Enantiomerically enriched tetrahydropyridine allyl chlorides. Karabiyikoglu S. I.; Brethomé, A. V.; Palacin, T.; Paton, R. S.; Fletcher, S. P. *Chem. Sci.* **2020**, *11*, 4125–4130.
- 125.** Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. Pieters, B. J. G. E.; Wuts, M. H. M.; Poater, J.; Kumar, K.; White, P. B.; Kamps, J. J. A. G.; Sherman, W.; Pruijn, G. J. M.; Paton, R. S.; Beuming, T.; Bickelhaupt, F. M.; Mecinović, J. *Commun. Chem.* **2020**, *3*, 69.
- 124.** Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins. Hintzen, J. C. J.; Poater, J.; Kumar, K.; Al Temimi, A. H. K.; Pieters, B. J. G. E.; Paton, R. S.; Bickelhaupt, F. M.; Mecinović, J. *Molecules* **2020**, *25*, 1918.
- 123.** Selective Halogenation Using Designed Phosphine Reagents. Levy, J. N.; Alegre-Requena, J. V.; Liu, R.; Paton, R. S.; McNally, A. *J. Am. Chem. Soc.* **2020**, *142*, 11295–11305
- 122.** Prediction of homolytic bond dissociation enthalpies for organic molecules at near chemical accuracy with sub-second computational cost. St John, P. C.; Guan, Y.; Kim, Y.; Kim, S.; Paton, R. S. *Nat. Commun.* **2020**, *11*, 2328.
- 121.** Fungal-derived brevianamide assembly by a stereoselective semipinacolase. Ye, Y.; Du, L.; Zhang, X.; Newmister, S. A.; McCauley, M.; Alegre-Requena, J. V.; Zhang W.; Mu, S.; Minami, A.; Fraley, A. E.; Adrover-Castellano, M. L.; Carney, N.; Shende, V. K.; Oikawa, H.; Kato H.; Tsukamoto, S.; Paton, R. S.; Williams R. M.; , Sherman, D. H.; Li, S. *Nat. Catal.* **2020**, *3*, 497–506.
- 120.** An Alkyne Linchpin Strategy for Drug: Pharmacophore Conjugation: Experimental and Computational Realization of a meta-Selective Inverse Sonogashira Coupling. Porey, S.; Zhang, X.; Bhowmick, S.; Singh, V. K.; Guin, S.; Paton, R. S.; Maiti, D. *J. Am. Chem. Soc.* **2020**, *142*, 3762–3774.
- 119.** Effects of substituents X and Y on the NMR chemical shifts of 2-(4-X phenyl)-5-Y pyrimidines. Yuan, H.; Chen, P.-W.; Li, M.-Y.; Zhang, Y.; Peng, Z.-W.; Liu, W.; Paton, R. S.; Cao, C. *J. Mol. Struct.* **2020**, *1204*, 127489.
- 118.** Unconventional Reactivity of Ethynylbenziodoxolone (EBX) Reagents and Thiols: Scope and Mechanism. Liu, B. Alegre-Requena, J. V.; Paton, R. S.; Miyake, G. *Chem. Eur. J.* **2020**, *26*, 2386–2394.
- 117.** Synthesis, Characterization, and Reactivity of Complex Tricyclic Oxonium Ions, Proposed Intermediates in Natural Product Biosynthesis. Chan, H. S. S.; Nguyen, Q. N. N.; Paton, R. S.; Burton, J. W. *J. Am. Chem. Soc.* **2019**, *141*, 15951–15962.
- 116.** A Pyridine-Pyridine Cross-Coupling Reaction via Dearomatized Radical Intermediates. Koniarczyk, J. L.; Greenwood, J. W.; Alegre-Requena, J. V.; Paton, R. S.; McNally, A. *Angew. Chem. Int. Ed.* **2019**, *58*, 14882–14886.
- 115.** Fungal Indole Alkaloid Biogenesis Through Evolution of a Bifunctional Reductase/Diels-Alderase. Dan, Q.; Newmister, S. A.; Klas, K. R.; Fraley, A. E.; McAfoos, T. J.; Somoza, A. D.; Sunderhaus, J. D.; Ye, Y.; Shende, V. V.; Yu, F.; Sanders, J. N.; Brown, W. C.; Zhao, L.; Paton, R. S.; Houk, K. N.; Smith, J. L.; Sherman, D. H.; Williams, R. M. *Nat. Chem.* **2019**, *11*, 972–980.
- 114.** Palladium-Catalyzed Directed meta-Selective C–H Allylation of Arenes: Unactivated Internal Olefins as Allyl Surrogates. Achar, T. K.; Zhang, X.; Mondal, R.; Shanavas, M. S.; Maity, S.; Paul, N.; Paton, R. S.; Maiti, D. *Angew. Chem. Int. Ed.* **2019**, *58*, 10353–10360.

- 113.** Retooling Asymmetric Conjugate Additions for Sterically Demanding Substrates with an Iterative Data-Driven Approach. Brethomé, A. V.; Paton, R. S.; Fletcher, S. P. *ACS Catal.* **2019**, *9*, 7179–7187.
- 112.** Structure Determination of a Chloroenyne from *Laurencia Majuscula* using Computational Methods and Total Synthesis. Shepherd, E. D.; Dyson, B. S.; Hak, W. E.; Nguyen, Q. N. N.; Lee, M.; Kim, M. J.; Sohn, T.-I.; Kim, D.; Burton, J. W.; Paton, R. S. *J. Org. Chem.* **2019**, *84*, 4971–4991.
- 111.** Iterative Arylation of Amino Acids and Aliphatic Amines via δ -C(sp³)-H Activation: Experimental and Computational Exploration. Guin, S.; Dolui, P.; Zhang, X.; Paul, S.; Singh, V. K.; Pradhan, S.; Chandrashekar, H. B.; Anjana, S. S.; Paton, R. S.; Maiti, D. *Angew. Chem. Int. Ed.* **2019**, *131*, 5689–5694.
- 110.** Hydrogen Bonding Phase-Transfer Catalysis with Potassium Fluoride: Enantioselective Synthesis of β -Fluoroamines. Pupo, G.; Vicini, A. C. Ascough, D. M. H.; Ibba, F.; Christensen, K. E.; Thompson, A. L.; Brown, J. M.; Paton, R. S.; Gouverneur, V. *J. Am. Chem. Soc.* **2019**, *141*, 2878–2883.
- 109.** Biosynthesis of Providencin: Understanding Photochemical Cyclobutane Formation with Density Functional Theory. Tang, B.; Paton, R. S. *Org. Lett.* **2019**, *21*, 1243–1247.
- 108.** Conformational Effects on Physical–Organic Descriptors – the Case of Sterimol Steric Parameters. Brethomé, A. V.; Fletcher, S. P.; Paton, R. S. *ACS Catalysis* **2019**, *9*, 2313–2323.
- 107.** Hydrogen bond enabled dynamic kinetic resolution of axially chiral amides mediated by a chiral counterion. Fugard, A.; Lahdenperä, A.; Mekareeya, A.; Tan, J.; Paton, R. S.; Smith, M. D. *Angew. Chem. Int. Ed.* **2019**, *58*, 2795–2798.
- 106.** Enantioselective rhodium-catalysed insertion of trifluorodiazethanes into tin hydrides. Hyde, S.; Veliks, J.; Ascough, D. M. H.; Szpera, R.; Paton, R. S.; Gouverneur, V. *Tetrahedron* **2019**, *75*, 17–25.
- 105.** Data-mining the diaryl (thio) urea conformational landscape: Understanding the contrasting behavior of ureas and thioureas with quantum chemistry. Luchini, G.; Ascough, D. M. H.; Alegre-Requena, J. V.; Gouverneur, V.; Paton, R. S. *Tetrahedron* **2019**, *75*, 697–702.
- 104.** Frontier Molecular Orbital Effects Control the Hole-Catalyzed Racemization of Atropisomeric Biaryls. Tan, J.; Paton, R. S. *Chem. Sci.* **2019**, *10*, 2285–2289.
- 103.** Hydrogen-bond dependent conformational switching: a computational challenge from experimental thermochemistry. Luccarelli, J.; Paton, R. S. *J. Org. Chem.* **2019**, *84*, 613–621.
- 102.** Non-Hydrolytic β -Lactam Antibiotic Fragmentation by L, D-Transpeptidases and Serine β -Lactamase Cysteine Variants. Lohans, C. T.; Chan, H. T. H.; Malla, T. R. Kumar, K.; Kamps, J. J. A. G.; McArdle, D. J. B.; van Groesen, E.; de Munnik, M.; Tooke, C. L.; Spencer, J.; Paton, R. S. Brem, J.; Schofield, C. J. *Angew. Chem. Int. Ed.* **2019**, *131*, 2012–2016.
- 101.** Heterobiaryl synthesis by contractive C–C coupling via P(V) intermediates. Hilton, M. C.; Zhang, X.; Boyle, B. T.; Alegre-Requena, J. V.; Paton, R. S.; McNally, A. *Science* **2018**, *362*, 799–804.
- 100.** Stereospecific 1,3-H Transfer of Indenols Proceeds via Persistent Ion-Pairs Anchored by NH \cdots π Interactions. Ascough, D. M. H.; Duarte, F.; Paton, R. S. *J. Am. Chem. Soc.* **2018**, *140*, 16740–16748.
- 99.** Selectivity in Transition Metal-catalyzed Cyclizations: Insights from Experiment and Theory. Anderson, E. A.; Paton, R. S. *CHIMIA* **2018**, *72*, 614–620.
- 98.** Catalytic Enantio- and Diastereoselective Mannich Addition of TosMIC to Ketimines. Franchino, A. Chapman, J.; Funes-Ardoiz, I.; Paton, R. S.; Dixon, D. J. *Chem. Eur. J.* **2018**, *24*, 17660–17664.
- 97.** Experimental and theoretical insight into the soot tendencies of the methylcyclohexene isomers. Kim, S.; Fiorinia, M. Park, J.-W.; Robichaud, D. J.; Dhruvajyoti, D. D.; St. John, P. C.; Lu, T.; McEnally, C.; Pfeifferle, L. D.; Paton, R. S.; Foust, T. D.; McCormick, R. L. *Proc. Combust. Inst.* **2018**, *37*, 1083–1090.
- 96.** Post-Translational Site-selective Protein α -Deuteration Protein Backbone Modification and Use as a Tool for Protein Mechanism. Galan, S. R. G.; Wickens, J. R.; Dadova, J.; Ng, W.-L.; Zhang, X.; Simion, R. A.; Quinlan, R.; Pires, E.; Paton, R. S.; Caddick, S.; Chudasama, V.; Davis, B. G. *Nature Chem. Biol.* **2018**, *14*, 955–963.
- 95.** Bifunctional iminophosphorane catalysed enantioselective sulfa-Michael addition of alkyl thiols to alkenyl

benzimidazoles. Formica, M.; Sorin, G.; Farley, A. J. M.; Diaz, J.; Paton, R. S.; Dixon, D. J. *Chem. Sci.* **2018**, *9*, 6969–6974.

94. Dynamic Intermediates in the Radical Cation Diels-Alder Cycloaddition: Lifetime and Suprafacial Stereoselectivity. Tan, J.; Hirvonen, V.; Paton, R. S. *Org. Lett.* **2018**, *20*, 2821–2825.

93. Asymmetric Nucleophilic Fluorination under Hydrogen Bonding Phase Transfer Catalysis. Pupo, G.; Ibba, F.; Ascough, D. M. H.; Vicini, A. C.; Ricci, P.; Christensen, K.; Morphy, J. R.; Brown, J. M.; Paton, R. S.; Gouverneur, V. *Science* **2018**, *360*, 638–642.

92. The true catalyst revealed: The intervention of chiral Ca and Mg phosphates in Brønsted acid promoted asymmetric Mannich reactions. Simón, L.; Paton, R. S. *J. Am. Chem. Soc.* **2018**, *140*, 5412–5420.

91. Cation– π interactions in protein-ligand binding: theory and data-mining reveal different roles for lysine and arginine. Kumar, K.; Woo, S. M.; Siu, T.; Cortopassi, W. A.; Duarte, F.; Paton, R. S. *Chem. Sci.* **2018**, *9*, 2655–2665.

90. Copper Catalysed Asymmetric Conjugate addition to β -substituted cyclopentenone forming quaternary centres with the aid of Quantitative Structure-Selectivity relationship. Ardkehan, R.; Mortimore, M.; Paton, R. S.; Fletcher, S. P. *Chem. Sci.* **2018**, *9*, 2628–2632.

89. A New Mechanism for β -Lactamases: Class D Enzymes Degrade Methyl Carbapenems via Lactone Formation. Lohans, C. T.; van Groesen, E.; Brem, J.; Kumar, K.; Paton, R. S.; Schofield, C. J. *Angew. Chem. Int. Ed.* **2018**, *57*, 1282–1285.

88. Recognition of Shorter and Longer Trimethyllysine Analogues by Epigenetic Reader Proteins. Al Temimi, A. H. K.; Belle, R.; Kumar, K.; Poater, J.; Betlem, P.; Pieters, B. J. G. E.; Paton, R. S.; Bickelhaupt, F. M.; Mecinović, J. *Chem. Commun.* **2018**, *54*, 2409–2412.

87. Direct sulfonylation of anilines mediated by visible light. Johnson, T. C.; Elbert, B. L.; Farley, A. J. M.; Gorman, T. W.; Genicot, C.; Lallemand, B.; Pasau, P.; Flasz, J.; Castro, J. L.; MacCoss, M.; Dixon, D. J.; Paton, R. S.; Schofield, C. J.; Smith, M. D.; Willis, M. C. *Chem. Sci.* **2018**, *9*, 629–633.

86. Experimental and Theoretical Study of Oxidative Stability of Alkylated Furans Used as Gasoline Blend Components. Christensen, E.; Fioroni, G. M.; Kim, S.; Fouts, L.; Gjersing, E.; Paton, R. S.; McCormick, R. *Fuel* **2018**, *212*, 576–585.

85. Asymmetric Total Syntheses and Structure Confirmation of Chlorofucins and Bromofucins. Kim, B.; Sohn, T.; Kim, D.; Paton, R. S. *Chem. Eur. J.* **2018**, *24*, 2634–2642.

84. Asymmetric Total Synthesis and Structure Confirmation of (+)-(3E)-Isolaurefucin Methyl Ether. Sohn, T.-I.; Kim, B.; Kim, D.; Paton, R. S. *Heterocycles* **2018**, *97*, 179–191.

- At Oxford -

83. Total synthesis of (–)-himalensine. Shi, H.; Michaelides, I.; Darses, B.; Jakubec, P.; Nguyen, Q. N.; Paton, R. S.; Dixon, D. J. *J. Am. Chem. Soc.* **2017**, *139*, 17755–17758.

82. Investigating D-Lysine Stereochemistry for Epigenetic Methylation, Demethylation and Recognition. Belle, R.; Al Temimi, A. H. K.; Kumar, K.; Pieters, B. J. G. E.; Dunford, J.; Tumber, A.; Johansson, C.; Brown, T.; Schofield, C. J.; Hopkinson, R. J.; Paton, R. S.; Kawamura, A.; Mecinović, J. *Chem. Commun.* **2017**, *53*, 13264–13267.

81. Construction of 6,10-syn- and anti-2,5-Dioxabicyclo[2.2.1]heptane Skeletons via Oxonium Ion Formation-Fragmentation: Prediction of Structure of (E)-Ocellenynone by NMR Calculation. Jeong, D.; Sohn, T.-I.; Kim, J. Y.; Kim, G.; Kim, D.; Paton, R. S. *Org. Lett.* **2017**, *19*, 6252–6255.

80. Asymmetric Induction in C-Alkylation of Tropane-Derived Enamines: Congruence Between Computation and Experiment. Li, Y.; Jackson, K. E.; Charlton, A.; Le Neve-Foster, B.; Khurshid, A.; Rudy, H.-K. A.; Thompson, A. L.; Paton, R. S.; Hodgson, D. M. *J. Org. Chem.* **2017**, *82*, 10479–10488.

79. A General C-H Cyanation of 6-Ring N-Containing Heteroaromatics. Elbert, B. L.; Farley, Gorman, T. W.; Johnson, T. C.; Genicot, C.; Lallemand, B.; Pasau, P.; Flasz, J.; Castro, J. L.; MacCoss, M.; Paton, R. S.; Schofield, C. J.; Smith, M. D.; Willis, M. C.; Dixon, D. J. *Chem. Eur. J.* **2017**, *23*, 14733–14737.

- 78.** Enantioselective conjugate addition catalyzed by a copper-phosphoramidite complex: Computational and experimental exploration of asymmetric induction. Ardhean, R.; Roth, P. M. C.; Maksymowicz, R. M.; Curran, A.; Peng, Q.; Paton, R. S.; Fletcher, S. P. *ACS Catalysis* **2017**, *7*, 6729–6737.
- 77.** Mechanistic insight into palladium-catalyzed cycloisomerization: A combined experimental and theoretical study. Mekareeya, A.; Walker, P. R.; Couce-Rios, A.; Campbell, C. D.; Steven, A.; Paton, R. S.; Anderson, E. A. *J. Am. Chem. Soc.* **2017**, *139*, 10104–10114.
- 76.** AMP binding stabilizes the KTN domain of the *Shewanella denitrificans* Kef potassium efflux system. Pliotas, C.; Grayer, S. C.; Ekkerman, S.; Chan, A. K. N.; Healy, J.; Marius, P.; Bartlett, W.; Khan, A.; Cortopassi, W. A.; Chandler, S. A.; Rasmussen, T.; Benesch, J. L. P.; Paton, R. S.; Claridge, T. D. W.; Miller, S.; Booth, I. R.; Naismith, J. H.; Conway, S. J. *Biochemistry* **2017**, *56*, 4219–4234.
- 75.** Visible light photocatalysis of 6π -heterocyclization. Münster, N.; Parker, N. A.; van Dijk, L.; Paton, R. S.; Smith, M. D. *Angew. Chem. Int. Ed.* **2017**, *56*, 9468–9472.
- 74.** Molecular Recognition in Asymmetric Counteranion Catalysis: Understanding Chiral Phosphate-Mediated Desymmetrization. Duarte, F.; Paton, R. S. *J. Am. Chem. Soc.* **2017**, *139*, 8886–8896.
- 73.** Structural and Stereoelectronic Insights into Oxygenase Catalyzed Formation of Ethylene from 2-Oxoglutarate. Zhang, Z.; Smart, T. J.; Choi, H.; Hardy, F.; Lohans, C. T.; Abboud, M. I.; Richardson, M. S. W.; Paton, R. S.; McDonough, M. A.; Schofield, C. J. *Proc. Nat. Acad. Sci.* **2017**, 4667–4672.
- 72.** Enantioselective Silver and Amine Co-catalyzed Desymmetrizing Cycloisomerization of Alkyne-linked Cyclohexanones. Manzano, R.; Datta, S.; Paton, R. S.; Dixon, D. J. *Angew. Chem. Int. Ed.* **2017**, *56*, 5834–5838.
- 71.** Phosphazene Catalyzed Addition to Electron-Deficient Alkynes: The Importance of Nonlinear Allenyl Intermediates upon Stereoselectivity. Simón, L.; Paton, R. S. *J. Org. Chem.* **2017**, *82*, 3855–3863.
- 70.** Dual Gold-Catalyzed Three-Component Reaction: Efficient Synthesis of Indene-Fused Esters, Acids, and Lactones through Gold Vinylidene Intermediates. Yu, C.; Ma, X.; Chen, B.; Tang, B.; Paton, R. S.; Zhang, G. *Eur. J. Org. Chem.* **2017**, *11*, 1561–1565.
- 69.** Divergent Photocyclization/1,4-Sigmatropic Rearrangements for the Synthesis of Sesquiterpenoid Derivatives. Gorobets, E.; Wong, N. E.; Paton, R. S.; Derksen, D. *J. Org. Lett.* **2017**, *19*, 484–487.
- 68.** Detailed Mechanistic Studies on Palladium-Catalyzed Selective C–H Olefination with Aliphatic Alkenes - A Significant Influence of Proton Shuttling. Deb, A.; Hazra, A.; Peng*, Q.; Paton, R. S.; Maiti, D. *J. Am. Chem. Soc.* **2017**, *139*, 763–775.
- 67.** Correlating Reactivity and Selectivity to Cyclopentadienyl Ligand Properties in Rh(III)-Catalyzed C–H Activation Reactions — An Experimental and Computational Study. Piou, T.; Romanov-Michailidis, F.; Romanova-Michaelides, M.; Jackson, K. E.; Semakul, N.; Taggart, T. D.; Newell, B. S.; Rithner, C. D.; Paton, R. S.; Rovis, T. *J. Am. Chem. Soc.* **2017**, *139*, 1296–1310.
- 66.** Heptamethyl Indenyl (Ind*) Enables Diastereoselective Benzamidation of Cyclopropenes via Rh(III)-Catalyzed C–H Activation. Semakul, N.; Jackson, K. E.; Paton, R. S.; Rovis, T. *Chem. Sci.* **2017**, *8*, 1015–1020.
- 65.** Cation– π interactions in CREBBP bromodomain inhibition: an electrostatic model for small-molecule binding affinity and selectivity. Cortopassi, W. A.; Kumar, K.; Paton, R. S. *Org. Biomol. Chem.* **2016**, *14*, 10926–10938.
- 64.** A Counterion-Directed Approach to the Diels-Alder Paradigm: Cascade Synthesis of Tricyclic Fused Cyclopropanes. Kiss, E.; Campbell, C. D.; Driver, R. W.; Jolliffe, J. D.; Lang, R.; Sergieiva, T.; Okovytyy, S.; Paton, R. S.; Smith, M. D. *Angew. Chem. Int. Ed.* **2016**, *55*, 13813–13817.
- 63.** Computing Organic Stereoselectivity – from Concepts to Quantitative Calculations and Predictions. Peng, Q.; Duarte, F.; Paton, R. S. *Chem. Soc. Rev.* **2016**, *45*, 6093–6107.
- 62.** Synthesis of Malhamensilipin A Exploiting Iterative Epoxidation/Chlorination: Experimental and Computational Analysis of Epoxide-Derived Chloronium Ions. Saska, J.; Lewis, W.; Paton, R. S.; Denton, R. *Chem. Sci.* **2016**, *7*, 7040–7049.
- 61.** Mechanisms of histone-modifying and reading enzymes: the role of the protein environment from a computational perspective. Cortopassi, W. A.; Kumar, K.; Duarte, F.; Pimentel, A. S.; Paton, R. S. *J. Mol. Graph.*

Model. **2016**, *67*, 69–84.

- 60.** Catalytic Control in Cyclizations: from Computational Mechanistic Understanding to Selectivity Prediction. Peng, Q.; Paton, R. S. *Acc. Chem. Res.* **2016**, *49*, 1042–1051.
- 59.** Furan production from light oxygenates in HZSM-5. Kim, S.; Evans, T. J.; Mukarakate, C.; Bu, L.; Beckham, G. T.; Nimlos, M. R.; Paton, R. S.; Robichaud, D. J. *ACS Sustain. Chem. Eng.* **2016**, *4*, 2615–2623.
- 58.** Investigations on Recyclization and Hydrolysis in Avibactam Mediated Serine β -Lactamase Inhibition. Choi, H.; Paton, R. S.; Park, H.; Schofield, C. J. *Org. Biomol. Chem.* **2016**, *14*, 4116–4128.
- 57.** Unraveling Innate Substrate Control in Site-Selective Palladium-Catalyzed C–H Heterocycle Functionalization. Choi, H.; Min, M.; Peng, Q.; Kang, D.; Paton, R. S.; Hong, S. *Chem. Sci.* **2016**, *7*, 3900–3909.
- 56.** Development of a True Transition State Force Field (TTSFF) from Quantum Mechanical Calculations. Madarász, A.; Berta, D.; Paton, R. S. *J. Chem. Theor. Comput.* **2016**, *12*, 1833–1844.
- 55.** DFT study on the enantioselectivity of spiroacetalization catalysed by an imidodiphosphoric acid catalyst: how confinement works. Simón, L.; Paton, R. S.; *Org. Biomol. Chem.* **2016**, *14*, 3031–3039.
- 54.** *Computational Ligand Design in Enantio- and Diastereoselective Ynamide 5+2. Cycloisomerizations*, Straker, R.; Peng*, Q.; Mekareeya, A.; Paton, R. S.; Anderson, E. A. *Nature Commun.* **2015**, *7*, 10109.
- 53.** Dioxxygen binding in the active site of histone demethylase JMJD2A and the role of protein environment. Cortopassi, W. E.; Simion, R. A.; Hornsby, C. E.; Costa Franca, T. C.; Paton, R. S. *Chem. Eur. J.* **2015**, *21*, 18983–18992.
- 52.** α - and α' -Lithiation–Electrophile trapping of N-thiopivaloyl and N-t-butoxythiocarbonyl α -substituted Azetidines: rationalisation of the regiodivergence using NMR and computation. Jackson, K. E.; Mortimer, C. L.; Odell, B.; McKenna, J. M.; Claridge, T. D. W.; Paton, R. S.; Hodgson, D. M. *J. Org. Chem.* **2015**, *80*, 9838–9846
- 51.** Substrate-Controlled Asymmetric Total Syntheses of Microcladallenes A, B, and C Based on the Proposed Structures. Sohn, T.-I.; Kim, D.; Paton, R. S. *Chem. Eur. J.* **2015**, *21*, 15988–15997.
- 50.** Role of Hydrogen Bonding Acceptors in Organo-Enamine Catalysis. Han, J.; Zhichao Lu, Z.; Flach, A. L.; Paton, R. S.; Hammond, G. B.; Xu, B. *Chem. Eur. J.* **2015**, *21*, 11687–11691.
- 49.** Coordination Diversity in Hydrogen-Bonded Homoleptic Fluoride–Alcohol Complexes Modulates Reactivity. Engle, K. M.; Pfeifer, L.; Pidgeon, G. W.; Giuffredi, G. T.; Thompson, A. L.; Paton, R. S.; Brown, J. M.; Gouverneur, V. *Chem. Sci.* **2015**, *6*, 5293–5302.
- 48.** Origins of asymmetric phosphazene organocatalysis: computations reveal a common mechanism for nitro- and phospho-aldol additions. Simón, L.; Paton, R. S. *J. Org. Chem.* **2015**, *80*, 2756–2766.
- 47.** Ethanol Dehydration in HZSM-5 studied by Density Functional Theory: Evidence for a Concerted Processes. Kim, S.; Robichaud, D. J.; Beckham, G. T.; Paton, R. S.; Nimlos, M. R. *J. Phys. Chem. A* **2015**, *119*, 3604–3614.
- 46.** Enantioselective Desymmetrization of Prochiral Cyclohexanones via Organocatalytic Intramolecular Michael Additions to α,β -Unsaturated Esters. Gammack-Yamagata, A. D.; Datta, S.; Jackson, K. E.; Stegbauer, L.; Paton, R. S.; Dixon, D. J. *Angew. Chem. Int. Ed.* **2015**, *127*, 4981–4985.
- 45.** Thermal and Photochemical Mechanisms for Cyclobutane Formation in Bielschowskysin Biosynthesis. Tang, B.; Simion, R. A.; Paton, R. S. *Synlett* **2015**, *26*, 501–507.
- 44.** Small molecule inhibitors of bromodomain-acetyl-lysine interactions. Brand, M.; Measures, A.; Wilson, B.; Cortopassi, W. A.; Alexander, R.; Hoss, M.; Hewings, D. S.; Paton, R. S.; Conway, S. J. *ACS Chem. Bio.* **2015**, *10*, 22–39.
- 43.** Catalytic Enantioselective Synthesis of Indanes via Cation-Directed 5-Endo-Trig Cyclization. Johnston, C. P.; Kothari, A.; Sergeieva, T.; Okovytyy, S. I.; Jackson, K. E.; Paton, R. S.; Smith, M. D. *Nat. Chem.* **2015**, *7*, 171–177.
- 42.** A series of potent CREBBP bromodomain ligands reveals an induced fit pocket stabilized by a cation- π interaction. Rooney, T. P. C.; Filippakopoulos, P.; Fedorov, O.; Picaud, S.; Cortopassi, W. A.; Hay, D. A.; Martin, S.; Tumber, A.; Rogers, C. M.; Philpott, M.; Wang, M.; Thompson, A. L.; Heightman, T. D.; Pryde, D. C.; Cook, A.; Paton, R. S.; Müller-Knapp, S.; Knapp, S.; Brennan, P. E.; Conway, S. J. *Angew. Chem. Int. Ed.* **2014**, *126*, 26,

6240–6244.

41. Cation-directed synthesis of pyrroloindolines and pyridoindolines via a hydrogen bond assisted isocyanide cyclization cascade. Knipe, P. C.; Gredičak, M.; Cernijenko, A.; Paton, R. S.; Smith, M. D. *Chem. Eur. J.* **2014**, *11*, 3005–3009.

40. Dissecting non-covalent interactions in oxazaborolidinium catalyzed cycloadditions of maleimides. Paton, R. S. *Org. Biomol. Chem.* **2014**, *12*, 1717–1720.

39. Natural product biosynthesis: It's all downhill from here. Hornsby, C. E.; Paton, R. S. *Nature Chem.* **2014**, *6*, 88–89.

38. Intramolecular Diels-Alder Reactions of Cycloalkenones: Stereoselectivity, Lewis Acid Influence, and Halogenation Effects. Pham, H.; Paton, R. S.; Ross, A. G.; Danishefsky, S. J.; Houk, K. N. *J. Am. Chem. Soc.* **2014**, *136*, 2397–2403.

37. Ligand Bite Angle-dependent Palladium-catalyzed Cyclization of Propargylic Carbonates to 2-Alkynyl Azacycles or Cyclic Dienamides. Daniels, D. S. B.; Jones, A. S.; Thompson, A. L.; Paton, R. S.; Anderson, E. A. *Angew. Chem. Int. Ed.* **2014**, *53*, 1915–1920.

36. Quantum mechanical calculations suggest that lytic polysaccharide monoxygenases employ a copper-oxygen rebound mechanism. Kim, S.; Sandgren, M.; Paton, R. S.; Beckham, G. T. *Proc. Nat. Acad. Sci.* **2014**, *111*, 149–154.

35. A mechanistic investigation of acid-catalyzed cleavage of aryl-ether linkages: Implications for lignin depolymerization in acidic environments. Sturgeon, M. R.; Kim, S.; Lawrence, K.; Paton, R. S.; Chmely, S. C.; Nimlos, M. R.; Foust, T. D.; Beckham, G. T. *ACS Sustain. Chem. Eng.* **2014**, *2*, 472–485.

34. Asymmetric Total Synthesis of (+)-Bermudenynol, a C15 Laurencia Metabolite with a Vinyl Chloride-Containing Oxocene Skeleton, via Intramolecular Amide Enolate Alkylation. Kim, G.; Sohn, T.-I.; Kim, D.; Paton, R. S. *Angew. Chem. Int. Ed.* **2014**, *53*, 272–276.

33. Diels-Alder Reactivities of Strained and Unstrained Cycloalkenes with Normal and Inverse-Electron-Demand Dienes: Activation Barriers and Distortion/Interaction Analysis. Liu, F.; Paton, R. S.; Kim, S.; Liang, Y.; Houk, K. N. *J. Am. Chem. Soc.* **2013**, *135*, 15642–15649.

32. Mechanistic investigations on the enantioselective Conia-ene reaction catalyzed by cinchona-derived amino urea pre-catalysts and Cu(I). Sladojevich, F.; Fuentes de Arriba, A. L.; Yang, T.; Ferrali, A.; Paton, R. S.; Dixon, D. *J. Chem. Eur. J.* **2013**, *19*, 14286–14295.

31. Structure Reassignment of Laurefurenynes A and B by Computation and Total Synthesis. Shepherd, D. J.; Broadwith, P. A.; Dyson, B. S.; Paton, R. S.; Burton, J. W. *Chem. Eur. J.* **2013**, *19*, 12644–12648.

30. Rapid Cross Metathesis for Protein Modifications via Chemical Access to Se-Allyl Selenocysteine in Proteins. Lin, Y. A.; Boutureira, O.; Lercher, L.; Bhushan, B.; Paton, R. S.; Davis, B. G. *J. Am. Chem. Soc.* **2013**, *135*, 12156–12159.

29. *Computational Organic Chemistry*, Jackson, K.; Jaffar, S.; Paton, R. S. *Annu. Rep. Prog. Chem., Sect. B*, **2013**, *109*, 235–255.

28. Mechanistic Study of a Ru-Xantphos Catalyst for Tandem Alcohol Dehydrogenation and Reductive Aryl-Ether Cleavage. Chmely, S. C.; Kim, S. C.; Ciesielski, P. N.; Jiménez-Osés, G.; Paton, R. S.; Beckham, G. T. *ACS Catal.* **2013**, *3*, 963–974.

27. Enhanced Reactivity in Dioxirane C-H Oxidations via Strain Release: A Computational and Experimental Study. Zhou, L.; Paton, R. S.; Eschenmoser, A.; Newhouse, T. R.; Baran, P. S.; Houk, K. N. *J. Org. Chem.* **2013**, *78*, 4037–4044.

26. C-Alkylation of Chiral Tropane- and Homotropene-Derived Enamines. Hodgson, D. M.; Charlton, A.; Paton, R. S.; Thompson, A. S. *J. Org. Chem.* **2013**, *78*, 1508–1518.

25. Synthesis of Cyclic Aminophosphonates through Copper Catalyzed Enamine Activation. Han, J.; Paton, R. S.; Xu, B.; Hammond, G. B. *Synthesis* **2013**, *45*, 463–470.

- 24.** Concise Substrate-Controlled Asymmetric Total Syntheses of Dioxabicyclic Marine Natural Products with 2,10-Dioxabicyclo-7.3.0.dodecene and 2,9-Dioxabicyclo6.3.0.undecene Skeletons. Kim, M. J.; Sohn, T.-I.; Kim, D.; Paton, R. S.; *J. Am. Chem. Soc.* **2012**, *134*, 20178–20188.
- 23.** Dinuclear Palladium Complexes – Precursors or Catalysts? Paton, R. S.; Brown, J. M. *Angew. Chem. Int. Ed.* **2012**, *51*, 10448–10450.
- 22.** Enzymatic Catalysis of Anti-Baldwin Ring-Closure in Polyether Biosynthesis. Hotta, K.; Chen, X.; Paton, R. S.; Minami, A.; Li, H. Swaminathan, K. T.; Mathews, I. I.; Watanabe, K.; Oikawa, H.; Houk, K. N.; Kim, C. Y. *Nature* **2012**, *483*, 355–358.
- 21.** An Efficient Computational Model to Predict the Synthetic Utility of Heterocyclic Arynes. Goetz, A. E.; Bronner, S. M.; Cisneros, J.; Melamed, J.; Paton, R. S.; Houk, K. N.; Garg, N. K. *Angew. Chem. Int. Ed.* **2012**, *51*, 2758–2762.
- 20.** Unusual Base-Induced Rearrangement of exo-9-Oxabicyclo4.2.1.non-7-ene Oxide to exo-8-Hydroxybicyclo3.3.0.octan-2-one. Hodgson, D. M.; Stent, M. A. H.; Paton, R. S.; Wilson, F. X. *Heterocycles* **2012**, *84*, 625–635.
- 19.** Computational Study of Bond Dissociation Enthalpies for a Large Range of Native and Modified Lignins. Kim, S.; Chmely, S. C.; Nimlos, M. R.; Bomble, Y. J.; Foust, T. D.; Paton, R. S.; Beckham, G. T. *J. Phys. Chem. Lett.* **2011**, *2*, 2846–2852.
- 18.** A stereoselective total synthesis of (±)-tormesol. Kim, H.; Bae, H.; Kim, S.; Kim, D.; Lee, D.; Paton, R. S. *Tetrahedron* **2011**, *67*, 10017–10025.
- 17.** Experimental Diels-Alder Reactivities of Cycloalkenones and Cyclic Dienes Explained Through Transition State Distortion Energies. Paton, R. S.; Kim, S.; Ross, A. G.; Danishefsky, S. J.; Houk, K. N. *Angew. Chem. Int. Ed.* **2011**, *50*, 10366–10368.

- PhD and Postdoctoral Studies -

- 16.** Gold-Catalyzed Intramolecular Oxygen Transfer Reactions of 2-Alkynyl-1,5-Diketones or 2-Alkynyl-5-Ketoesters. Scope, Expansion and Mechanistic Investigations on A Novel 4+2. Cycloaddition. Liu, L.; Malhotra, D.; Jin, Z.; Paton, R. S.; Houk, K. N.; Hammond, G. B. *Chem. Eur. J.* **2011**, *17*, 10690–10699.
- 15.** Unraveling the Mechanism of Cascade Reactions of Zincke Aldehydes. Paton, R. S.; Steinhardt, S. E.; Vanderwal, C. D.; Houk, K. N. *J. Am. Chem. Soc.* **2011**, *133*, 3895–3905.
- 14.** Indolyne Experimental and Computational Studies: Synthetic Applications and Origins of Selectivities of Nucleophilic Additions. Im, G.-Y. J.; Bronner, S. M.; Goetz, A. E.; Paton, R. S.; Cheong, P.-H. Y.; Houk, K. N. Garg, N. K. *J. Am. Chem. Soc.* **2010**, *132*, 17933–17944.
- 13.** The 4+2., not 2+2., Mechanism Occurs in the Gold-Catalyzed Intramolecular Oxygen Transfer Reaction of 2-Alkynyl-1,5-Diketones. Liu, L.-P.; Malhotra, D.; Paton, R. S.; Houk, K. N.; Hammond, G. B. *Angew. Chem. Int. Ed.* **2010**, *49*, 9132–9135.
- 12.** Origins of Stereoselectivity in the trans-Diels-Alder Paradigm. Paton, R. S.; Mackey, J. L.; Kim, W.H.; Lee, J. H.; Danishefsky, S. J.; Houk, K. N. *J. Am. Chem. Soc.* **2010**, *132*, 9335–9340.
- 11.** Indolyne and Aryne Distortions and Nucleophilic Regioselectivities. Cheong, P. H. Y.; Paton, R. S.; Bronner, S. M.; Im, G. Y.; Garg, N. K.; Houk, K. N. *J. Am. Chem. Soc.* **2010**, *132*, 1267–1269.
- 10.** Origins of Regioselectivity of Diels–Alder Reactions for the Synthesis of Bisanthraquinone Antibiotic BE-43472B A. Hayden, A. E.; Paton, R. S.; Becker, J.; Lim, Y. H.; Nicolaou, K. C.; Houk, K. N. *J. Org. Chem.* **2010**, *75*, 922–928.
- 9.** Gold(I)-Catalyzed Intermolecular Hydroalkoxylation of Allenes: a DFT Study. Paton, R. S.; Maseras, F. *Org. Lett.* **2009**, *11*, 2237–2240.
- 8.** Hydrogen Bonding and Pi-Stacking: How Reliable are Force Fields? A Critical Evaluation of Force Field Descriptions of Non-Bonded Interactions. Paton, R. S.; Goodman, J. M. *J. Chem. Inf. Model.* **2009**, *49*, 944–955.
- 7.** Mechanistic Insights into the Catalytic Asymmetric Allylboration of Ketones: Bronsted or Lewis Acid Activation?

Paton, R. S.; Goodman, J. M.; Pellegrinet, S. C. *Org. Lett.* **2009**, *11*, 37–40.

6. A DFT Study of the Asymmetric Alkenylation of Enones Catalyzed by Binaphthols. Paton, R. S.; Goodman, J. M.; Pellegrinet, S. C. *J. Org. Chem.* **2008**, *73*, 5078–5089.

5. Stereostructure Assignment of Flexible Five-Membered Rings by GIAO ¹³C NMR Calculations: Prediction of the Stereochemistry of Elatenyne. Smith, S. G.; Paton, R. S.; Burton, J. W.; Goodman, J. M. *J. Org. Chem.* **2008**, *73*, 4053–4062.

4. 1,5-Anti Stereocontrol in the Boron-Mediated Aldol Reactions of β-Alkoxy Methyl Ketones: the Role of the Formyl Hydrogen Bond. Paton, R. S.; Goodman, J. M. *J. Org. Chem.* **2008**, *73*, 1253–1263.

3. Exploration of the Accessible Chemical Space of Acyclic Alkanes. Paton, R. S.; Goodman, J. M. *J. Chem. Inf. Model.* **2007**, *47*, 2124–2132.

2. Enantioselectivity in the boron aldol reactions of methyl ketones. Goodman, J. M.; Paton, R. S. *Chem. Commun.* **2007**, 2124–2126.

1. Understanding the Origins of Remote Asymmetric Induction in the Boron Aldol Reactions of β-Alkoxy Methyl Ketones. Paton, R. S.; Goodman, J. M. *Org. Lett.* **2006**, *8*, 4299–4302.

- Books and Book Chapters -

5. Ligand Design for Asymmetric Catalysis: Combining Mechanistic and Chemoinformatics Approaches, Ardhean, R.; Fletcher, S. P.; Paton, R. S. *In Topics in Organometallic Chemistry*, Springer, Berlin, Heidelberg **2020** pp 1–37.

4. *NMR Prediction*, Jackson, K. E.; Paton, R. S.; *In Applied Theoretical Organic Chemistry, World Scientific (Europe)*, **2018** pp 165–189.

3. *Computational Design of New Protein Catalysts*, Kiss, G.; Johnson, S. A.; Nosrati, G.; Çelebi-Ölçüm, N.; Kim, S.; Paton, R. S.; Houk, K. N. in *Modeling of Molecular Properties* (ed P. Comba), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany **2011**, chapter 16

2. *Theoretical Studies of Asymmetric Gold Catalysis*, Paton, R. S.; Maseras, F. *in Science and Supercomputing in Europe* **2008**, pp. 140–142

1. *Chemistry Olympiad Support Booklet*, Copley, P.; Hersey, T.; McCaw, C.; Paton, R. S.; Scott, K.; Worrall, A.; Wothers, P.; Woodley, E. *Royal Society of Chemistry* **2008**, ISBN: 978-1-84755-866-4

Invited Lectures

134. June 2027: [Physical Organic Chemistry GRC](#), Holderness, NH

133. September 2026: Plenary: IUPAC International Conference on Physical Organic Chemistry, Munich, Germany

132. July 2026: Plenary: BOSS XIX: 19th Belgian Organic Synthesis Symposium, Leuven, Belgium

131. June 2026: 5th HRC, Pittsburgh, PA

130. June 2026: 14th International Symposium on Organic Free Radicals (ISOFR-14), Bologna, Italy

129. March 2026: Distinguished Speaker, Naval Research Laboratory, USA

128. January 2026: 8th International Mini-Symposium: Molecular Machine Learning

127. November 2025: Kyung Hee University, Seoul, Korea

126. October 2025: Lu Jiaxi Lecture, Xiamen University, China

125. October 2025: Plenary: AI for Chemistry in iHarbor Symposium, Xi'an Jiaotong University, China

124. October 2025: Shanghai Institute for Organic Chemistry, China

123. October 2025: Keynote: International Conference of Computational Organic Catalysis, Shenzhen, China

122. September 2025: CAMLC25, Zaragoza, Spain

121. June 2025: HRC 2025, TU Dresden, Germany

120. June 2025: Machine Learning and Artificial Intelligence in Synthetic Chemistry Summer School, University of Helsinki

119. May 2025: Plenary: Machine Learning in Chemical and Materials Sciences 2025, Santa Fe

118. March 2025: Machine Learning for Molecular Simulation & Design, ACS National Meeting, San Diego
117. December 2024: University of Seoul, Korea
116. November 2024: University of Cambridge Chemical Society
115. October 2024: Sygnature Discovery, Nottingham, UK
114. September 2024: European Conference on Organic Free Radicals, Manchester, UK
113. August 2024: IUPAC Conference on Physical Organic Chemistry, Beijing, China
112. August 2024: Wuhan University, Wuhan
111. August 2024: SUSTech, Shenzhen
110. August 2024: HRC 2024, Zhejiang University, Hangzhou
109. July 2024: Frontiers of Computational Reaction Prediction, University of Chicago
108. June 2024: Cheminformatics, Automation and Machine Learning in Chemistry, Jaca
107. June 2024: ICIQ, Spain
106. June 2024: University of Girona, Spain
105. June 2024: Autonomous University of Barcelona, Spain
104. May 2024: Brazilian Chemical Society Lecture, Sao Paulo, Brazil
103. May 2024: Student Seminar Series, University of Minnesota, MN
102. February 2024: University of Pennsylvania, PA
101. February 2024: FDA Center for Drug Evaluation and Research
100. January 2024: AstraZeneca
99. November 2023: University of North Carolina at Chapel Hill
98. November 2023: Chemistry Graduate Student Association Invited Lecturer, Northeastern University
97. October 2023: Whitman College
96. October 2023: Vanderbilt University
95. August 2023: Data Science for Catalysis: Automated-Synthesis, Process Optimization & Catalyst Discovery, ACS National Meeting, San Francisco, CA
94. July 2023: International Conference on Chemical Bonding, Kauai
93. July 2023: Accelerating Reaction Discovery, Telluride
92. June 2023: 23rd Tetrahedron Symposium, Gothenburg, Sweden
91. March 2023: Theoretical and Experimental Approaches to Catalyst Development, ACS National Meeting, Indianapolis
90. December 2022: Syngenta Catalysis Network Lecture 2022
89. December 2022: ISQBS 2022, Ibaraki University, Japan
88. December 2022: University of Pittsburgh
87. November 2022: Carnegie Mellon University
86. August 2022: Roitberg Symposium, ACS National Meeting, Chicago
85. August 2022: Houk Symposium, UCLA
84. July 2022: [Gordon Conference on Stereochemistry](#)
83. July 2022: [Gordon Conference on Computational Chemistry](#)
82. July 2022: [WATOC](#)
81. May 2022: Deargen, Daejeon, South Korea
80. May 2022: PKNU, Busan, South Korea
79. May 2022: Department of Chemistry, Stanford University
78. April 2022: Molecule Maker Lab Institute (MMLI)
77. April 2022: 36th Annual Symposium of the Rocky Mountain Catalysis Society, Colorado School of Mines
76. March 2022: From Theory to Therapy: New Developments in Quantum Mechanical Calculations for Driving Best Chemistry in Academia and Industry, ACS National Meeting, San Diego
75. March 2022: Presidential Workshop: Everything Chemists Always Wanted To Know About Machine Learning, ACS National Meeting, San Diego
74. January 2022: [15th Winter Conference on Medicinal & Bioorganic Chemistry](#), Steamboat Springs

73. December 2021: Department of Chemistry, Montana State University
72. October 2021: Department of Chemistry, Lawrence University
71. October 2021: Department of Chemistry, California Polytechnic State University
70. September 2021: Department of Chemistry, Truman State University
69. August 2021: IUPAC World Chemistry Congress, Montreal, Canada
68. July 2021: [VISTA Symposium on Artificial-Intelligence and Data-Science assisted Synthesis](#)
67. May 2021: International Consortium for Innovation and Quality in Pharmaceutical Development
66. April 2021: Houk International Alumni Meeting
65. November 2020: Genentech
64. August 2020: GSK
63. June 2020: 24th Annual ACS Green Chemistry & Engineering Conference
62. May 2020: Canadian Chemistry Conference and Exhibition (CCCE), Winnipeg
61. February 2020: Department of Chemistry and Biochemistry, University of Missouri – St. Louis
60. November 2019: Department of Chemistry, University of Denver
59. November 2019: Frontiers in Physical Organic Chemistry, Southwest & Rocky Mountain Regional ACS Meeting, El Paso
58. November 2019: Department of Chemistry, Princeton University, NJ
57. October 2019: Department of Chemistry and Biochemistry, UCLA, CA
56. September 2019: Machine Learning and Informatics for Chemistry and Materials, Telluride, CO
55. September 2019: Mechanistic Homogeneous Catalysis – A Meeting between Theory and Experiment, Stockholm, Sweden
54. July 2019: [ISTCP X](#), Tromsø, Norway
53. January 2019: University of Vienna, Austria
52. November 2018: University of Colorado, Denver, USA
51. July 2018: Hanyang University, Seoul, South Korea
50. July 2018: Pukyong National University, South Korea
49. June 2018: [Computational Catalysis for Sustainable Chemistry](#), ICIQ, Tarragona, Spain
48. June 2018: [37th Reaction Mechanisms Conference](#), University of British Columbia, Canada
47. May 2018: [2nd International Symposium on Organic Reaction Mechanism](#), Peking University, Shenzhen Graduate School, China
46. April 2018: [Predictive Catalysis](#) 2018, Girona, Spain
45. March 2018: Complutense University of Madrid, Spain
44. February 2018: Colorado School of Mines, Golden, USA
43. June 2017: [11th EUCO-TCC](#), Barcelona, Spain
42. June 2017: [Challenges in Computational Homogeneous Catalysis](#), Stockholm, Sweden
41. April 2017: [V ENEQUI](#), University of Coimbra, Portugal
40. February 2017: University of Cologne, Germany
39. October 2016: University of Liverpool, UK
38. August 2016: KAIST, South Korea
37. July 2016: [IX International School On Organometallic Chemistry](#), San Sebastian, Spain
36. June 2016: ECS 2016, University of Strathclyde, UK
35. June 2016: [RCOM9](#), Marseilles, France
34. June 2016: RSC Awards Symposium, Queens University Belfast, UK
33. April 2016: Hans Suschitzky Symposium, University of Salford, UK
32. March 2016: RSC South East Regional Meeting, University of East Anglia, UK
31. March 2016: UK-Japanese Symposium on Asymmetric Catalysis, University of Manchester, UK
30. February 2016: Department of Chemistry, University of Cambridge, UK
29. February 2016: Department of Condensed Matter Physics, University of Cambridge, UK
28. February 2016: Federal University of São Carlos, Brazil

27. December 2015: Department of Chemistry, Warwick University, UK
26. December 2015: Department of Chemistry, Heriot-Watt University, UK
25. November 2015: Department of Chemistry, University of Oxford, UK
24. October 2015: University of Geneva, Switzerland
23. October 2015: Department of Chemistry, POSTECH, Pohang, South Korea
22. September 2015: [International Symposium on Synthesis and Catalysis](#), Evora, Portugal
21. August 2015: Colorado State University, USA
20. July 2015: NSCCS Computational Workshop for Synthetic Chemists, Imperial College London, UK
19. May 2015: University of Helsinki, Finland
18. March 2015: [Computational Molecular Science](#), Warwick, UK
17. February 2015: ICIQ, Tarragona, Spain
16. February 2015: Imperial College London, UK
15. February 2015: RWTH Aachen, Germany
14. August 2014: [ACS Organic Division Young Investigators Award Symposium](#), San Francisco, USA
13. February 2014: RSC South-West Regional Meeting – Oxford, UK
12. December 2013: University of California, Los Angeles, USA
11. October 2013: University College London, UK
10. August 2013: [Transatlantic Frontiers of Chemistry](#) – Kloster Seeon, Germany
9. July 2013: [Asia-Pacific Conference of Theoretical/Computational Chemistry](#) – Gyeongju, South Korea
8. April 2013: [UK Young Chemists 2013](#) – Imperial College London, UK
7. March 2013: Seoul National University, South Korea
6. February 2013: University of Bristol, UK
5. January 2013: LCC University of Toulouse, France
4. June 2012: Quantum Mechanics and Molecular Dynamics of Chemical and Biological Reactivity, UCLA, USA
3. March 2012: University of Birmingham, UK
2. January 2011: University of Nottingham, UK
1. January 2011: United States Food and Drug Administration – Irvine, USA

Teaching

Colorado State University:

- *Created a new senior-level course in computational chemistry and cheminformatics.*
- *Created a graduate-level course in organic spectroscopy focused on problem-solving approaches.*
- *Created a graduate-level course in computational organic chemistry*
- *Taught service organic chemistry classes to non-major students (200 students) and organic chemistry courses to chemistry majors.*

CHEM480A5: Computational Chemistry and Cheminformatics (3 credits, Spring 2025)

CHEM241: Foundations of Organic Chemistry (4 credits, Spring 2023, 2024, 2025)

CHEM343: Organic Chemistry II (3-credits, Spring 2020, 2021, 2022).

CHEM346: Organic Chemistry II. (3-credits, Spring 2019).

CHEM651C: Computational Organic Chemistry. (1 credit, Fall 2018, 2019, 2020, 2021, 2022).

CHEM541: Organic Spectroscopy (2 credits, Spring 2019, 2020, 2021, 2022, 2023, 2024).

University of Oxford:

- *Created a hands-on graduate course in DFT and mechanism, and a new class on electronic structure theory.*
- *Developed the undergraduate organic spectroscopy course.*
- *Taught introductory organic chemistry (orbitals and mechanism) to chemistry and biochemistry cohorts.*
- *Tutor with responsibility for all aspects of organic chemistry across the undergraduate curriculum.*

DFT and Mechanism: (Fall 2014, 2015, 2016, 2017).

Electronic Structure Theory: (Fall 2014, 2015, 2016, 2017).

Foundation Mathematics: (Fall 2014, 2015, 2016, 2017).

Orbitals and Mechanism: (Fall 2011, 2012-2013, 2014, 2015, 2016, 2017).

Organic Spectroscopy: (Fall 2010, 2011, 2013).

Tutorial Fellowship in Organic Chemistry, *Responsible for teaching 6 hours per week of organic chemistry to groups of two or three students.* (Fall/Spring 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017).

Workshops and Summer Schools:

- *Cheminformatics, Automation and Machine Learning in Chemistry (CAMLC 2024)*
- *Fixman Summer School in Theoretical and Computational Chemistry (2018, 2023)*
- *Brazilian Summer School on Chemistry: Computational Organic Chemistry (2016)*

Mentoring

Ph.D. Thesis Students:

25. Grace Bergan (2025 – current)
24. Megha Sasidaran (2025 – current)
23. Laura-Charlotte Underwood (2024 – current)
22. William Hughes (2024 – current)
21. Jake King (2023 – current)
20. Alex Platt (2022 – current)
19. Abhijeet Bhadauria (2022 – current)
18. Niket Manoj (2022 – current)
17. Dr. Shree Sowndarya (2019 – 2024) – *now Bristol Myers Squibb, Princeton, NJ*
 - ACS COMP Division Excellence Award for Graduate Students Spring 2024
 - NSF CCAS Diversity Fellowship 2023-2024
 - NREL internship summer 2023
 - Abbie Internship summer 2022
16. Dr. Louis de Lescure (2019 – 2024) – *now Sanofi Pharmaceuticals, Cambridge, MA*
15. Dr. Liliana Gallegos (2018 – 2023) – *now Postdoc (Isayev/Gomes), Carnegie Mellon University, PA*
 - ACS COMP Division Excellence Award for Graduate Students Fall 2023
 - NSF CCAS Diversity Fellowship 2022-2023
 - Frontera Computational Science Fellowship 2021-2022
 - ACS Bridge Career & Professional Development Award 2021
14. Dr. Heidi Klem (2018 – 2023) – *now NRC Postdoctoral Fellow, NIST, CO*
 - National Research Council Postdoctoral Research Associateship, 2023-2025
 - Chemical Structure Association Trust Grant Recipient, 2023
 - ACS Graduate Student Leadership Award in Mentoring, 2022
13. Dr. Guilian Luchini (2018 – 2023) – *now Bristol Myers Squibb, San Diego, CA*
 - ACS CINF Division Scholarship for Scientific Excellence 2022
 - GSK Internship, 2023
 - Chemical Structure Associate Trust Grant 2019
12. Dr. Owen Smith (2017 – 2021) – *now Pharmaron, Hoddesdon, UK*
11. Dr. Jacqueline Tan (2016 – 2020) – *now Institute of High Performance Computing (A*STAR), Singapore*
10. Dr. Xinglong Zhang (2016 – 2019) – *now Assistant Professor, Chinese University of Hong Kong*
9. Dr. Alex Brethomé (2016 – 2019) – *now Infineum, Paris, France*
 - Eugène Schueller Prize for Ph.D. dissertation, 2020
8. Dr. David Ascough (2016 – 2019) – *now Emerald Cloud Lab, San Francisco, CA*
7. Dr. Kiran Kumar (2015 – 2019) – *now Johnson & Johnson, Philadelphia, PA*
6. Dr. Ruchuta Ardkhean (2015 - 2019) – *now Lecturer, HRH Princess Chulabhorn College of Medical Science*
5. Dr. Hannah Patel (2015- 2019) – *now Mathematics teacher, Eton College, UK*

4. Dr. Wilian Cortopassi (2013 – 2017) – *now* Associate Director, Takeda, Boston
3. Dr. Kelvin Jackson (2012 - 2016) – *now* Prytania Solutions, London, UK
2. Dr. Robert Simion (2012 – 2016) – *now* Enzbond, London, UK
1. Dr. Sami Jaffar (2011 – 2015) – *now* EY-Parthenon, London, UK

Postdoctoral Associates:

15. Dr. Eve Xianwei Xu (2026 – current)
14. Dr. Ambre Carpentier (2025 – current)
13. Dr. Graham Haug (2023 – current)
12. Dr. Mihai Popescu (2022 – 2026) - *now* Group Leader, University of Vienna
11. Dr. Zhitao Feng (2023 – 2025) – *now* Associate Professor, Central South University, China
10. Dr. Santeri Aikonen (2021 – 2022) – *now* Johnson & Johnson, Philadelphia, PA
 - ACS Postdoctoral Scholars Recognition: leadership in Diversity, Equity, Inclusion, and Respect, 2022
9. Dr. Yingzi Li (2019 - 2022) – *now* Beatriu de Pinós Fellow (Maseras), ICIQ, Spain
8. Dr. Juan V. Alegre-Requena (2018 – 2022) – *now* tenured scientist, University of Zaragoza, Spain
 - Juan de la Cierva Fellowship, 2022
 - Chemical Structure Association (CSA) Trust Grant, 2022
 - ACS COMP Division Wiley Computers in Chemistry Outstanding Postdoc Award, 2019
7. Dr. Sreenithya Avadakkam (2019 – 2021) – *now* Postdoc (Pitko) at TU Delft, Netherlands
6. Dr. Yanfei Guan (2018 – 2019) – *now* Pfizer, Cambridge, MA
5. Dr. Nhu Nguyen (2017 – 2019) – *now* Terray Therapeutics, CA
4. Dr. Kelvin Jackson (2016 – 2017) – *now* Prytania Solutions, London, UK
3. Dr. Fernanda Duarte (2015 – 2017) – *now* Associate Professor, University of Oxford, UK
2. Dr. Qian Peng (2014 – 2016) – *now* Professor, Nankai University, China
1. Dr. Bencan Tang (2012 – 2016) – *now* Professor, University of Nottingham, Ningbo, China

Undergraduate Students:

35. Ashlynn Estal (2024)
34. Fiona Richards (REU 2024) – admitted to PhD program, Michigan
33. Aum Patel (REU 2024)
32. Trey Roupp (2023 – 2024)
31. Claire Jepsen (2023 – 2024) – admitted to PhD program, University of Edinburgh
30. Kim Nguyen (2023 – 2024)
29. Wonjin Ko (REU 2023)
28. Tobin Patterson (2020 – 2022)
27. Kate Fieseler (2021 – 2022) – admitted to PhD program, University of Oxford, UK
26. Turki Alturaifi (2020 – 2021) – admitted to PhD program, University of Pittsburgh
25. Cameron Nelson (2020)
24. Erin Connolly (REU 2019)
23. Thomas Schilling (2018 – 2019)
22. Wil Adams (REU 2018) – admitted to PhD program, McMaster University, Canada
21. Charlotte Miles (2017 – 2018)
20. Jan-Niklas Boyn (2016 – 2017) – admitted to PhD program, University of Chicago
19. Connor Brogan (2016 – 2017)
18. Will Hak (2015 – 2016)
17. Matthew Raybould (2015 – 2016) – admitted to PhD program, University of Oxford, UK
16. Shinny Woo (2015 – 2016)
15. Callum Arnold (2014 – 2015) – admitted to PhD program, Penn State
14. Michael Kennedy (2014 – 2015)
13. Susan Leung (2014 – 2015) – admitted to PhD program, University of Oxford, UK

12. Sophie Mathew-Jones (2014 – 2015)
11. Sam Hall (NVIDIA Summer scholarship 2013)
10. Alex Anthony (2013 – 2014)
9. Charlie Hornsby (2013 – 2014)
8. Alan Wise (2013 – 2014)
7. Wenbo Xie (Oxford-UGA student exchange program 2012)
6. Alex Curran (2012 – 2013)
5. Katie Hansel (2012 – 2013) – admitted to PhD program, Imperial College London, UK
4. Rosie Lang (2012 – 2013)
3. Kelvin Jackson (2011 – 2012) – admitted to PhD program, University of Oxford, UK
2. Christoph Schnedermann (2011 – 2012) – admitted to PhD program, University of Oxford, UK
1. Erin Shepherd (2011 – 2012) – admitted to PhD program, University of Oxford, UK

Hosted Researchers:

17. Maik Niedziella (Münster, 2024)
16. Susana Portela (Madrid, 2023)
15. Dr. Lucas Sigmund (TU Berlin, 2022)
14. Dr. Lisa Michelat (CNRS Orleans, 2022)
13. Wojtek Treyde (Max Planck Heidelberg, 2021-2022)
12. Dr. Meire Kawamura (Sao Carlos, 2019-2020)
11. Prof. Hua Yuan (Hunan, 2019-2020)
10. Dr. Mihai Popescu (Oxford, 2019)
9. Dr. Markus Rauhalati (Helsinki, 2018)
8. Dr. Adam Madarasz (Budapest, 2014)
7. Dr. Yago Rodeja (Madrid, 2017)
6. Prof. Jesús Díaz Álvarez (Extramadura, 2017)
5. Dr. Bruno Servilha (Sao Paulo, 2017)
4. Dr. Ignacio Funes (ICIQ, 2015)
3. Dr. Almudena Couce (Barcelona, 2015)
2. Prof. Sergiy Okovytyy (Dnipropetrovsk, 2014)
1. Dr. Tetiana Sergeiva (Dnipropetrovsk, 2014)

External Thesis Assessor:

8. University of Liege (2025)
7. IIT Bhubaneswar (2024)
6. University of Oxford (2022)
5. University of Mauritius (2021)
4. University of Bristol (2019)
3. University of Cambridge (2017)
2. University of Helsinki (2015)
1. Heriot-Watt University (2015)

Professional Service

Professional Memberships: American Chemical Society COMP and CINP divisions, Royal Society of Chemistry (Fellow).

Professional Committees:

- ACS National Award Selection Committee (2024-2026 award cycle).
- ACS COMP Division Awards Co-chair
- ACS COMP Executive Committee & Alternate Councillor
- Health & Environmental Sciences Institute for Genetic Toxicology Technical Committee, Nitrosamines

Steering Team

Editorial Advisory Boards:

- *Trends in Chemistry*
- *Tetrahedron: Chemistry*
- *Chemistry – Methods*
- *Essential Chem*
- *Magnetic Resonance in Chemistry*

Journal Reviewing: <https://orcid.org/0000-0002-0104-4166>, ResearcherID profile: top 1 percentile reviewer in Chemistry 2017, 2018, 2019.

Grant Reviewing:

- DOE BES ad hoc reviews (2026)
- NSF CAT Panel (2026)
- DOE INCITE: Chemistry Panel (2025)
- DFG SPP Panel (2025, Germany)
- NSF DMREF *ad hoc* reviews (2024)
- NSF CSDM Panel (2024)
- NSF ACCESS Panel (2023 – current)
- NIH NIGMS MIRA Panel (2023, 2024)
- DFG CRC Panel (2023, Germany)
- DOE INCITE: Biological Science Panel (2023, 2024)
- DFG SPP Panel (2021, Germany)
- NSF CCI Phase II Panel (2021)
- RSC Subject Expert Grant Assessment Panel (2018 – 2022)
- NIH SBCB Study Section (2019)
- NSF GOALI Reviewer (2019)
- ACS PRF Grant Program Reviewer (2018 – present)
- *Ad hoc* reviews for the Leverhulme Trust, Royal Society, European Research Council, Flanders: Research Foundation, Belgium, Swiss National Science Foundation
- Selection panel for Tutorial Fellowship in Physics at St Hilda's College (2017)
- Selection panel for St Hilda's College Junior Research Fellowships (2015 – 2017)
- External specialist Assessor to the Research Fellowship appointments panel for University of Cambridge colleges (Corpus Christi, Churchill College, Kings College, Trinity Hall)

Conference and Symposium Organization:

- **2028:** Chair – IUPAC Conference on Physical Organic Chemistry, Colorado
- **2022 – 2024:** Co-chair – Gordon Conference on Computational Chemistry
- **2023:** Co-chair – Houk 80th Symposium, ACS National Meeting, San Francisco
- **2023:** Discussion leader – Gordon conference on Physical Organic Chemistry
- **2022:** Discussion leader – Gordon conference on Stereochemistry
- **2019 – present:** Co-chair: Telluride Workshop “Machine Learning and Informatics for Chemistry and Materials”
- **2019:** Symposium Organizer *Immersive Virtual Reality for Molecular Design*, ACS National Meeting, San Diego
- **2019:** Symposium Organizer *Probing Reactive Intermediates through Chemical Computations*, ACS National Meeting, Orlando

Outreach:

- **2023:** Video interview with *ChemTalk*, a non-profit organization dedicated to science education and outreach
- **2021:** Coding Camp for 10th and 11th grade students at Colorado State University

- **2015:** Visited high schools in inner London to conduct chemistry workshops introducing students to IR spectroscopy and career routes for chemists.
- **2014:** Gave career talks for graduate and postdoctoral scientists in Oxford; I was also featured in a recent careers piece in *Chemistry World*.
- **2014 – 2018:** Chemistry tutor for residential courses (Linacre Trust) aimed at increasing participation in higher-education. I lectured high-school students from schools under-represented in higher education: 70% of students attending obtained offers from Oxford/Cambridge/Imperial. I have written a book on Chemistry problems distributed by the RSC throughout UK schools, served on the RSC Olympiad Committee, and was head-mentor for the UK at the International Chemistry Olympiad.

University Service

Colorado State University

2025 Spring: Statistics Chair Search Committee

2024 Fall: Chemistry Operating Budget Strategy Committee

2024 Fall: Statistics Standing Committee on Promotion & Tenure, Committee member

2024 Fall: Chemistry Standing Committee on Promotion & Tenure, Committee member

2022 – 2023: Chair, Chemistry Faculty Search (resulted in hiring Prof. Yuyang Dong)

2022 – present: Chair, Chemistry Undergraduate and Graduate Student Awards Committee

2022 – present: Faculty Council Committee on Information Technology

2018 – present: Chair, Organic Chemistry Division

2018 – present: College of Natural Sciences Scholarship Review Committee

2018 – present: Faculty Advisor to Chemistry Majors

2022 – 2023: College of Natural Sciences Faculty Council Representative

2018 – 2023: Departmental Executive Committee

University of Oxford

2017 – 2018: Department of Chemistry Outreach Committee

2015 – 2018: Department of Chemistry Consultative Committee

2014 – 2018: St Hilda's College IT committee

2014 – 2018: St Hilda's College Academic Disciplinary Committee

2012 – 2014: St Hilda's College College Library Committee

2011 – 2013: Department of Chemistry, Organizer of Organic Colloquia

2011 – 2013: Department of Chemistry, Organiser of the Symposium of Final Year PhD Talks

2010 – 2012: Department of Chemistry Staff-Student Consultative Committee

2010 – 2018: St Hilda's College Tutorial Fellow in Organic Chemistry

2010 – 2018: St Hilda's College Governing Body

2010 – 2018: St Hilda's College Academic Committee

Consulting & Advising

Consultant: Verdox (2021 – current)

Expert Witness: Herbert Smith Freehills (2022)

Expert Witness: Bartlit Beck LLP (2019 – 2021)