

## 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

- 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

- 186.** Fluorochemicals from PFAS via a Phosphate-enabled Mechanochemical Process. Yang, L.; Chen, Z.; Goult, C. A.; Tan, J.; Schlatzer, T.; Paton, R. S.; Gouverneur, V. *Nature* **2024**, *in revision*

- 185.** 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.* **2024**, *in revision*
- 184.** 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**, *in revision*
- 183.** C–F bond activation by an organic photoredox catalyst. Liu, X.; Green, A.; Pompetti, N. F.; Sau, A.; Li, Y.; Zhao, Y.; Paton, R. S.; Damrauer, N. H.; Miyake, G. M. *Nature* **2024**, *in revision*
- 182.** 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.* **2024**, *accepted*.
- 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**, 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  $\delta$  and  $\gamma$  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**, DOI: 10.1016/j.chempr.2024.07.001
- 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.; Corcilus, L.; Payne, R. J. *Angew. Chem. Int. Ed.* **2023**, *62*, e202313037.
- 164.** Fluorochemicals from fluor spar with a phosphate-enabled mechanochemical process bypassing HF. Patel, C.; André-Joyaux, E.; Leitch, J. A.; Martínez de Irujo-Labelde, 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  $\sigma$ -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**, DOI: 10.1002/wcms.1663.
- 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  $6\pi$  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.; Larance, 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.** <sup>18</sup>F-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 NO<sub>3</sub> 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 <sup>1</sup>H and <sup>13</sup>C 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.; Scora, 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 sp<sup>2</sup>–sp<sup>3</sup> 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.*

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**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  $\gamma$ -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 Alkylation 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.
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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 <sup>13</sup>C 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, Ardskhean, 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**

113. November 2024: University of Cambridge Chemical Society
112. October 2024: Sygnature Discovery, Nottingham, UK
111. September 2024: European Conference on Organic Free Radicals, Manchester, UK
110. August 2024: IUPAC Conference on Physical Organic Chemistry, Beijing, China
109. August 2024: Wuhan University, Wuhan
108. August 2024: SUSTech, Shenzhen
107. August 2024: HRC 2024, Zhejiang University, Hangzhou
106. July 2024: Frontiers of Computational Reaction Prediction, University of Chicago
105. June 2024: Cheminformatics, Automation and Machine Learning in Chemistry, Jaca
104. June 2024: ICIQ, Spain

103. June 2024: University of Girona, Spain
102. June 2024: Autonomous University of Barcelona, Spain
101. May 2024: Brazilian Chemical Society Lecture, Sao Paolo, Brazil
100. May 2024: Student Seminar Series, University of Minnesota, MN
100. February 2024: University of Pennsylvania, PA
100. February 2024: FDA Center for Drug Evaluation and Research
99. January 2024: AstraZeneca
98. November 2023: University of North Carolina at Chapel Hill
97. 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: Daejeon, 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:**

22. Jake King (2023 – current)
21. Alex Platt (2022 – current)
20. Abhijeet Bhadauria (2022 – current)
19. Niket Manoj (2022 – current)
18. Brandon Portela (2021 – current)
17. 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
  - Abbvie Internship summer 2022
16. Dr. Louis de Lescure (2019 – current) – *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 CINP 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* Gilead Sciences, San Francisco, CA
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:**

14. Dr. Ambre Carpentier (2025 – current)
13. Dr. Zhitao Feng (2023 – current)
12. Dr. Graham Haug (2023 – current)
11. Dr. Mihai Popescu (2022 – current)
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* Postdoc (Maseras), ICIQ, Spain
8. Dr. Juan V. Alegre-Requena (2018 – 2022) – *now* tenured scientist, CSIC, 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* Associate Professor, University of Nottingham, Ningbo, China

***Undergraduate Students:***

35. Ashlynn Estal (2024 – present)
34. Fiona Richards (REU 2024)
33. Aum Patel (REU 2024)
32. Trey Roupp (2023 – 2024)
31. Claire Jepsen (2023 – present) – 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 (NVVIA 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, 2021-2-2022)
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:**

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 CINF 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:**

- 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:**

- **2022 – 2024:** Co-chair – Gordon Conference on Computational Chemistry
- **2023:** Co-chair – Houk 80<sup>th</sup> 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 10<sup>th</sup> and 11<sup>th</sup> 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*

**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 – 2022)

Expert Witness: Herbert Smith Freehills (2022)

Expert Witness: Bartlit Beck LLP (2019 – 2021)