Abigail Gutmann Doyle
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A. FIELD OF SPECIALIZATION

Organic Chemistry, Catalysis, Organometallic Chemistry, Physical Organic Chemistry & Data Science, Radiochemistry, Asymmetric Catalysis

B. EDUCATION

2003-2008	**Harvard University, Department of Chemistry and Chemical Biology**
	Degree awarded: Ph.D., NDSEG, NSF, and Harvard Merit Pre-Doctoral Fellow
	Research Advisor: Professor Eric N. Jacobsen
	"Engaging Alkyl Halides and Oxocarbenium Ions in Asymmetric Catalysis"
2002-2003	**Stanford University, Department of Chemistry**
	NDSEG Pre-Doctoral Fellow
	Research Advisor: Professor Justin Du Bois
1998-2002	**Harvard University, Department of Chemistry and Chemical Biology**
	Degree awarded: A.B. and A.M. with Highest Honors, summa cum laude
	Research Advisor (2000-2002): Professor Eric N. Jacobsen

C. PROFESSIONAL AND ACADEMIC EXPERIENCE

Saul Winstein Endowed Chair in Organic Chemistry, UCLA (July 2021 to present)

A. Barton Hepburn Professor of Chemistry, Princeton University (July 2017 to June 2021)

- Provide a team of 16 graduate students and postdoctoral scholars with leadership, personalized mentoring, scientific vision, financial support, and administrative guidance. I have set in place numerous mechanisms to promote creativity and encourage scientific breadth & depth in my co-workers, to foster a healthy, encouraging, and inclusive environment to pursue science, to mentor students on how to effectively communicate their work in written and oral form, and to enhance their professional development. Doyle lab members have gone on to careers in academia, process and medicinal chemistry, data science, and energy and materials science.
- Established a research area at the interface of machine learning and synthetic chemistry with the goal of using ML to facilitate reaction prediction, optimization, and mechanistic elucidation.
- Elucidated the photophysics of organometallic Ni complexes relevant to cross coupling and metallaphotoredox catalysis (collaboration with Scholes lab). Identified Ni as an underexplored alternative to precious metal photocatalysts relevant to solar energy research and chemical synthesis.
- Discovered a new strategy for direct radical generation and C–O activation from alcohol and carboxylic feedstocks via photoredox catalysis with phosphine mediators (collaboration with Rovis lab).
- Discovered a new class of monodentate phosphine ligands (TyrannoPhos and TriceraPhos) that afford unprecedented reactivity for Ni-catalyzed Suzuki cross-coupling.
- Designed a strategy for effecting S_N1 substitutions from $C(sp_3)$–H and $C(sp_3)$–CO_2X substrates via photoredox catalysis that enables the mild synthesis of tertiary fluorides, ethers, and C–C bond formation. Translated the strategy to the incorporation of ^{18}F into previously inaccessible radiotracers.

Senior Editor, Accounts of Chemical Research (November 2016 to present)

Associate Professor of Chemistry, Princeton University (July 2013 to June 2017)

- Identified a new cross-coupling paradigm in which the combination of photoredox catalysis and nickel catalysis enables C(sp^3)–C bond formation from simple and readily available organic molecules (collaboration with MacMillan lab). Independent studies by our group have established this activation mode as general for C–H functionalization under exceptionally mild conditions.
- Invented new methods for the introduction of ^{18}F into organic substrates that feature uncommonly mild, rapid, and operationally convenient procedures. The processes enable access to experimental and clinically-validated radiotracers by late-stage radiofluorination and have led to a number of collaborations with industrial and academic groups for the development of new PET tracers.
- Identified novel ligands for Ni catalysis that enable unprecedented reactivity or activity – phosphines featuring remote steric hindrance and the electron-deficient olefin ligand FroDO.
- Invented two new chemicals (one a fluorination reagent and the other a Ni pre-catalyst) that have been commercialized and have seen widespread adoption by the community including on kilo scale.
- Developed a collection of new synthetic methods for C(sp^3)–C bond formation that afford access to valuable heterocycles and acyclic amines and ethers.

Assistant Professor of Chemistry, Princeton University (July 2008 to June 2013)

- Mentored 4 postdoctoral fellows, 12 graduate students, and 8 undergraduate researchers.
- Discovered the first asymmetric catalytic methods for nucleophilic fluorination, including cooperative catalytic systems for asymmetric ring opening of epoxides and aziridines, and two Pd-catalyzed protocols for enantio- and regioselective allylic fluorination.
- Identified catalytic cross-coupling reactions with styrenyl epoxides and aziridines as electrophiles. The methodologies feature unique ligand effects for nickel catalysis that enable regioselective Csp^3–O and Csp^3–N activation and mild C_{alkyl}–C bond formation.
- Elucidated a new entry to alkyl cross coupling that involves oxidative interaction of a nickel catalyst with iminium and oxocarbenium electrophiles; this approach has led to the identification of enantioselective methods for the preparation of important chiral heterocyclic products.

Summer Intern, Bristol-Myers Squibb, Discovery Chemistry (Metabolic Diseases, May to August 2000)

D. TEACHING EXPERIENCE

Chemistry 303: Organic Chemistry I (undergraduate-level)

Chemistry 521: Organometallic Chemistry (graduate-level)

Chemistry 530: Synthetic Organic Chemistry (graduate-level)

Chemistry 532: Mechanistic and Physical Organic Chemistry (under/graduate-level)

Chemistry 536: Methods for Complex Organic Synthesis (graduate-level)

E. PUBLICATIONS

60. Żurański, A. M.; Martinez Alvarado, J. I.; Shields, B. J.; Doyle, A. G. **"Predicting Reaction Yields via Supervised Learning."** *Acc. Chem. Res.* **2021**, *54*, 1856–1865.

59. Shen, Y.; Borowski, J. E.; Hardy, M. A.; Sarpong, R.; Doyle, A. G.; Cernak, T**. "Automation and computer-assisted planning for chemical synthesis."** *Nat. Rev. Methods Primers* **2021**, *1*, 23.

58. Shields, B. J.; Stevens, J.; Li, J.; Parasram, M.; Damani, F.; Martinez-Alvarado, J.; Janey, J.; Adams, R. P.; Doyle, A. G. **Bayesian Reaction Optimization as a Tool for Chemical Synthesis.** *Nature* **2021**, *590*, 89–96.

57. Kariofillis, S. K.; Doyle, A. G. **"Synthetic and Mechanistic Implications of Chlorine Photoelimination in**

Nickel/Photoredox C(sp^3)–H Cross-Coupling." *Acc. Chem. Res.* **2021**, *54*, 988–1000.

56. Proppe, A. H.; Li, Y. C.; Aspuru-Guzik, A.; Berlinguette, C. P.; Chang, C. J.; Cogdell, R.; Doyle, A. G.; Flick, J.; Gabor, N. M.; van Grondelle, R.; Hammes-Schiffer, S.; Jaffer, S. A.; Kelley, S. O.; Leclerc, M.; Leo, K.; Mallouk, T. E.; Narang, P.; Schlau-Cohen, G. S.; Scholes, G. D.; Vojvodic, A.; Yam, V. W.; Yang, J. Y.; Sargent, E. H. **Bioinspiration in Light Harvesting and Catalysis.** *Nat. Rev. Mater.* **2020**, *5*, 828–846.

55. Webb, E. W.; Park, J. B.; Cole, E. L.; Donnelly, D. J.; Bonacorsi, S. J.; Ewing, W. R.; Doyle, A. G. **"Nucleophilic (Radio)Fluorination of Redox-Active Esters via Radical-Polar Crossover Enabled by Photoredox Catalysis."** *J. Am. Chem. Soc.* **2020**, *142*, 9493–9500.

54. Parasram, M.; Shields, B. J.; Ahmad, O.; Knauber, T.; Doyle, A. G. **"Regioselective Cross-Electrophile Coupling of Epoxides and (Hetero)aryl Iodides via Ni/Ti/Photoredox Catalysis"** *ACS Catal.* **2020**, *10*, 5821–5827.

53. Estrada, J. G.; Williams, W. L.; Ting, S. I.; Doyle, A. G. **"Role of Electron-Deficient Olefin Ligands in a Ni-Catalyzed Aziridine Cross Coupling to Generate Quaternary Carbons."** *J. Am. Chem. Soc.* **2020**, *142*, 8928–8937.

52. Kariofillis, S. K.; Shields, B. J.; Tekle-Smith, M. A.; Zacuto, M. J.; Doyle, A. G. **"Nickel/Photoredox-Catalyzed Methylation of (Hetero)aryl Chlorides Using Trimethyl Orthoformate as a Methyl Radical Source."** *J. Am. Chem. Soc.* **2020**, *142*, 7683–7689.

51. Steiman, T. J.; Liu, J.; Mengiste, A.; Doyle, A. G. **"Synthesis of β-Phenethylamines via Ni/Photoredox Cross-Electrophile Coupling of Aliphatic Aziridines and Aryl Iodides."** *J. Am. Chem. Soc.* **2020**, *142*, 7598–7605.

50. Ting, S. I.; Garakyaraghi, S.; Taliaferro, C. M.; Scholes, G. D.; Castellano, F. N.; Doyle, A. G. **"Excited States of Ni Complexes Relevant to Photoredox Catalysis: Characterization and Mechanistic Implications."** *J. Am. Chem. Soc.* **2020**, *142*, 5800–5810.

49. Martinez Alvarado, J. I.; Ertel, A. B.; Stegner, A.; Stache, E. E.; Doyle, A. G. **"Direct Use of Carboxylic Acids in the Photocatalytic Hydroacylation of Styrenes to Generate Dialkyl Ketones."** *Org. Lett.* **2019,** *21*, 9940–9944.

48. Seff, S.; Zhou, W.; Damani, F.; Doyle, A. G.; Adams, R. P. **"Discrete Object Generation with Reversible Inductive Construction"** arXiv:1907.08268 [cs.LG]

47. Estrada, J. G.; Ahneman, D. T.; Sheridan, R. P.; Dreher, S. D.; Doyle, A. G. **Response to Comment on "Predicting Reaction Performance in C–N Cross-Coupling Using Machine Learning".** *Science* **2018,** *362*, eaat8763.

46. Stache, E. E.; Ertel, A. B.; Rovis, T.; Doyle, A. G. **C–O Generation of Phosphoranyl Radicals via Photoredox Catalysis Enables Voltage-Independent Activation of Strong C–O Bonds**. *ACS Catalysis* **2018**, *8*, 11134–11139.

45. Ackerman, L. K. G.; Martinez Alvarado, J. I.; Doyle, A. G. **Direct C–C Bond Formation from Alkanes Using Ni-Photoredox Catalysis.** *J. Am. Chem. Soc.* **2018**, *140*, 14059–14063.

44. Nielsen, M. K.; Ahneman, D. T.; Riera, O.; Doyle, A. G. **Deoxyfluorination with Sulfonyl Fluorides: Navigating Reaction Space with Machine Learning.** *J. Am. Chem. Soc.* **2018**, *140*, 5004–5008.

43. Ahneman, D. T.; Estrada, J. G.; Lin, S.; Dreher, S. D.; Doyle, A. G. **Predicting reaction performance in C–N cross-coupling using machine learning.** *Science* **2018**, *360*, 186–190.

42. Shields, B. J.; Kudisch, B.; Scholes, G. D.; Doyle, A. G. **Long-Lived Charge Transfer States of Nickel(II) Aryl Halide Complexes Facilitate Bimolecular Photoinduced Electron Transfer**. *J. Am. Chem. Soc.* **2018,** *140*, 3035–3039.

41. Heinz, C.; Lutz, J. P.; Simmons, E. M.; Miller, M. M.; Ewing, W. R.; Doyle, A. G. **Ni-Catalyzed Carbon–Carbon Bond-Forming Reductive Amination.** *J. Am. Chem. Soc.* **2018**, *140*, 2292–2300.

40. Nielsen, M. K.; Shields, B. J.; Liu, J. Williams, M. J.; Zacuto, M. J; Doyle, A. G. **"Mild, Redox-Neutral Formylation of Aryl Chlorides via Photocatalytic Generation of Chlorine radicals"** *Angew. Chem. Int. Ed.* **2017**, *129*, 7297–7300.

39. Woods, B. P.; Orlandi, M.; Huang, C.-Y. Sigman, M. H.; Doyle, A. G. **"Nickel-Catalyzed Enantioselective Reductive Cross-Coupling of Styrenyl Aziridines"** *J. Am. Chem. Soc.* **2017,** *139*, 5688–5691.

38. Stache, E. E.; Rovis, T.; Doyle, A. G. **"Nickel-photoredox catalyzed enantioselective desymmetrization of meso cyclic anhydrides."** *Angew. Chem. Int. Ed.* **2017**, *56*, 3679–3683.

37. Wu, K.; Doyle, A. G. **"Parameterization of phosphine ligands demonstrates enhancement of nickel catalysis via remote steric effects"** *Nature Chem.* **2017,** *9*, 779–784.

36. Shields, B. J.; Doyle, A. G. **Direct C(sp^3)–H Cross Coupling Enabled by Catalytic Generation of Chlorine Radicals.** *J. Am. Chem. Soc.* **2016**, *138*, 12719–12722.

35. Gray, E. E.; Nielsen, M. K.; Choquette, K. A.; Kalow, J. A.; Graham, T. J. A.; Doyle, A. G. **Nucleophilic (Radio)Fluorination of α-Diazocarbonyl Compounds Enabled by Copper-Catalyzed H–F Insertion.** *J. Am. Chem. Soc.* **2016,** *138,* 10802–10805.

34. Ahneman, D. T.; Doyle, A. G. **C–H functionalization of amines with aryl halides by nickel-photoredox catalysis**. *Chem. Sci.* **2016***, 7*, 7002–7006.

33. Lutz, J. P.; Chau, S. T.; Doyle, A. G. **Nickel-Catalyzed Enantioselective Arylation of Pyridine**. *Chem. Sci.* **2016**, *7*, 7105–7109.

32. Joe, C. L.; Doyle, A. G. **Direct Acylation of C(sp^3)–H Bonds Enabled by Nickel and Photoredox Catalysis.** *Angew. Chem. Int. Ed.* **2016** *55*, 4040–4043.

31. Nielsen, M. K.; Ugaz, C. R.; Li, W.; Doyle, A. G. **PyFluor: A Low-Cost, Stable, and Selective Deoxy-fluorination Reagent.** *J. Am. Chem. Soc.* **2015,** ***137,*** 9571−9574.

30. Arendt, K. M.; Doyle, A. G. **Dialkyl Ether Formation via Nickel-Catalyzed Cross Coupling of Acetals and Aryl Iodides.** *Angew. Chem. Int. Ed.* **2015**, *54*, 9876-9880.

29. Huang, C.-Y.; Doyle, A. G. **Electron-Deficient Olefin Ligands Enable Generation of Quaternary Carbons by Ni-Catalyzed Cross Coupling.** *J. Am. Chem. Soc.* **2015**, *137*, 5638–5641.

28. Shields, J. D.; Gray, E. E.; Doyle, A. G. **A Modular, Air-Stable Nickel Precatalyst.** *Org. Lett.* **2015**, *17*, 2166–2169.

27. Zuo, Z.; Ahneman, D.; Chu, L.; Terrett, J.; Doyle, A. G.; MacMillan, D. W. C. **Merging photoredox with nickel catalysis: Coupling of α-carboxyl sp3-carbons with aryl halides.** *Science* **2014**, *345*, 437–440.

26. Huang, C.-Y. (Dennis); Doyle, A. G. **The Chemistry of Transition Metals with Three-Membered Ring Heterocycles.** *Chem. Rev.* **2014**, *114*, 8153–8198.

25. Graham, T. J. A.; Lambert, R. F.; Ploessl, K.; Kung, H. F.; Doyle, A. G. **Enantioselective radiosynthesis of positron emission tomography (PET) tracers containing [^{18}F]fluorohydrins**. *J. Am. Chem. Soc.* **2014**, *136*, 5291–

5294.

24. Katcher, M. H.; Norrby, P.-O.; Doyle, A. G. **Mechanistic Investigations of Palladium-Catalyzed Allylic Fluorination.** *Organometallics.* **2014**, *33*, 2121–2133.

23. Shields, J. D.; Ahneman, D. T.; Graham, T. J. A.; Doyle, A. G. **Enantioselective, Nickel-Catalyzed Suzuki Cross-Coupling of Quinolinium Ions.** *Org. Lett.* **2013**, *16*, 142–145.

22. Nielsen, D. K.; Huang, C.-Y. (Dennis); Doyle, A. G. **Directed Nickel-Catalyzed Negishi Cross Coupling of Alkyl Aziridines.** *J. Am. Chem. Soc.* **2013**, *135*, 13605–13609.

21. Braun, M.-G.; Doyle, A. G. **Palladium-Catalyzed Allylic C–H Fluorination.** *J. Am. Chem. Soc.* **2013**, *135*, 12990–12993.

20. Chau, S. T.; Lutz, J. P.; Wu, K.; Doyle, A. G. **Nickel-Catalyzed Enantioselective Arylation of Pyridinium Ions: Harnessing an Iminium Ion Activation Mode.** *Angew. Chem., Int. Ed.* **2013**, *52*, 9153–9156.

19. Kalow, J. A.; Doyle, A. G. **Enantioselective fluoride ring opening of aziridines enabled by cooperative Lewis acid catalysis.** *Tetrahedron*, **2013**, *69*, 5702–5709.

18. Braun, M.-G.; Katcher, M. H.; Doyle, A. G. **Carbofluorination via a Palladium-Catalyzed Cascade Reaction.** *Chemical Science*, **2013**, *4*, 1216–1220.

17. Sylvester, K. T.; Wu, K.; Doyle, A. G. **Mechanistic Investigations of the Nickel-Catalyzed Suzuki Reaction of *N,O*-Acetals: Evidence for Boronic Acid-Assisted Oxidative Addition and an Iminium Activation Pathway**. *J. Am. Chem. Soc.* **2012**, *134*, 16967–16970.

16. Kalow, J. A.; Schmitt, D. E.; Doyle, A. G. **Synthesis of β-Fluoroamines by Lewis Base-Catalyzed Hydrofluorination of Aziridines**. *J. Org. Chem.* **2012**, *77*, 4177–4183.

15. Huang, C.-Y. (Dennis); Doyle, A. G. **Nickel-Catalyzed Negishi Alkylations of Styrenyl Aziridines**. *J. Am. Chem. Soc.* **2012**, *134*, 9541–9544.

14. Graham, T. J. A.; Doyle, A. G. **Nickel-Catalyzed Cross Coupling of Chromene Acetals and Boronic Acids**. *Org. Lett.* **2012**, *14*, 1616–1619.

13. Katcher, M. H.; Sha, A.; Doyle, A. G. **Regio- and Enantioselective Fluorination of Acyclic Allylic Halides**. *J. Am. Chem. Soc.* **2011**, *133*, 15902–15905.

12. Kalow, J. A.; Doyle, A. G. **Mechanistic Investigations of Cooperative Catalysis in the Enantioselective Fluorination of Epoxides**. *J. Am. Chem. Soc.* **2011**, *133*, 16001–16012.

11. Nielsen, D. K.; Doyle, A. G. **Nickel-Catalyzed Cross Coupling of Styrenyl Epoxides with Boronic Acids**. *Angew. Chem., Int. Ed.* **2011**, 50, 6056–6059.

10. Graham, T. J. A.; Doyle, A. G. **Transition Metal-Catalyzed Cross Coupling with *N*-Acyliminium Ions Derived from Quinolines and Isoquinolines**. *Chem. Sci.* **2011**, *2*, 980–984.

9. Shaw, T. W.; Kalow, J. A.; Doyle, A. G. **Fluoride ring-opening kinetic resolution of terminal epoxides: preparation of *(S)*-2-fluoro-1-phenylethanol**. *Org. Syn.* **2012**, *89*, 9–18.

8. Katcher, M. H.; Doyle, A. G. **Palladium-Catalyzed Asymmetric Synthesis of Allylic Fluorides**. *J. Am. Chem. Soc.* **2010**, *132*, 17402–17404.

7. Kalow, J. A.; Doyle, A. G. **Enantioselective Ring-Opening of Epoxides by Fluoride Anion Promoted by a Cooperative Dual Catalyst System**. *J. Am. Chem. Soc.* **2010**, *132*, 3268–3269.

6. Reisman, S. E.; Doyle, A. G.; Jacobsen, E. N. **Enantioselective Thiourea-Catalyzed Additions to Oxocarbenium Ions.** *J. Am. Chem. Soc.* **2008**, *130*, 7198–7199.

5. Doyle, A. G.; Jacobsen, E. N. **Small-Molecule H-Bond Donors in Asymmetric Catalysis**. *Chem. Rev.* **2007**, *107*, 5713–5743.

4 Doyle, A. G.; Jacobsen, E. N. **Enantioselective Alkylation of Acyclic α,α–Disubstituted Tributyltin Enolates Catalyzed by a Cr(salen) Complex.** *Angew. Chem. Int. Ed.* **2007**, *46*, 3701–3705.

3. Doyle, A. G.; Jacobsen, E. N. **Enantioselective Alkylations of Tributyltin Enolates Catalyzed by Cr(salen)Cl: Access to Enantiomerically Enriched All-Carbon Quaternary Centers.** *J. Am. Chem. Soc.* **2005**, *127*, 62–63.

2. Ellsworth, B. A.; Doyle, A. G.; Patel, M.; Caceres-Cortes, J.; Meng, W.; Deshpande, P. P.; Pullockaran, A.; Washburn, W. N. **C-Arylglucoside synthesis: triisopropylsilane as a selective reagent for the reduction of an anomeric C-phenyl ketal.** *Tetrahedron-Asymmetry* **2003**, *14*, 3243–3247.

1. White, M. C.; Doyle, A. G.; Jacobsen, E. N. **A Synthetically Useful, Self-Assembling MMO Mimic System for Catalytic Alkene Epoxidation with Aqueous H_2O_2.** *J. Am. Chem. Soc.* **2001**, *123*, 7194–7195.

F. HONORS, PRIZES, & FELLOWSHIPS

- Camille and Henry Dreyfus Foundation Machine Learning in the Chemical Sciences and Engineering Award (2021)
- American Chemical Society Fellow (2020)
- RSC Fluorine Award (2019)
- 15th Hirata Prize (2019)
- BMS Unrestricted Grant in Synthetic Organic Chemistry (2016)
- Phi Lambda Upsilon National Fresenius Award (2014)
- Presidential Early Career Award for Scientists and Engineers (2014)
- Novartis Chemistry Lectureship (2014/2015)
- Bayer Excellence in Science Award (2013)
- Arthur C. Cope Scholar Award (2013)
- Camille-Dreyfus Teacher Scholar Award (2013)
- Thieme Chemistry Journals Award (2013)
- Amgen Young Investigator Award (2012)
- Alfred P. Sloan Foundation Fellowship (2012)
- NSF CAREER Award (2012-2017)
- Roche Early Excellence in Chemistry Award (2012)
- Eli Lilly Grantee Award (2012-2014)
- Boehringer Ingelheim New Investigator Award (2012)
- Merck Award for Selective Fluorination (2010-2012)
- ACS PRF Doctoral New Investigator Grant (2009)
- Sanofi Aventis New Faculty Award (2008)
- Eli Lilly New Faculty Award (2008)
- Harvard Merit Fellowship (2007)
- Sigma-Aldrich Graduate Student Innovation Award (2006)

- Christensen Prize for Outstanding Research Achievement (2005)
- National Science Foundation Pre-Doctoral Fellowship (2004-2007)
- National Defense Science and Engineering Pre-Doctoral Fellowship (2002-2004)
- Harvard College Certificate of Distinction in Teaching (2004)
- Phi Beta Kappa Junior Inductee (2001)
- Pfizer Undergraduate Summer Research Fellowship (2001)
- Harvard College Research Fellowship Award (2001)
- Harvard Detur Prize Recipient (1999)

G. INVITED TALKS (select examples)

131. Gordon Research Conference, Natural Products, Andover, NH (July 2022)
130. Gordon Research Conference, Stereochemistry, Newport, RI (August 2022)
129. 2021 International Chemical Congress of Pacific Basin Societies (Pacifichem), 2 invited lectures (December 2021)
128. VISTA symposium (July 2021)
127. Big Data and Machine Learning for Chemistry, EPFL/ETHZ Summer School (June 2021)
126. Award Lecture, RSC Fluorine Symposium (June 2021)
125. 25th Annual Green Chemistry & Engineering Conference (June 2021)
124. Unchained Labs Webinar (May 2021)
123. CDT Conference in Data Driven Chemical Synthesis (April 2021)
122. Society of Chemical Industry Webinar (February 2021)
121. Plenary Speaker, Batcheva de Rothschild Seminar on Strong Bond Activation, Dead Sea, Israel (postponed)
120. SCS Lectureship Award, Switzerland (postponed)
119. Plenary Speaker, International Symposium on Organic Free Radicals, Munster, Germany (postponed)
118. Plenary Speaker, 3rd International Conference on Hydrogen Atom Transfer, Rome, Italy (postponed)
117. ACS National Meeting, Symposium in Honor of Sarah Reisman, Philadelphia, PA (postponed)
116. 19th Hirata Prize, Nagoya, Japan (December 2019)
115. Center for Light Energy Activated Redox Processes, Northwestern University (November 2019)
114. Scripps Research Institute, La Jolla, CA (September 2019)
113. Gordon Research Conference, Organic Reactions & Processes, Easton, MA (July 2019)
112. "New Directions in Catalysis" Symposium, Canadian Society for Chemistry, Quebec City (June 2019)
111. Grassmere Conference, UK (May 2019)
110. 54th SCS Conference on Stereochemistry, Bürgenstock Conference, Switzerland (May 2019)
109. Harvard University, Cambridge, MA (April 2019)
108. Machine Learning for the Chemical Sciences, Dreyfus Foundation Symposium, New York, NY (April 2019)
107. "Accelerating drug discovery through enabling chemistry technologies" Symposium, Spring ACS National Meeting, Orlando, FL (March 2019)
106. Student-Invited Speaker, UC Berkeley, Berkeley, CA (February 2019)
105. NYU, New York, NY (February 2019)
104. BioHub Symposium, Cambridge, MA (August 2018)
103. Apple & Co. (September 2018)
102. Plenary Speaker, 21st International Symposium on Homogenous Catalysis, Amsterdam, The Netherlands (June 2018)
101. BMS Lecturer, Columbia University, New York, NY (June 20188)
100. Colorado State University, Fort Collins, CO (May 2018)
99. Aldrich Lecturer, University of Nebraska, Lincoln, NE (April 20188)
98. Plenary Speaker, Banff Organic Chemistry Symposium, Banff, Canada (October 2017)
97. Merck, West Point, PA (September 2017)
96. Stanford University, Palo Alto, CA (September 2017)
95. Plenary Speaker, Oxford Synthesis Symposium, Oxford, UK (June 2017)
94. Gordon Research Conference, Heterocyclic Chemistry, Newport, RI (June 2017)

93. Symposium in honor of Prof. Matt Sigman's Creativity in Organic Synthesis Award, Spring ACS Meeting, San Francisco, CA (April 2017)
92. Duke University, Durham, NC (February 2017)
91. Vanderbilt University, Nashville, TN (January 2017)
90. Bristol Chemical Synthesis – Syngenta Award, Bristol, UK (January 2017)
89. Cambridge University, Cambridge, UK (January 2017)
88. Creativity in Synthesis North Jersey ACS Section, NJ (December 2016)
87. NESACS Process Chemistry Symposium, Novartis, Cambridge, MA (October 2016)
86. Emory University, Atlanta, GA (October 2016)
85. University of Utah, Salt Lake City, UR (September 2016)
84. Diversity in Chemistry Symposium and JOC/Organometallics Award Lecture Symposium, ACS Fall National Meeting, Philadelphia, PA (August 2016)
83. Gordon Research Conference, Organometallics, Newport, RI (July 2016)
82. Celgene, NJ (June 2016)
81. Philadelphia Organic Chemistry Committee Student Lecture, Philadelphia, PA (April 2016)
80. Plenary Spekaer, Florida Heterocycles Conference, Gainesville, FL (March 2016)
79. National Organic Symposium, College Park, MD (July 2015)
78. Novartis, Basel, Switzerland (June 2015)
77. ETH, Zürich, Switzerland (June 2015)
76. University of Illinois, Urbana Champaign (April 2015)
75. Distinguished Women in Chemistry Seminar Series, Stanford University, Palo Alto, CA (April 2015)
74. Fresenius Award Lecture Symposium, ACS Spring National Meeting, Denver, CO (March 2015)
73. University of Wisconsin, Madison, WI (February 2015)
72. Yale University, New Haven, CT (January 2015)
71. Stereochemistry Gordon Research Conference, Newport RI (August 2014)
70. French American Chemical Society, Avignon, France (June 2014)
69. Harvard University, Cambridge, MA (May 2014)
68. Novartis, Cambridge, MA (May 2014)
67. MIT, Cambridge, MA (May 2014)
66. Columbia University, New York, NY (April 2014)
65. Eli Lilly Grantee Award Symposium, Indianapolis, IN (March 2014)
64. AbbVie, North Chicago, IL (November 2013)
63. Gilead, Foster City, CA (October 2013)
62. Indiana University, Bloomington, IN (September 2013)
61. Modern Methods in Fluorination Chemistry Symposium, 246th American Chemical Society National Meeting, Indianapolis, IN (September 2013)
60. High-Throughput Chemistry & Chemical Biology GRC (June 2013)
59. California Institute of Technology, Pasadena, CA (May 2013)
58. GlaxoSmithKline, Research Triangle, North Carolina (April 2013)
57. Fluorine in Medicinal Chemistry Symposium, 245th American Chemical Society National Meeting, New Orleans, LA (April 2013)
56. DuPont Crop Protection, Newark, DE (March 2013)
55. University of California, Irvine, CA (March 2013)
54. The Scripps Research Institute, La Jolla, CA (March 2013)
53. University of Ottawa, Ottawa, Canada (January 2013)
52. Bristol–Myers Squibb, Wallingford, CT (November 2012)
51. Swarthmore, Swarthmore, PA (November 2012)
50. University of North Carolina, Chapel Hill, NC (November 2012)
49. Amgen, Thousand Oaks, CA (October 2012)
48. New Jersey Biotechnology Chemistry Consortium (October 2012)
47. University of Utah, Salt Lake City, UT (October 2012)

47. University of California, Berkeley, CA (September 2012)
46. UT Southwestern, Dallas, TX (September 2012)
45. Texas A&M, College Station, TX (September 2012)
44. University of Texas, Austin, Austin, TX (September 2012)
43. Keynote Address, 2012 Chemistry Forum, Pfizer, Groton, CT (September 2012)
42. Boehringer Ingelheim, Connecticut (July 2012)
41. Bristol-Myers Squibb, Lawerenceville, NJ (July 2012)
40. Bristol-Myers Squibb, Hopewell, NJ (July 2012)
39. Bristol-Myers Squibb, New Brunswick, NJ (July 2012)
38. Johnson & Johnson, San Diego, CA (June 2012)
37. Plenary Lecture, International Symposia on Advancing the Chemical Sciences 7, Challenges in Organic Chemistry and Chemical Biology, Edinburgh, Scotland (June 2012)
36. 42nd Annual NSF Workshop on Synthesis, Dedham, MA (May 2012)
35. Plenary Lecture, Roche Excellence in Chemistry Symposium, Nutley, NJ (May 2012)
34. The City College of New York, New York, NY (May 2012)
33. Merck Laboratories, West Point, PA (May 2012)
32. Organic Chemistry Day, University of Missouri-Columbia, Missouri, Columbia (April 2012)
31. University of Louisville, Louisville, KY (April 2012)
30. Boston College, Boston, MA (April 2012)
29. Boston University, Boston, MA (April 2012)
28. Princeton Local ACS Meeting, Princeton, NJ (April 2012)
27. Symposium in honor of Jeffrey Johnson's Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator, ACS National Meeting, San Diego, CA (March 2012)
26. Merck Laboratories, Rahway, NJ (March 2012)
25. Lehigh University, Bethlehem, PA (February 2012)
24. University of California, Los Angeles, Los Angeles, CA (January 2012)
23. Novartis Lecture, University of Michigan, Ann Arbor, MI (December 2011)
22. University of Washington, Seattle, Seattle, WA (October 2011)
21. University of Pennsylvania, Philadelphia, PA (September 2011)
20. Bristol-Myers Squibb, 2011 Green Symposium Series, New Brunswick, NJ (August 2011)
19. Merck Laboratories, Kenilworth, NJ (July 2011)
18. Gordon Research Conferences – Natural Products, Smithfield, RI (July 2011)
17. Gordon Research Conferences – Organic Reactions and Processes, Smithfield, RI (July 2011)
16. Gordon Research Conferences – Heterocycles, Newport, RI (June 2011)
15. Eli Lilly and Company, Indianapolis, IN (June 2011)
14. Avid Radiopharmaceuticals, Philadelphia, PA (May 2011)
13. Abbott Laboratories, Abbott Park, IL (May 2011)
12. City University of New York, Brooklyn College, Brooklyn, NY (April 2011)
11. Colby College, Waterville, ME (April 2011)
10. Symposium in honor of David MacMillan's ACS Award for Creative Work in Synthetic Organic Chemistry, ACS National Meeting, Anaheim, CA (March 2011)
9. Pacifichem Conference, Honolulu, Hawaii (December 2010)
8. Kyoto University, Kyoto, Japan (October 2010)
7. Osaka University, Osaka, Japan (October 2010)
6. Sixth International Symposium on Integrated Synthesis, Kobe, Japan (October 2010)
5. International Symposium on Environmentally Benign Synthesis, Osaka, Japan (October 2010)
4. Gordon Research Conferences – Stereochemistry (short talk), Newport, RI (August 2010)
3. ACS National Meeting (oral presentation #10689), Boston, MA (August, 2010)
2. Sanofi-Aventis, Bridgewater, NJ (February 2009)
1. ACS National Meeting (oral presentation #76), San Francisco, CA (September 2006)

H. SERVICE

Outside Service

- Governing Committee, Open Reaction Database (https://docs.open-reaction-database.org/en/latest/index.html)
- Senior Editor, Accounts of Chemical Research (Nov 2016-present)
- Chirality 2018 (Princeton University, Princeton, NJ), co-chair
- ACS National Award Selection Committee
- Editorial Advisory Board member for *ACS Central Science* (current) & *Organic Letters* & *Advanced Synthesis & Catalysis* (2014-2020)
- Study section, SBCA, SBCB, NIGMS
- Grant reviewer for National Science Foundation (2012-present)
- Grant reviewer for American Chemical Society Petroleum Research Fund (2009-present)
- Co-organizer of the 42nd National Organic Chemistry Symposium (2010-2011) and Chirality Conference (2016)
- Session chair for ACS National Meeting (Boston, MA) & Gordon Research Conferences (2009-present)
- Organized and performed chemistry demonstrations for children at Trenton Science Museum's Super Science Saturday (2011-present)
- Faculty mentor for Mercer County Community College honors chemistry program
- Outside reader and examiner for graduate students in the Chemistry Department at Columbia University
- Reviewer for ACS, Wiley, Elsevier, Nature Publishing Group, and Royal Society of Chemistry journals
- Member of the American Chemical Society (2002-present)

Princeton University Service

- Director of Graduate Studies (2017-2020)
- Chemistry Diversity Committee (2014-2021)
- Panelist, Tigers with Cubs (2015)
- Women in STEM Working Group at Princeton (2014-2021)
- Committee of Committees (2013-2015)
- Chair of the Organic Chemistry Seminar Series (2008-2013)
- Chair of the Organic Graduate Admissions Committee (2008-2013)
- Graduate Work Committee (2008-2021)
- Junior Faculty Search Committee (2008-2015); chair in 2015
- Instrumentation Committee (2010-2021)
- Staffing and Long Range Planning Committee (2014-present)
- Created new graduate course "Chem 536," offered as part of Princeton University's Industrial Affiliates Program (2009-present)
- Created a Student Invited Lecture Series (SILS) in collaboration with the Chemistry Graduate Student Organization (2009-2021)
- Grader for incoming Chemistry graduate student's organic placement exam (2008-2011)
- Faculty panel member for Princeton's incoming women in science, engineering, and mathematics (2009-2021)
- Roundtable discussion facilitator for Princeton's undergraduate chemistry club dinner series (2011-2021)
- Grader for undergraduate organic prize exams (2010-2021)
- Reader and external grader for organic undergraduate senior theses (2010-2021)

Outreach efforts

- Trenton Science Museum, Super Science Saturday (Spring 2011–2015)
- Faculty mentor for Mercer Country Community College Honors Chemistry Program (2012-present)
- Faculty panel member for Princeton's incoming women in science, engineering, and mathematics (2009-present)
- Roundtable discussion facilitator for Princeton's undergraduate chemistry club dinner series (2011-present)

I. COLLABORATORS

- Professor Gregory Scholes (Princeton University)
- Professor Tomislav Rovis (Columbia University)
- Professor Ryan Adams (Department of Computer Science, Princeton University)
- Professor Matt Sigman (Department of Chemistry, University of Utah)
- Professor Hank Kung (Department of Radiology, University of Pennsylvania)
- Professor David MacMillan (Princeton University)
- Dr. Eric Hostetler (Translational Imaging Biomarkers, Merck Research Laboratories)
- Drs. Sam Bonacorsi and David Donnelly (Radiochemistry group, BMS Company)
- Drs. Spencer Dreher, Shane Krska, Heather Johnson, and Thomas Lyons (Merck Research Laboratories)
- Professor Phil Castellano (NC State)
- Professor Robert Paton (Colorado State University)
- Professor Olaf Wiest (Notre Dame)
- Professor Nitesh Chawla (Notre Dame)
- Dr. Kian Tan (Novartis)
- Professor Richmond Sarpong (UC Berkeley)