ERIC M. SIMMONS

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SUMMARY

Organic chemist with backgrounds in total synthesis, organometallic chemistry, synthetic methodology and process development. Extensive experience in the synthesis of complex molecules through the design, execution and optimization of multi-step sequences. Skilled in the development and scale-up of novel metal-catalyzed transformations of pharmaceutical intermediates and in conducting small-scale air-sensitive organometallic chemistry using glovebox techniques.

EDUCATION

University of Illinois at Urbana-Champaign, Urbana, IL *and* **Aug. 2009 to Jul. 2011**
University of California at Berkeley, Berkeley, CA **Aug. 2011 to Nov. 2011**
NIH Ruth L. Kirschstein NRSA Postdoctoral Fellow

University of California at Berkeley, Berkeley, CA **Aug. 2004 to June 2009**
Ph.D. in organic chemistry (received May 2009)

Tufts University, Medford, MA **Sept. 2000 to May 2004**
B.A. *magna cum laude* in chemistry and Spanish (received May 2004)

PROFESSIONAL EXPERIENCE

Catalysis Group Lead, Chemical & Synthetic Development, Bristol-Myers Squibb, New Brunswick, NJ

Senior Research Investigator II (Supervisor: Dr. Jacob Janey) **Sep. 2018 to present**

Catalysis R&D Group, Chemical & Synthetic Development, Bristol-Myers Squibb, New Brunswick, NJ

Senior Research Investigator II (Supervisors: Dr. Jacob Janey and Dr. Yi Xiao) **Dec. 2016 to Aug. 2018**
Senior Research Investigator I (Supervisor: Dr. Yi Xiao) **Jan. 2016 to Dec. 2016**

Catalysis R&D Group, Early Phase Chemical Development, Bristol-Myers Squibb, New Brunswick, NJ

Senior Research Investigator I (Supervisor: Dr. Yi Xiao) **May 2014 to Jan. 2016**
Research Investigator II (Supervisor: Dr. Yi Xiao) **Dec. 2011 to May 2014**

- Engaged in the rapid development of conditions for robust, scalable catalytic transformations, facilitated by the design and execution of high-throughput experiments to simultaneously examine multiple reaction parameters, and in conducting kinetic and mechanistic studies to probe the mechanism of these reactions
- Experienced in process development, pilot plant execution and tech transfer of catalytic processes

University of Illinois at Urbana-Champaign, Urbana, IL *and* **Aug. 2009 to Jul. 2011**
University of California at Berkeley, Berkeley, CA **Aug. 2011 to Nov. 2011**

Postdoctoral Research Associate (Advisor: Prof. John F. Hartwig)

- Identified an iridium-catalyzed, hydroxyl group-directed *ortho*-silylation of aromatic C–H bonds and established conditions for functionalization of the resulting benzoxasilole products
- Developed a method for the 1,4-hydroxyl group-directed oxygenation of unactivated aliphatic C–H bonds suitable for complex molecule synthesis, based on an iridium-catalyzed C–H silylation/oxidation sequence

University of California at Berkeley, Berkeley, CA

Graduate Research Assistant (Advisor: Prof. Richmond Sarpong) **Oct. 2004 to June 2009**

- Developed an enyne cycloisomerization reaction for the construction of benzocycloheptadienes and investigated their application in the total synthesis of complex natural products
- Completed the total synthesis of four natural products in the icetexane diterpenoid family, leading to two structural revisions

- Designed and carried out a synthetic route to the pentacyclic core of the cortistatin natural product family and completed a formal total synthesis of cortistatin A

Graduate Student Instructor **Aug. 2004 to May 2007**

- Assisted in the teaching of Chemistry 3A (fall 2004) and Chemistry 112A (fall 2005), undergraduate organic chemistry lecture and laboratory courses
- Taught the Chemistry 112B Scholars section (spring 2007), a supplemental lecture course in undergraduate organic chemistry

Tufts University, Medford, MA **Sept. 2003 to May 2004**

Undergraduate Research Assistant (Advisor: Prof. Marc d'Alarcao)

- Performed independent undergraduate research in the field of organic synthesis

PROFESSIONAL HONORS AND ACHIEVEMENTS

- Bristol-Myers Squibb Research Leveraging Technology (LevTech) Innovation Award, 2019
- American Chemical Society Young Investigator, 2017
- Bristol-Myers Squibb Chemistry Leadership Award, 2015
- NIH Ruth L. Kirschstein National Research Service Award, 2009-2011
- American Chemical Society Division of Medicinal Chemistry Fellowship, 2007-2008
- Roche Pharmaceuticals Fellowship, University of California, 2006-2007
- Member, American Chemical Society, 2006-present
- Gerald E. K. Branch Fellowship, University of California, 2005-2006
- The Durkee Scholarship, Tufts University, 2004
- American Chemical Society Certificate, 2004

PUBLICATIONS

ORCID: 0000-0002-3854-1561

(30) Beutner, G. L.; Coombs, J. R.; Green, R. A.; Inankur, B.; Lin, D.; Qiu, J.; Roberts, F.; **Simmons, E. M.**; Wisniewski, S. R. "Palladium-Catalyzed Amidation and Amination of (Hetero)aryl Chlorides under Homogeneous Conditions Enabled by a Soluble DBU/NaTFA Dual-Base System" *Org. Process Res. Dev.* **2019**, *23,* 1529-1537.

(29) Sherwood, T. C.; Xiao, H-Y.; Bhaskar, R. G.; **Simmons, E. M.**; Zaretsky, S.; Rauch, M. P.; Knowles, R. R.; Dhar, T. G. M. "Decarboxylative intramolecular arene alkylation using N-(acyloxy)phthalimides, an organic photocatalyst, and visible light" *J. Org. Chem.* **2019**, *84,* 8360-8379.

(28) Wisniewski, S. R.; Savage, S. A.; Romero, E. O.; Eastgate, M. D.; Tan, Y.; **Simmons, E. M.**; Plata, R. E.; Sowa, Jr., J. R.; Blackmond, D. G. "Utilizing Native Directing Groups: Mechanistic Understanding of a Direct Arylation Leads to Formation of Tetracyclic Heterocycles via Tandem Intermolecular, Intramolecular C−H Activation" *J. Org. Chem.* **2019**, *84,* 7961-7970.

(27) Coombs, J. R.; Green, R. A.; Roberts, F.; **Simmons, E. M.**; Stevens, J. M.; Wisniewski, S. R. "Advances in Base-Metal Catalysis: Development of a Screening Platform for Nickel-Catalyzed Borylations of Aryl (Pseudo)halides with $B_2(OH)_4$" *Organometallics* **2019**, *38,* 157-166.

(26) Hayler, J. D.; Leahy, D. K.; **Simmons, E. M** "A Pharmaceutical Industry Perspective on Sustainable Metal Catalysis" *Organometallics* **2019**, *38,* 36-46.

(25) Strotman, N. A.; Ramirez, A.; **Simmons, E. M.**; Soltani, O.; Parsons, A. T.; Fan, Y.; Sawyer, J. R.; Rosner, T.; Janey, J. M.; Tran, K.; Li, J.; La Cruz, T. E.; Pathirana, C.; Ng, A. T.; Deerberg, J. "Enantioselective Synthesis of a γ‑Secretase Modulator via Vinylogous Dynamic Kinetic Resolution" *J. Org. Chem.* **2018**, *83,* 11133-11144.

(24) Maity, P.; Ramana Reddy, V. V.; Mohan, J.; Korapati, S.; Narayana, H.; Cherupally, N.; Chandrasekaran, S.; Ramachandran, R.; Sfouggatakis, C.; Eastgate, M. D.; **Simmons, E. M.**; Vaidyanathan, R. "Development of a Scalable Synthesis of BMS-978587 Featuring a Stereospecific Suzuki Coupling of a Cyclopropane Carboxylic Acid" *Org. Process Res. Dev.* **2018**, *22,* 888-897.

(23) Beutner, G.; Carrasquillo, R.; Geng, P.; Hsiao, Y.; Huang, E. C.; Janey, J.; Katipally, K.; Kolotuchin, S.; La Porte, T.; Lee, A.; Lobben, P.; Lora-Gonzalez, F.; Mack, B.; Mudryk, B.; Qiu, Y.; Qian, X.; Ramirez, A.; Razler, T. M.; Rosner, T.; Shi, Z.; **Simmons, E.**; Stevens, J.; Wang, J.; Wei, C.; Wisniewski, S. R.; Zhu, Y. "Adventures in Atropisomerism: Total Synthesis of a Complex Active Pharmaceutical Ingredient with Two Chirality Axes" *Org. Lett.* **2018**, *20,* 3736-3740.

(22) Wertjes, W.; Ayers, S.; Gao, Q.; **Simmons, E. M.**; Beutner, G. L. "A Divergent Nickel-Catalyzed Synthesis of Quinazolinediones and Benzoxazinone Imines" *Synthesis* **2018**, *50,* 4453-4461.

(21) Young, I. S.; **Simmons, E. M.**; Fenster, M. D. B.; Zhu, J. J.; Katipally, K. R. "Palladium-Catalyzed C–O Coupling of a Sterically Hindered Secondary Alcohol with an Aryl Bromide and Significant Purity Upgrade in the API Step" *Org. Process Res. Dev.* **2018**, *22,* 585-594.

(20) Schmidt, M. A.; **Simmons, E. M.**; Wei, C. S.; Park, H.; Eastgate, M. D. "An Enantioselective Total Synthesis of (+)-Duocarmycin SA" *J. Org. Chem.* **2018**, *83,* 3928-3940.

(19) 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.

(18) Leahy, D. K.; **Simmons, E. M.**; Hung, V.; Sweeney, J. T.; Fleming, W. F.; Miller, M. "Design and Evolution of the BMS Process Greenness Scorecard" *Green Chem.* **2017**, *19,* 5163-5171.

(17) **Simmons, E. M.**; Mudryk, B.; Lee, A. G.; Qiu, Y.; Razler, T. M.; Hsiao, Y. "Development of a Kilogram-Scale Process for the Enantioselective Synthesis of 3-Isopropenyl-cyclohexan-1-one via Rh/DTBM-SEGPHOS-Catalyzed Asymmetric Hayashi Addition Enabled By 1,3-Diol Additives" *Org. Process Res. Dev.* **2017**, *21,* 1659-1667.

(16) Ayothiraman, R.; Rangaswamy, S.; Maity, P.; **Simmons, E. M.**; Beutner, G. L.; Janey, J.; Treitler, D. S.; Eastgate, M. D.; Vaidyanathan, R. "Zinc Acetate-Promoted Buchwald−Hartwig Couplings of Heteroaromatic Amines" *J. Org. Chem.* **2017**, *82,* 7420-7427.

(15) Coombs, J. R.; Fraunhoffer, K. J.; **Simmons, E. M.**; Stevens, J. M.; Wisniewski, S. R.; Yu, M. "Improving Robustness: In Situ Generation of a Pd(0) Catalyst For the Cyanation of Aryl Bromides" *J. Org. Chem.* **2017**, *82,* 7040-7044.

(14) Wei, C. S.; **Simmons, E. M.**; Hsiao, Y.; Eastgate, M. D. "Development of Robust, Scaleable Catalytic Processes through Fundamental Understanding of Reaction Mechanisms" *Top. Catal.* **2017**, *60,* 620-630.

(13) Beutner, G. L.; Hsiao, Y.; Razler, T.; **Simmons, E. M.**; Wertjes, W. "Nickel-Catalyzed Synthesis of Quinazolinediones" *Org. Lett.* **2017**, *19,* 1052-1055.

(12) Li, J.; **Simmons, E. M.**; Eastgate, M. D. "A data-driven strategy for predicting greenness scores, rationally comparing synthetic routes and benchmarking PMI outcomes for the synthesis of molecules in the pharmaceutical industry" *Green Chem.* **2017**, *19*, 127-139.

(11) Cheng, C.; **Simmons, E. M.**; Hartwig, J. F. "Iridium-Catalyzed, Diastereoselective Dehydrogenative Silylation of Terminal Alkenes with $(TMSO)_2MeSiH$" *Angew. Chem. Int. Ed.* **2013**, *52*, 8984-8989.

(10) Cortez, F. de J.; Lapointe, D.; Hamlin, A. M.; **Simmons, E. M.**; Sarpong, R. "Synthetic studies on the icetexones: enantioselective formal syntheses of icetexone and *epi*-icetexone" *Tetrahedron* **2013**, *69*, 5665-5676.

(9) **Simmons, E. M.**; Hartwig, J. F. "On the Interpretation of Deuterium Kinetic Isotope Effects in C–H Bond Functionalizations by Transition-Metal Complexes" *Angew. Chem. Int. Ed.* **2012**, *51*, 3066-3072.

(8) **Simmons, E. M.**; Hartwig, J. F. "Catalytic functionalization of unactivated primary C–H bonds directed by an alcohol" *Nature* **2012**, *483*, 70-73.

(7) **Simmons, E. M.**; Hartwig, J. F. "Iridium-Catalyzed Arene *Ortho*-Silylation by Formal Hydroxyl-Directed C–H Activation" *J. Am. Chem. Soc.* **2010**, *132*, 17092-17095.

(6) Hardin-Narayan, A. R.[‡]; **Simmons, E. M.**[‡]; Sarpong, R. "Synthetic Strategies Directed Towards the Cortistatin Family of Natural Products" *Eur. J. Org. Chem.* **2010**, 3553-3567.

(5) **Simmons, E. M.**; Hardin-Narayan, A. R.; Guo, X.; Sarpong, R. "Formal total synthesis of (±)-cortistatin A" *Tetrahedron* **2010**, *66*, 4696-4700.

(4) **Simmons, E. M.**; Sarpong, R. "Structure, biosynthetic relationships and chemical synthesis of the icetexane diterpenoids" *Nat. Prod. Rep.* **2009**, *26*, 1195-1217.

(3) **Simmons, E. M.**; Hardin, A. R.; Guo, X.; Sarpong, R. "Rapid Construction of the Cortistatin Pentacyclic Core" *Angew. Chem. Int. Ed.* **2008**, *47,* 6650-6653.

(2) **Simmons, E. M.**; Yen, J. R.; Sarpong, R. "Reconciling Icetexane Biosynthetic Connections with Their Chemical Synthesis: Total Synthesis of (±)-5,6-Dihydro-6α-hydroxysalviasperanol, (±)-Brussonol, and (±)-Abrotanone" *Org. Lett.* **2007**, *9*, 2705-2708.

(1) **Simmons, E. M.**; Sarpong, R. "Ga(III)-Catalyzed Cycloisomerization Strategy for the Synthesis of Icetexane Diterpenoids: Total Synthesis of (±)-Salviasperanol" *Org. Lett.* **2006**, *8,* 2883-2886.

ORAL PRESENTATIONS

(7) **Simmons, E**. "Non-Mass Based Metrics: Assessing Environmental, Health and Safety Impacts of Chemical Processes" 22nd Annual Green Chemistry & Engineering Conference, Portland, OR, United States, June 18-20, 2018.

(6) **Simmons, E.** "Discovery, Development and Mechanistic Study of Catalytic Transformations for the Multi-Kilogram Scale Synthesis of Pharmaceutical Intermediates" 254th ACS National Meeting, Washington, DC, United States, August 20-24, 2017.

(5) **Simmons, E.** "Process Development and Application of a Pd-Catalyzed Direct Arylation in the Commercial Synthesis of the HCV NS5B Inhibitor Beclabuvir" Gordon Research Conference on Organic Reactions and Processes, Easton, MA, July 23-28, 2017.

(4) **Simmons, E.** "Mechanistic Studies of a Multi-Kilogram Scale Direct Arylation Process En Route to Beclabuvir" Gordon Research Conference on Inorganic Reaction Mechanisms, Galveston, TX, March 5-10, 2017.

(3) Fleming, W.; Hung, V.; Leahy, D.; Miller, M.; **Simmons, E**.; Sweeney, J. "Design and Evolution of the BMS Process Greenness Scorecard" 19th Annual Green Chemistry & Engineering Conference, N. Bethesda, MD, United States, July 14-16, 2015.

(2) **Simmons, E. M.**; Hartwig, J. F. "Iridium-catalyzed, hydroxyl group-directed dehydrogenative silylation of aromatic and aliphatic C-H bonds" 241st ACS National Meeting, Anaheim, CA, United States, March 27-31, 2011.

(1) **Simmons, E. M.**; Hardin, A. R.; Guo, X.; Yen, J. R.; Sarpong, R. "Application of a cycloisomerization strategy to the synthesis of icetexane and cortistatin natural products and structural analogs" 236th ACS National Meeting, Philadelphia, PA, United States, Aug. 17-21, 2008.

POSTER PRESENTATIONS

(6) Beutner, G. L.; Coombs, J. R.; Green, R. A.; Inankur, B.; Lin, D.; Qiu, J.; Roberts, F.; **Simmons, E. M.**; Wisniewski, S. R. "Covering Our Bases: Development of Homogeneous Conditions for Scalable and Reproducible Cross-Coupling Reactions" Gordon Research Conference on Organic Reactions & Processes, Easton, MA, July 21-26, 2019.

(5) **Simmons, E.**; Chan, C.; DelMonte, A.; Hang, C.; Hsiao, Y.; Ramirez, A. "Mechanistic Studies of a Pd-Catalyzed, Intramolecular Direct Arylation En Route to Beclabuvir" Gordon Research Conference on Organometallic Chemistry, Newport, RI, July 10-15, 2016.

(4) **Simmons, E**.; Chan, C.; DelMonte, A.; Hang, C.; Hsiao, Y.; Ramirez, A. "Mechanistic Studies on the Pd-Catalyzed, Intramolecular Direct Arylation of BMS-809940" Gordon Research Conference on Organic Reactions & Processes, Lewiston, ME, July 19-24, 2015.

(3) **Simmons, E. M.**; Hartwig, J. F. "Iridium-Catalyzed, Dehydrogenative Silylation of sp^2 and sp^3 C–H Bonds" Gordon Research Conference on Heterocyclic Compounds, Newport, RI, June 26-July 1, 2011.

(2) **Simmons, E. M.**; Hardin, A. R.; Guo, X.; Sarpong, R. "Progress Toward the Total Synthesis of Cortistatin A" Gordon Research Conference on Natural Products, Tilton, NH, July 20-25, 2008.

(1) **Simmons, E. M.**; Sarpong, R. "Total synthesis of icetexane diterpenoids via a metal-mediated cycloisomerization" 232nd ACS National Meeting, San Francisco, CA, United States, Sept. 10-14, 2006.

PATENTS

(1) Benkovics, T.; Chen, K.; Deerberg, J.; Dummeldinger, M.; Galella, M. A.; Inankur, B.; Kolotuchin, S. V.; Li, J.; Lin, D.; Rogers, A. J.; Rosso, V. W.; **Simmons, E. M**.; Smith, M. J.; Soumeillant, M. C. D.; Strotman, N. A.; Treitler, D. S.; Tymonko, S.; Wang, J.; Zhang, Y.; Zheng, B. "PROCESS FOR THE PREPARATION OF 6-(CYCLOPROPANEAMIDO)-4-((2-METHOXY-3-(1-METHYL-1H-1,2,4-TRIAZOL-3-YL)PHENYL)AMINO)-N-(METHYL-D3)PYRIDAZINE-3-CARBOXAMIDE" WO 2018/183649 A1.