Brandon E. Haines, Ph.D.

Curriculum Vitae

Westmont College
Department of Chemistry
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Santa Barbara, CA

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EDUCATION

2009 – 2014: University of Notre Dame, Ph.D. Chemistry, Advisor: Dr. Olaf Wiest
Computational Studies on the Mechanism of HMG-CoA reductase and Grignard $S_{RN}1$ Reaction

2005 – 2009: Grand Valley State University, B.S. Chemistry

PROFESSIONAL APPOINTMENTS

2018 – present: Westmont College, Assistant Professor, Department of Chemistry

2014 – 2018: Emory University, Post-doctoral Fellow, Emerson Center for Scientific Computation and the Chemistry Department, Advisor: Dr. Jamal Musaev

COURSES TAUGHT

Westmont College
Sprint 2020, *current semester*: General Chemistry II w/ Lab (CHM-006-1); Organic Chemistry Lab (CHM-102L-1/2/3), enrollment 11/12/15; Chemical Research (CHM-198), enrollment 5
Fall 2019: General Chemistry I w/ Lab (CHM-005-2); General Chemistry I Lab (CHM-005L-4/5); Physical Chemistry I Lab (CHM-132); Chemical Research (CHM-198), enrollment 3
Spring 2018: General Chemistry I w/ Lab (CHM-006-2), enrollment 35; General Chemistry II Lab (CHM-006L-3/4), enrollment 20/22; Chemical Research (CHM-198), enrollment 2
Fall 2018: General Chemistry I w/ Lab (CHM-005-2), enrollment 50; General Chemistry I Lab (CHM-005L-3/4), enrollment 22/23; Physical Chemistry I Lab (CHM-132), enrollment 6

Research Mentoring through Stauffer Summer Research Program
Summer 2019: 2 students

HONORS

2019: NSF Career Workshop attendee, Alexandria, VA
2017: Emerson Center Symposium Poster Award, Emerson Center Symposium, Atlanta, GA
2013: 63rd Lindau Nobel Laureate Meeting, Young Researcher, US Delegation, Sponsor: Oak Ridge Associated Universities
2013: Jeremiah P. Freeman Award for Teaching in Organic Chemistry, University of Notre Dame, Notre Dame, IN
2010 – 2012: Ruth L. Kirschstein National Research Service Award, Chemistry-Biochemistry-Biology Interface (CBBI) Program, University of Notre Dame, Notre Dame, IN

GRANT SUPPORT

7/1/2019 – 7/1/2020: "Investigation of Enantioselectivity, Stereo-electronic effects and New Ligands in Transition-metal Catalysis" XSEDE XRAC (Computational Resources), 26,600 node hours.

PEER-REVIEWED PUBLICATIONS, ORCID: 0000-0002-5013-8396

Mentored Work

24. Xu, L. P.; Haines, B. E.; Ajitha, M. J.; Murakami, K.; Itami, K.; Musaev, D. G. "Roles of Base in the Pd-Catalyzed Annulative Chlorophenylene Dimerization" *ACS. Catal.* **2020***, 10,* 3059-3073*,* DOI: 10.1021/acscatal.9b05328
23. Quinn, T. R.; Steussy, C. N.; Haines, B. E.; Lei, J.; Wang, W.; Sheong, F. K.; Stauffacher, C. V.; Huang, X.; Norrby, P.-O.; Helquist, P.; Wiest, O. "Microsecond Timescale Simulations at the Transition State of PmHMGR Predict Remote Allosteric Residues" *ChemRxiv,* **2019,** preprint, DOI: 10.26434/chemrxiv.9999545.v1
22. Gair, J. J.; Haines, B. E.; Filatov, A. S.; Musaev, D. G.; Lewis, J. C. "Di-Palladium Complexes are Active Catalysts for Mono-N-Protected Amino Acid Accelerated Enantioselective C-H Functionalization" *ACS. Catal.* **2019***, 9,* 11386-11397*,* DOI: 10.1021/acscatal.9b03887
21. Haines, B. E.; Nelson, B. M.; Grandner, J. M.; Kim, J.; Houk, K. N.; Movassaghi, M.; Musaev, D. G. "Mechanism of Permanganate-Promoted Dihydroxylation of Complex Diketopiperazines: Critical Roles of Counter-cation and Ion-Pairing" *J. Am. Chem. Soc*. **2018**, *140,* 13375-13386, DOI: 10.1021/jacs.8b08371
20. Haines, B. E.; Sarpong, R.; Musaev, D. G. "Generality and Strength of Transition Metal β-Effects" *J. Am. Chem. Soc*. **2018**, *140*, 10612-10618, DOI: 10.1021/jacs.8b06817
19. Wilkerson-Hill, S.; Haines, B. E.; Musaev, D. G.; Davies, H. M. L. "Synthesis of [3a,7a]-Dihydroindoles by a Tandem Arene Cyclopropanation/3,5-Sigmatropic Rearrangement Reaction" *J. Org. Chem*. **2018**, 83, 7939-7949, DOI: 10.1021/acs.joc.8b00812
18. Usui, K.; Haines, B. E.; Musaev, D. G.; Sarpong, R. "Understanding Regiodivergence in a Pd(II)-Mediated Site-Selective C–H Alkynylation" *ACS. Catal.* **2018**, *8*, 4516-4527, DOI: 10.1021/acscatal.8b01116
17. Haines, B. E.; Yu J.-Q.; Musaev, D. G. "Mechanistic Details of Ni(II)-Catalyzed C–H Iodination with Molecular Iodine" *Chem. Sci*. **2018**, *9*, 1144-1154*,* DOI: 10.1039/C7SC04604A
16. Varela-Alvarez, A.; Haines, B. E.; Musaev, D. G. "Key Mechanistic Insights into the Intramolecular C-H Bond Amination and Double Bond Aziridination in Sulfamate Esters Catalyzed by Dirhodium Tetracarboxylate Complexes" *J. Organomet. Chem.* **2018**, *867,* 183-192*,* DOI: 10.1016/j.jorganchem.2017.12.013 – *Beletskaya 85th Special Issue*
15. Gair, J. J.; Haines, B. E.; Filatov, A. S.; Musaev, D. G.; Lewis, J. C. "Mono-*N*-Protected Amino Acid Ligands Stabilize Dimeric Palladium(II) Complexes of Importance to C-H Functionalization" *Chem. Sci*. **2017**, *8*, 5746-5756, DOI: 10.1039/C7SC01674C
14. Plata, R. E.; Hill, D. E.; Haines, B. E.; Musaev, D. G.; Chu, L.; Hickey, D. P.; Sigman, M. S.; Yu, J.- Q.; Blackmond, D. G. "A Role for Pd(IV) in Catalytic Enantioselective C-H

Functionalization With Monoprotected Amino Acid Ligands Under Mild Conditions" *J. Am. Chem. Soc*. **2017**, *139*, 9238-9245, DOI: 10.1021/jacs.7b03716

13. Haines, B. E.; Yu J.-Q.; Musaev, D. G. "Enantioselectivity Model for Pd-Catalyzed C–H Functionalization Mediated by the Mono-*N*-protected Amino Acid (MPAA) Family of Ligands" *ACS Catal*. **2017**, *7*, 4344-4354, DOI: 10.1021/acscatal.7b01281
12. Haines, B. E.; Kawakami, T.; Kuwata, K.; Murakami, K.; Itami, K.; Musaev, D. G. "Cu-Catalyzed Aromatic C–H Imidation with *N*-fluorobenzenesulfonimide: Mechanistic Details and Predictive Models" *Chem. Sci*. **2017**, *8*, 988-1001, DOI: 10.1039/C6SC04145K – *Highlighted in C&E News, November 7, 2016*
11. Haines, B. E.; Saito, Y.; Segawa, Y.; Itami, K.; Musaev, D. G. "Flexible Reaction Pocket on Bulky Diphosphine-Ir Complex Controls Regioselectivity in *para*-selective C–H Borylation of Arenes" *ACS Catal*. **2016**, *6*, 7536-7546, DOI: 10.1021/acscatal.6b02317
10. Haines, B. E.; Berry, J. F.; Yu J.-Q.; Musaev, D. G. "Factors Controlling Stability and Reactivity of Dimeric Pd(II) Complexes in C–H Functionalization Catalysis" *ACS Catal*. **2016**, *6*, 829-839, DOI: 10.1021/acscatal.5b02447
9. Haines, B. E.; Xu, H.; Verma, P.; Wang, X.-C.; Yu J.-Q.; Musaev, D. G. "Mechanistic Details of Pd(II)-Catalyzed C–H Iodination with Molecular I_2: Oxidative Addition vs. Electrophilic Cleavage" *J. Am. Chem. Soc.* **2015**, *137*, 9022-9031, DOI: 10.1021/jacs.5b03410
8. Haines, B. E.; Musaev, D. G. "Factors Impacting the Mechanism of the Mono-*N*-Protected Amino Acid Ligand-Assisted and Directing-Group-Mediated C–H Activation Catalyzed by Pd(II) Complex" *ACS Catal*. **2015**, *5*, 830-840, DOI: 10.1021/cs5014706
7. Clausen, D. J.; Smith, W. B.; Haines, B. E.; Wiest, O.; Bradner, J. E.; Willams, R. M. "Modular Synthesis and Biological Activity of Pyridyl-based Analogs of the Potent Class I Histone Deacetylase Inhibitor Largazole" *Bioorg. Med. Chem*. **2015**, *23*, 5061-5074, DOI: 10.1016/j.bmc.2015.03.063
6. Decroos, C.; Clausen, D. J.; Haines, B. E.; Wiest, O.; Williams, R. M.; Christianson, D. W. "Variable Active Site Loop Conformations Accommodate the Binding of Macrocyclic Largazole Analogues to HDAC8" *Biochemistry*, **2015**, *54*, 2126-2135, DOI: 10.1021/acs.biochem.5b00010
5. Haines, B. E.; Wiest, O. "SET-Induced Biaryl Cross-Coupling: An $S_{RN}1$ Reaction" *J. Org. Chem*. **2014**, *79*, 2771-2774, DOI: 10.1021/jo500222d
4. Haines, B. E.; Wiest, O.; Stauffacher, C. V. "The Increasingly Complex Mechanism of HMG-CoA Reductase" *Acc. Chem. Res*. **2013**, *46*, 2416-2426, DOI: 10.1021/ar3003267
3. Haines, B. E.; Steussy, C. N.; Stauffacher, C. V.; Wiest, O. "Molecular Modeling of the Reaction Pathway and Hydride Transfer Reactions of HMG-CoA Reductase" *Biochemistry*, **2012**, *51*, 7983-7995, DOI: 10.1021/bi3008593
2. Ngassa, F. N.; Gomez, J. M.; Haines, B. E.; Ostach, M. J.; Hector, J. W.; Hoogenboom, L. J.; Page, C. E. "Facile Cu-free Sonogashira Cross-coupling of Nucleoside C-6 Arylsulfonates with Terminal Alkynes" *Tetrahedron*, **2010**, *66*, 7919-7926, DOI: 10.1016/j.tet.2010.08.032)
1. Ngassa, F. N.; Lindsay, E. A.; Haines, B. E. "The first Cu- and Amine-free Sonogashira-type Cross-coupling in the C-6-alkynylation of Protected 2′-deoxyadenosine" *Tetrahedron*, **2009**, *65*, 4085-4091, DOI: 10.1016/j.tet.2009.03.064

CONFERENCE PRESENTATIONS

6. Haines, B. E.; Yu, J.-Q.; Musaev, D. G. "Enantioselectivity Model for Pd-Catalyzed C–H Functionalization Mediated by the Mono-N-Protected Amino Acid (MPAA) Family of Ligands" Poster Presentation, Emerson Center Symposium, Atlanta, GA, November 2, 2017
5. Haines, B. E.; Yu, J.-Q.; Musaev, D. G. "Enantioselectivity Model for Pd-Catalyzed C–H Functionalization Mediated by the Mono-N-Protected Amino Acid (MPAA) Family of Ligands" Poster Presentation, Gordon Research Conference, Physical Organic Chemistry, Holderness, NH, June 25-30, 2017
4. Haines, B. E.; Musaev, D. G. "Key mechanistic details of the Cu-catalyzed aryl C–H imidation with Nfluorobenzenesulfonimide (NFSI)" Oral Presentation, ORG 393, 252nd ACS National Meeting, Philadelphia, PA, August 23, 2016
3. Haines, B. E.; Musaev, D. G. "Pd(II)-Catalyzed C–H Iodination with Molecular I_2 as the Only Oxidant: Oxidative Addition vs. Electrophilic Cleavage" Oral Presentation, ORG 366, 250th ACS National Meeting, Boston, MA, August 18, 2015
2. Haines, B. E.; Musaev, D. G. "Pd(II)-Catalyzed C–H Iodination with Molecular I_2 as the Only Oxidant: Oxidative Addition vs. Electrophilic Cleavage" Oral Presentation, 4th Georgia Area Inorganic Network (GAIN) Symposium, Atlanta, GA, August 1, 2015
1. Haines, B. E.; Steussy, C. N.; Stauffacher, C. V.; Wiest, O. "Mechanism of HMG-CoA Reductase and the Development of Quantum Mechanically Trained Force Fields for the Reaction" Poster Presentation COMP 251, 246th ACS National Meeting, Indianapolis, IN, September 8-12, 2013

SERVICE

Westmont College
Institutional
Fall 2019: Salary and Budget Committee (Semester Replacement)