

Kelly M. Hines, Ph.D.

Department of Medicinal Chemistry
University of Washington
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Education

Vanderbilt University

Ph.D. in Chemistry

Dissertation: Biomolecular Signatures of Disease via Ion Mobility and Mass Spectrometry Techniques

Advisor: John A. McLean, Stevenson Professor of Chemistry

Nashville, TN

May 2014

University of Florida

Bachelor of Science in Chemistry, *Cum Laude*

Gainesville, FL

May 2009

Research Experience

University of Washington Department of Medicinal Chemistry

Senior Fellow

Advisor: Professor Libin Xu

Seattle, WA

07/2015 - Present

- Established calibrants for accurate measurement of lipid collision cross sections by traveling wave ion mobility-mass spectrometry (IM-MS)
- Developed lipidomics methods using hydrophilic interaction chromatography (HILIC) with IM-MS for mammalian and bacterial lipids
- Measured the collision cross sections of 1,400 drugs and drug-like molecules using a novel high-throughput flow injection analysis (FIA)-IM-MS approach
- Characterized the lipidomes of daptomycin-resistant Gram-positive pathogens with HILIC-IM-MS to determine the effects of resistance on individual lipid species

Mayo Clinic Regional Metabolomics Core

Division of Endocrinology, Diabetes, Metabolism and Nutrition

Postdoctoral Fellow

Advisor: Dr. K. Sreekumaran Nair, M.D., Ph.D.

Rochester, MN

06/2014-07/2015

- Developed a high-resolution Orbitrap mass spectrometry method for the determination of low-abundance [ring-¹³C₆]-phenylalanine enrichment in individual muscle proteins isolated by 2D-gel electrophoresis.
- Established targeted LC-MS/MS methods for the quantitation of hexosyl ceramides, acyl carnitines, and small molecules in biological matrices including plasma, cerebrospinal fluid, and tissue.
- Evaluated differential mobility spectrometry (DMS)-MS for the separation of glucosyl- and galactosyl ceramides in plasma and cerebrospinal fluid

Vanderbilt University Department of Chemistry

Graduate Research Assistant

Advisor: Professor John A. McLean

Nashville, TN

08/2009 – 05/2014

- Investigated the molecular features distinguishing diabetic from non-diabetic wound fluids isolated from a model system of diabetic wound healing using an untargeted ion mobility-mass spectrometry (IM-MS) platform.
- Examined the metabolic profiles of human breast cancer tissues in an untargeted manner using a polar extraction strategy and UPLC-IM-MS/MS.
- Identified six novel sites of phosphorylation in Asef2, a protein involved in cell migration, with 95% sequence coverage and 100% coverage of possible phosphorylation sites.

Honors, Awards and Fellowships

- **05/2018 – Awarded the ACS Dan Su Travel Award** for the top four female candidates invited to attend the 2018 ACS Postdoc to Faculty Workshop in Boston, MA (Aug. 2018). The award provided \$1,000 to cover travel expenses to attend the workshop.
- **01/2018 – Awarded Young Investigator Travel Grant by The Association for Mass Spectrometry: Applications to the Clinical Lab (MSACL)** for the abstract titled “Lipid signatures as diagnostic predictors of β -lactam “seesaw effect” in glycopeptide, lipopeptide, and lipoglycopeptide resistance.” Award covered travel expenses to attend and present at the 2018 MSACL conference.
- **01/2017 – Awarded Young Investigator Travel Grant by The Association for Mass Spectrometry: Applications to the Clinical Lab (MSACL)** for the abstract titled “Identification of Altered Lipidome in Lipopeptide-Resistant Bacteria by HILIC-IM-MS.” Award covered travel expenses to attend and present at the 2017 MSACL conference.
- **12/2015 – Awarded 2015-16 USP Global Fellowship**
Selected by the U.S. Pharmacopeia as one of three 2015-16 USP Global Fellows for the project titled “Ion Mobility-Mass Spectrometry as an Orthogonal Technique for Identification and Characterization of Drugs by Structure.” Fellowship included \$30,000 to fund the proposed research for one year.
- **09/2014 –** The publication, “Structural mass spectrometry of tissue extracts to distinguish cancerous and non-cancerous breast diseases,” was featured on the November cover of *Molecular BioSystems*.
- **06/2013 –** The wound healing in diabetes work was highlighted in an interview article in The Analytical Scientist “Wound Healing in Diabetes.” The Analytical Scientist has a circulation of 52,000 electronic copies and 21,000 printed copies internationally.

Publications

Journal Articles

15. **Kelly M. Hines** and Libin Xu, “Lipidomic consequences of phospholipid synthesis defects in *Escherichia coli* revealed by HILIC-ion mobility-mass spectrometry,” *Chemistry and Physics of Lipids*, 2019, 219, 15-22.
14. Elijah J. Weber, Kevin A. Lidberg, Lu Wang, Theo K. Bammler, James W. MacDonald, Mavis J. Li, Michelle Redhair, William M. Atkins, Cecilia Tran, **Kelly M. Hines**, Josi Herron, Libin Xu, Maria Beatriz Monteiro, Susanne Ramm, Vishal Vaidya, Martti Vaara, Timo Vaara, Jonathan Himmelfarb, Edward J. Kelly, “Human kidney on a chip assessment of polymyxin antibiotic nephrotoxicity,” *JCI Insight*, 2018, 3, e123673.
13. Josi Herron, **Kelly M. Hines**, and Libin Xu, “Assessment of altered cholesterol homeostasis by xenobiotics using ultra-high performance liquid chromatography-tandem mass spectrometry,” *Current Protocols in Toxicology*, 2018, 78, e65.
12. David R. Raleigh, Navdar Sever, Pervinder K. Choksi, Monika Abedin Sigg, **Kelly M. Hines**, Bonne M. Thompson, Daniel Elnatan, Priyadarshini Jaishankar, Paola Bisignano, Francesc R. Garcia-Gonzalo, Alexis Leigh Krup, Markus Eberl, Eamon F. X. Byrne, Christian Siebold, Sunny Y. Wong, Adam R. Renslo, Michael Grabe, Jeffrey G. McDonald, Libin Xu, Philip A. Beachy, Jeremy F. Reiter, “Cilia-associated oxysterols activate Smoothed,” *Molecular Cell*, 2018, 72 (2), 316-327.
11. Steven J. Fliesler, Neal S. Peachy, Josi Herron, **Kelly M. Hines**, Nadav I. Weinstock, Sriganesh Ramachandra Rao, Libin Xu, “Prevention of Retinal Degeneration in a Rat Model of Smith-Lemli-Opitz Syndrome,” *Scientific Reports*, 2018, 8 (1), 1286. Author Correction: 2018, 8 (1), 4289.
10. **Kelly M. Hines**, Adam Waalkes, Kelsi Penewit, Elizabeth A. Holmes, Stephen J. Salipante, Brian J. Werth, Libin Xu, “Characterization of the Mechanisms of Daptomycin Resistance among Gram-Positive Bacterial Pathogens by Multidimensional Lipidomics,” *mSphere*, 2017, 2 (6), e00492-17.
9. **Kelly M. Hines**, Dylan H. Ross, Kimberly L. Davidson, Matthew F. Bush, Libin Xu, “Large-Scale Structural Characterization of Drug and Drug-like Compounds by High-Throughput Ion Mobility-Mass Spectrometry,” *Analytical Chemistry*, 2017, 89 (17), 9023-9030.
8. **Kelly M. Hines**, Josi Herron, Libin Xu, “Assessment of altered lipid homeostasis by HILIC-ion mobility-mass spectrometry-based lipidomics,” *Journal of Lipid Research*, 2017, 58, 809-819.
7. Carrie J. Finno, Matthew H. Bordbari, Stephanie J. Valberg, David Lee, Josi Herron, **Kelly Hines**, Tamer Monsour, Erica Scott, Danika L. Bannasch, James Mickelson, Libin Xu, “Transcriptome profiling of equine vitamin E deficient neuroaxonal dystrophy identifies upregulation of liver X receptor target genes,” *Free Radical Biology and Medicine*, 2016, 101, 261-271.

6. **Kelly M. Hines**, Jody C. May, John A. McLean, Libin Xu, "Evaluation of Collision Cross Section Calibrants for Structural Analysis of Lipids by Traveling Wave Ion Mobility-Mass Spectrometry," *Analytical Chemistry*, 2016, *88* (14), 7329-7336.
5. **Kelly M. Hines**, G. Charles Ford, Katherine Klaus, Brian Irving, Beverly Ford, Kenneth Johnson, Ian Lanza, K. Sreekumaran Nair, "Application of high-resolution mass spectrometry to measure low abundance isotope enrichment in individual muscle proteins," *Analytical and Bioanalytical Chemistry*, 2015, *407* (14), 4045-4052.
4. **Kelly M. Hines**, Billy R. Ballard, Dana M. Marshall and John A. McLean, "Structural mass spectrometry of tissue extracts to distinguish cancerous and non-cancerous breast diseases," *Molecular BioSystems*, 2014, *10* (11), 2827-3032.
3. J. Corey Evans, **Kelly M. Hines**, Jay G. Forsythe, Begum Erdogan, Mingjian Shi, Salisha Hill, Kristie L. Rose, John A. McLean and Donna J. Webb, "Phosphorylation of Serine 106 in Asef2 Regulates Cell Migration and Adhesion Turnover," *Journal of Proteome Research*, 2014, *13* (7), 3303-3313.
2. **Kelly M. Hines**, Samir Ashfaq, Jeffrey M. Davidson, Susan R. Opalenik, John P. Wikswo and John A. McLean, "Biomolecular Signatures of Diabetic Wound Healing by Structural Mass Spectrometry," *Analytical Chemistry*, 2013, *85* (7), 3651-3659.
1. Alexander P. Lamers, Mary E. Keithly, Kwangho Kim, Paul D. Cook, Donald F. Stec, **Kelly M. Hines**, Gary A. Sulikowski, and Richard N. Armstrong, "Synthesis of Bacillithiol and the Catalytic Selectivity of FosB-Type Fosfomycin Resistance Proteins," *Organic Letters*, 2012, *14* (20), 5207-5209.

Invited Book Chapters

2. Sarah M. Stow, Nichole M. Lareau, **Kelly M. Hines**, C. Ruth McNees, Cody R. Goodwin, Brian O. Bachmann, and John A. McLean, "Structural separations for natural product characterization by ion mobility-mass spectrometry: Fundamental theory to emerging applications," Invited chapter for inclusion in "Natural Products Analysis: Instrumentation, Methods and Applications," Vladimir Havlicek and Jaroslav Spizek, Eds. *John Wiley & Sons, Inc.* 2013.
1. **Kelly M. Hines**, Jeffrey R. Enders, and John A. McLean, "Multidimensional Separations by Ion Mobility-Mass Spectrometry," Invited chapter for inclusion in "Encyclopedia of Analytical Chemistry (online)," Robert Myers and David Muddiman, Eds. *John Wiley & Sons, Ltd.* December 2012.

Select Presentations

7. **Kelly M. Hines**, Tianwei Shen, Adam Waalkes, Kelsi Penewit, Elizabeth A. Holmes, Stephen J. Salipante, Brian J. Werth, and Libin Xu, *Lipid signatures associated with glycopeptide, lipopeptide, and lipoglycopeptide cross-resistance and the β -lactam "seesaw effect" in MRSA*, 66th American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Diego, CA (June 2018).
6. **Kelly M. Hines**, Adam Waalkes, Kelsi Penewit, Elizabeth A. Holmes, Stephen J. Salipante, Brian J. Werth, Libin Xu, *Alteration of membrane lipids is associated with glycopeptide, lipopeptide and lipoglycopeptide cross-resistance and the β -lactam "seesaw effect" in MRSA*, University of Washington Postdoctoral Association Annual Research Symposium, Seattle, WA (April 2018). **Oral presentation.**
5. **Kelly M. Hines**, Adam Waalkes, Kelsi Penewit, Elizabeth A. Holmes, Stephen J. Salipante, Brian J. Werth, Libin Xu, *Lipid signatures as diagnostic predictors of β -lactam "seesaw effect" in glycopeptide, lipopeptide, and lipoglycopeptide resistance*, Mass Spectrometry: Applications to the Clinical Lab 2018 US Annual Conference & Exhibits, Palm Springs, CA (January 2018). **Oral presentation, Young Investigator Travel Grant**
4. **Kelly M. Hines**, Brian J. Werth, Libin Xu, *Lipidomics Analysis of Antimicrobial-Resistant Bacteria by HILIC-Ion Mobility-Mass Spectrometry*, Federation of Analytical Chemistry and Spectroscopy Societies SciX Conference, Reno, NV (October 2017). **Invited presentation.**
3. **Kelly M. Hines**, Brian J. Werth, Libin Xu, *Monitoring Alterations of Bacterial Lipidome in Antimicrobial Resistance with HILIC-IM-MS*, 65th American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN (June 2017). **Oral presentation.**
2. **Kelly M. Hines**, Brian J. Werth, Libin Xu, *Identification of Altered Lipidome in Lipopeptide-Resistant Bacteria by HILIC-IM-MS*, Mass Spectrometry: Applications to the Clinical Lab 2017 US Annual Conference & Exhibits, Palm Springs, CA (January 2017). **Oral presentation, Young Investigator Travel Grant**
1. **Kelly M. Hines**, Jody C. May, John A. McLean, Libin Xu, *Evaluation of Collision Cross Section Calibrants for Structural Analysis of Lipids by Traveling Wave IM-MS*, 64th American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Antonio, TX (June 2016).

Teaching Experience

Mentoring – University of Washington, Department of Medicinal Chemistry

- Directed the research of four graduate students: Josi Herron, Dylan H. Ross, Amy Li, and Tianwei Shen
- Instructed graduate students in lipid extraction from biological samples, LC-MS/MS method development and operation, ion mobility-mass spectrometry, and data analysis
- Josi Herron was second author on: Kelly M. Hines, Josi Herron, Libin Xu, “Assessment of altered lipid homeostasis by HILIC-ion mobility-mass spectrometry-based lipidomics,” *Journal of Lipid Research*, 2017, 58, 809-819.
- Dylan H. Ross was second author on: Kelly M. Hines, Dylan H. Ross, Kimberly L. Davidson, Matthew F. Bush, Libin Xu, “Large-Scale Structural Characterization of Drug and Drug-like Compounds by High-Throughput Ion Mobility-Mass Spectrometry,” *Analytical Chemistry*, 2017, 89 (17), 9023-9030.

Teaching Assistant – Vanderbilt University, Department of Chemistry

- Forensic Chemistry Laboratory, January - May 2011, January - May 2012
- Organic Chemistry Laboratory, August 2009 - August 2010, August - December 2011
- Instrumental Analysis Laboratory, August - December 2010.

Assistant TA – University of Florida, Department of Chemistry

- Analytical Chemistry Lab, January - December 2008

Professional Memberships

- **2018 – Present** Member, American Society for Microbiology
- **2012 – Present** Member, American Chemical Society
- **2010 – Present** Member, American Society for Mass Spectrometry

Professional Service

- **01/2018** – Chair of “Microbiology Metabolomics” session at Mass Spectrometry: Applications to the Clinical Lab (MSACL) 2018 Conference
- **2016 – Present** Ad hoc reviewer for Mayo Clinic Metabolomics Resource Core Pilot and Feasibility Program grants

References

Libin Xu, Ph.D.

Postdoctoral Advisor

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John A. McLean, Ph.D.

Graduate Advisor

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Brian J. Werth, Pharm.D.

Research Collaborator

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K. Sreekumaran Nair, M.D., Ph.D

Postdoctoral Advisor

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Director of Mayo Clinic Metabolomics Resource Core
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