BIOGRAPHICAL SKETCH

Provide the following information for the Senior/key personnel and other significant contributors. Follow this format for each person. **DO NOT EXCEED FIVE PAGES**.

NAME: Koelmel, Jeremy P

eRA COMMONS USER NAME (credential, e.g., agency login): JEREMY.KOELMEL

POSITION TITLE: Postdoctoral Research Fellow

EDUCATION/TRAINING (Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.)

INSTITUTION AND LOCATION	DEGREE	Completion Date MM/YYYY	FIELD OF STUDY
Hampshire College	B.A.	05/2011	Environmental Chemistry
University of Florida	Ph. D.	12/2017	Analytical Chemistry
Yale University	PostDoc		Environmental Toxicology/ Exposure Assessment

A. Personal Statement

My long-term research interests are to develop my own laboratory and academic career developing and applying techniques in exposomics. Exposomics covers the interaction between environmental exposures, including from contaminants, diet, and drugs, with biological consequences. My specific interests within exposomics are to develop mass spectral and informatics approaches to more comprehensively characterize both the exposome (exogenous compounds) and endogenous (biological) molecules. I am also interested in the interaction between exogenous compounds and endogenous compounds which can lead to novel compounds, for example DNA adducts, small molecule adducts, and oxidation products. As oxidation products are a nearly universal indication of biological stress, developing tools to improve the coverage of oxidized molecules will aid in numerous applications. Through my future research, I aim to develop techniques that more comprehensively covering molecules which are indicative of our exposures and biological response, allowing researchers to determine mechanisms and markers linking health and the environment. Ideally, the research and mentoring during my career will result in changes in policy and education, and development of new treatments, which will reduce harmful exposures and their consequences.

My interest in mass spectrometry and the measurement of xenobiotic compounds started in my undergraduate career where I designed and undertook research measuring trace metals in plants resulting in several first author publications. After my undergraduate, I received a Fulbright to India to study biotechnologies (plants and microbial species) to remediate contaminated environments. During my work in India I came across communities devastated from improper industrial waste management, and realized the importance of organic mass spectrometry in characterizing these diverse pollutants.

For my doctorate I joined the Yost group at the University of Florida in 2013 and learned state-of-the-art techniques for analyzing organic compounds by liquid chromatography high resolution tandem mass spectrometry. I spent my PhD focusing on developing data-acquisition strategies and software for lipidomics which resulted in both numerous open source software (with 5 software focused publications to date) and development of this software by Agilent technologies (Lipid Annotator, published). During my PhD and a following research position with the Southeast Center for Integrated Metabolomics (SECIM) I applied the lipidomics software I developed to numerous clinical and environmental applications including: Parkinson's disease, stress and fetal development, an inflammatory disease in wildlife in South Africa, and nonalcoholic fatty liver disease.

I enjoy teaching and mentoring, and have taught as a science teacher in multiple capacities including as a camp director and camp counselor. I have received multiple awards for my teaching endeavors. In 2017 I was recognized for my outstanding mentorship of undergraduates by the University of Florida's division of graduate

student affairs in the Graduate Student Mentoring Award, which is only awarded annually to 6 of 12,500 graduate students at the University of Florida. My work with 6 undergraduates from multiple disciplines resulted in 5 publications with undergraduates as authors, including two publications with undergraduates as co-first authors. I am passionate to both develop useful tools for exposomics, apply them, and mentor and train young researchers to forward the field.

At Yale, through hosting free seminars and sending out online brochures, I have been able to build a multidisciplinary team of talented undergraduates to work with me to forward the field of measurement science. I continued the work on fatty liver disease under Vasilis Vasiliou (50% effort), where I expanded and applied the lipidomics informatics techniques to mouse models of alcoholic fatty liver disease. I was able to determine early indications of liver damage and plasma biomarkers before changes using traditional visual histology were observed. This work is being submitted to Nature Methods. With Krystal Pollitt (50% effort) I developed informatics techniques for passive samplers in order to measure thousands of personal exposures and link these chemicals to sources, uses, and predicted toxicity data. We have applied these workflows to people all across the world, including in India, China, South Africa, United States and Canada, gaining an extensive picture of universal and location specific chemical exposures of concern. In addition, I developed the first software for perfluorinated chemical suspect screening using predicted library generation. I am keen to combine my new expertise in exposure assessment with my expertise in lipidomics and metabolomics for a true exposomics approach in my next year at Yale.

B. Positions and Honors

Positions and Employment

- 2020 Scientific Board FreshAir Inc.
- 2019 CEO Innovative Omics Inc.
- 2019 Postdoctoral student. Yale University
- 2018 2020 Scientific advisor, Lipid Annotator development team. Agilent Technologies, Santa Clara, CA
- 2018 2019 Adjunct Research Scientist. Southeast Center for Integrated Metabolomics, University of Florida, Gainesville, FL
- 2013 2017 PhD student, Analytical Division, University of Florida, Gainesville, FL
- 2012 2013 Nehru Fulbright scholar, University of Hyderabad, Gachibowli, Hyderabad, India
- 2011 2012 Autism personal support worker, Amherst, MA
- 2011 Environmental Chemistry Research Apprentice, Hampshire College, Amherst, MA

Other Experience and Professional Memberships

2013 - Member, American Society of Mass Spectrometry (ASMS)

<u>Honors</u>

2019 Sanibel Student Travel Award, American Society for Mass Spectrometry (ASMS) Steven A. Hofstadler Award, Clinical and Pharmaceutical Solutions for Analysis (CPSA) 2017 2017 Graduate Student Mentoring Award, University of Florida, Division of Graduate Student Affairs 2016 NACRW Student Scholarship Award, North American Chemical Residue Workshop Townes R. Leigh Prize, University of Florida, Graduate Standards Committee 2014 2013-2017 Graduate School Fellowship, University of Florida, Department of Chemistry 2012-2013 Nehru Fulbright Scholar. Institute of International Education 2011 Ingenuity Award, Hampshire College Community Campus Leadership and Activities 2010 NSF REU Grantee, National Science Foundation

C. Contribution to Science

I have co-authored 30 articles and book chapters, five technical reports, and nine software to date in the fields of measuring xenobiotics, and detection of biological molecules for clinical and environmental applications. Ten of my publications were published during my PhD candidacy, and twelve are first author publications. I have given over 40 academic talks, including nine invited talks. I have also presented my work at both public and industrial venues.

- 1. My early publications (undergraduate and as a Fulbright scholar in India) focused on developing and applying analytical techniques for trace metal and nanoparticle imaging and analysis in soil and aquatic systems. The techniques were applied to the field of phytoremediation the use of plants to extract, contain, or volatize trace metals for soil and water remediation.
 - a. **Koelmel, J.P.**, Amarasiriwardena, D.: Imaging of metal bioaccumulation in Hay-scented fern (*Dennstaedtia punctilobula*) rhizomes growing on contaminated soils by laser ablation ICP-MS. Environmental Pollution. 168, 62–70 (2012). doi:10.1016/j.envpol.2012.03.035
 - b. **Koelmel, J.P.**, Leland, T., Wang, H., Amarasiriwardena, D., Xing, B.: Investigation of gold nanoparticles uptake and their tissue level distribution in rice plants by laser ablation-inductively coupled-mass spectrometry. Environmental Pollution. 174, 222–228 (2013). doi:10.1016/j.envpol.2012.11.026
 - c. Koelmel, J.P., Prasad, M.N.V., Pershell, K.: Bibliometric analysis of phytotechnologies for remediation: global scenario of research and applications. International Journal of Phytoremediation. 17, 145–153 (2015). doi:10.1080/15226514.2013.862207
 - d. **Koelmel, J.P.**, Sebastian, A., Prasad, M.N.V.: Chapter 26 Synthetic Biology: An Emerging Field for Developing Economies. In: Bioremediation and Bioeconomy. pp. 665–685. Elsevier (2016)
- 2. After my Fulbright scholarship, I completed my PhD under Dr. Richard A. Yost at the University of Florida, focusing on the development of lipidomics workflows. During and after my doctoral studies, I developed computer algorithms, software, and instrumental acquisition methods to improve the accuracy and coverage of lipid measurements. The five major pieces of software that I have developed can be found at: http://secim.ufl.edu/secim-tools/
 - a. Koelmel, J.P., Kroeger, N.M., Ulmer, C.Z., Bowden, J.A., Patterson, R.E., Cochran, J.A., Beecher, C.W.W., Garrett, T.J., Yost, R.A.: LipidMatch: an automated workflow for rule-based lipid identification using untargeted high-resolution tandem mass spectrometry data. BMC Bioinformatics. 18, 331 (2017). doi:10.1186/s12859-017-1744-3
 - b. Ulmer, C.Z., Koelmel, J.P., Ragland, J.M., Garrett, T.J., Bowden, J.A.: LipidPioneer: A Comprehensive User-Generated Exact Mass Template for Lipidomics. Journal of American Society for Mass Spectrometry. 1–4 (2017). doi:10.1007/s13361-016-1579-6
 - c. Koelmel, J.P., Kroeger, N.M., Gill, E.L., Ulmer, C.Z., Bowden, J.A., Patterson, R.E., Yost, R.A., Garrett, T.J.: Expanding Lipidome Coverage Using LC-MS/MS Data-Dependent Acquisition with Automated Exclusion List Generation. Journal of American Society for Mass Spectrometry. 28, 908–917 (2017). doi:10.1007/s13361-017-1608-0
 - d. Koelmel, J. P., Cochran, J. A., Ulmer, C. Z., Levy, A. J., Patterson, R. E., Olsen, B. C., Yost, R. A., Bowden, J. A., Garrett, T. J. Software Tool for Internal Standard Based Normalization of Lipids, and Effect of Data-Processing Strategies on Resulting Values. BMC Bioinformatics 20, 1, (2019). doi: 10.1186/s12859-019-2803-8.
- 3. During my PhD and thereafter, I was also involved in setting guidelines for lipidomics analyses with the goal of harmonizing lipidomics practices for clinical and other applications. This work included developing methods and publishing work to describe best practices for experimental design, working with industry to create quality software workflows, as well as helping to develop inter-laboratory studies through a collaboration with Dr. John A. Bowden at the National Institute for Standards and Technology (NIST):
 - a. Koelmel, J.P., Ulmer, C.Z., Jones, C.M., Yost, R.A., Bowden, J.A.: Common cases of improper lipid annotation using high-resolution tandem mass spectrometry data and corresponding limitations in biological interpretation. Biochimica et Biophysica Acta (BBA) - Molecular and Cell Biology of Lipids. 1862, 766–770 (2017). doi:10.1016/j.bbalip.2017.02.016
 - b. Bowden, J.A., Heckert, A., Ulmer, C.Z., Jones, C.M., Koelmel, J.P., et. al.: Harmonizing Lipidomics: NIST Interlaboratory Comparison Exercise for Lipidomics using Standard Reference Material 1950 Metabolites in Frozen Human Plasma. Journal of Lipid Research. jlr.M079012 (2017). doi:10.1194/jlr.M079012
 - c. **Koelmel, J.P.**, Schock, T.B., Jones, C.M., Ulmer, C.Z., Garrett, T.J., Yost, R.A., Bowden, J.A.: Examining Heat Treatment for Stabilization of the Lipidome. Bioanalysis (2018). doi: 10.4155/bio-2017-0209
 - d. **Koelmel, J.P.**, Sartain, M., Salcedo, J., Murali, A., Li, X., Stow, S.: Improving Coverage of the Plasma Lipidome Using Iterative MS/MS Data Acquisition Combined with Lipid Annotator Software and 6546 LC/Q-TOF. (2019) doi:10.3390/metabo10030101

- 4. Continuing my work on lipidomics with my collaborator Dr. John A. Bowden and others after my PhD, I began to focus on environmental applications of lipidomics.
 - a. Koelmel, J. P.; Ulmer, C. Z.; Fogelson, S.; Jones, C. M.; Botha, H.; Bangma, J. T.; Guillette, T. C.; Luus-Powell, W. J.; Sara, J. R.; Smit, W. J.; et al. Lipidomics for Wildlife Disease Etiology and Biomarker Discovery: A Case Study of Pansteatitis Outbreak in South Africa. Metabolomics (2019). doi: 10.1007/s11306-019-1490-9
 - Koelmel, J.P., Campbell, J.E., Guingab-Cagmat, J., Meke, L., Garrett, T.J., Stingl, U.: Re-modeling of foliar membrane lipids in a seagrass allows for growth in phosphorus-deplete conditions. PLoS One. 14, (2019). doi: 10.1371/journal.pone.0218690
 - c. **Koelmel, J. P.**, Napolitano, M. P., Ulmer, C. Z., Vasiliou, V., Garrett, T. J., Yost, R. A., Prasad, M. N. V., Godri Pollitt, K. J., Bowden, J. A.: Environmental lipidomics: understanding the response of organisms and ecosystems to a changing world. Metabolomics (2020), 16. doi: 10.1007/s11306-020-01665-3
- 5. In addition, as an assistant research scientist at the South East Center for Integrated Metabolomics under Dr. Timothy J. Garrett, I began to incorporate lipidomics to answer questions about human diseases, especially disease with environmental exposures as high risk factors including Parkinson's, fatty liver disease, and stress induced health effects. I continued this work at Yale with 50% of my effort at the first year of Yale with Dr. Vasilis Vasiliou focusing on lipidomics to assess mechanisms and markers of alcoholic fatty liver disease (two manuscripts in preparation). This work serves as a bridge to my work with Dr. Krystal Pollitt combining lipidomics and environmental exposure monitoring for human health applications:
 - a. Patterson, R.E., Kirpich, A.S., Koelmel, J.P., Kalavalapalli, S., Morse, A.M., Cusi, K., Sunny, N.E., McIntyre, L.M., Garrett, T.J., Yost, R.A.: Improved experimental data processing for UHPLC–HRMS/MS lipidomics applied to nonalcoholic fatty liver disease. Metabolomics (2017). doi:10.1007/s11306-017-1280-1
 - b. Gill, E.L., Koelmel, J.P., Meke, L., Yost, R.A., Garrett, T.J., Okun, M.S., Flores, C., Vedam-Mai, V.: Ultrahigh-Performance Liquid Chromatography–High-Resolution Mass Spectrometry Metabolomics and Lipidomics Study of Stool from Transgenic Parkinson's Disease Mice Following Immunotherapy. J. Proteome Res. (2019). doi: 10.1021/acs.jproteome.9b00605
 - c. Walejko, J.M., **Koelmel, J.P.**, Garrett, T.J., Edison, A.S., Keller-Wood, M.: Multi-omics Approach Reveals Metabolic Changes in the Heart at Birth. Am. J. Physiol. Endocrinol. Metab. (2018). Doi: 10.1152/ajpendo.00297.2018
 - d. Walejko, J.M., Antolic, A., Koelmel, J.P., Garrett, T.J., Edison, A.S., Keller-Wood, M.: Chronic maternal cortisol excess during late gestation leads to metabolic alterations in the newborn heart. Am. J. Physiol. Endocrinol. Metab. 316, E546–E556 (2019). https://doi.org/10.1152/ajpendo.00386.2018

Complete List of Published Work in Google Scholar Citations (29 publications; 527 citations)

https://scholar.google.com/citations?user=jLbx6gcAAAAJ