Jeremy P. Koelmel, PhD Chemistry

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CURRENT EMPLOYMENT

Team/Project Leader. Yale School of Public Health, Yale University, New Haven, CT

CEO. Innovative Omics Inc. (Informatics solutions for non-targeted biological and environmental mass spectrometry http://innovativeomics.com/)

EDUCATION

Yale University, New Haven, CT, Postdoctoral Research Fellow, 2019-2020

University of Florida, Gainesville, FL, Ph. D. in Analytical Chemistry, 2013-2017

Hampshire College, Amherst, MA, Bachelors of Arts Degree in Environmental Chemistry, 2007-2011

RESEARCH AND TEACHING VISION

Me and my teams' mission, both in my academic role at Yale and as CEO of Innovative Omics, is to detect hundreds to tens of thousands of contaminants simultaneously using a single platform consisting of high-resolution tandem mass spectrometry and associated techniques. We focus on emerging and legacy contaminants where software solutions are lacking. While instrumentation exists to provide a wealth of data on various chemical structures, processing this data to provide useful information on contaminants is challenging. We develop and employ novel data-acquisition and data-processing algorithms to automatically predict structures and fluxes of contaminants in both point and non-point pollution sources and apply methods both in developed countries and in developing countries. Furthermore, we are working with the EPA to link comprehensive measurement of contaminants and exposures to predicted and experimental measurements of toxicity, to rapidly screen for compound with the highest health risk.

Furthermore, I am interested in linking contaminant exposure in wildlife and humans to changes in biology using genomics, lipidomics, and metabolomics. I have developed a suite of lipidomics software tools during my career, and am well versed in various lipidomics workflows. I believe the link between health and the environment is essential for leveraging political and public support for increasing funding for environmental research, environmental regulation and remediation.

Public awareness and involvement in science is an important step to make sure that the direction of scientific research is one which meets the public's needs and desires, and to ensure the growth of science through increased funding and people entering scientific careers. I am interested in the communication of scientific findings to the public. Specifically, I hope to work with teams generating media and visiting different institutions to engage the public in education, sponsoring, and participating in scientific discoveries related to health and the environment.

Currently, I have closely mentored over 20 undergraduates, PhD students, and other researchers, including a number of students who were not currently in the physical sciences. It has been a pleasure to lead multidisciplinary teams across computer programming, chemistry, biology, epidemiology, and various other disciplines, having undergraduates take lead roles, including first author roles in publications (see publication section). Through my mentorship, I have given bright and creative students a productive venue to cultivate themselves as budding researchers. I hope that the science they produce provides valuable products, more efficient use of resources, and/or a cleaner environment. More importantly, I know that, just as the bar was set very high for me by the selfless service of my mentors, these students in turn may apply themselves fully as

mentors as they continue their endeavors.

PUBLICATIONS

Manuscripts (Total Citations, google scholar: 950+)
Mentees for which I was the main mentor for this project are highlighted in blue
§denotes share first author
*denotes corresponding author

38. **Koelmel, J.P.** §, **Stelben, P.J.** §, McDonough, C.A., Dukes, D.A., **Aristizabal-Henao, J.J.**, Nason, S.L., Li, Y., Sternberg, S., Lin, E., Beckmann, M., Williams, A.J., Draper, J., Finch, J.P., Munk, J.K., Deigl, C., Rennie, E.E., Bowden, J.A.*, Godri Pollitt, K.J.*: FluoroMatch 2.0 – Making Automated and Comprehensive Non-Targeted PFAS Annotation a Reality. Anal. Bioanal. Chem. Accepted (2021).

37. Hagstrom, A.L., Anastas, P., Boissevain, A., Borrel, A., Deziel, N.C., Fenton, S.E., Fields, C., Fortner, J.D., Franceschi-Hofmann, N., Frigon, R., Jin, L., Kim, J.-H., Kleinstreuer, N.C., **Koelmel, J.P.**, Lei, Y., Liew, Z., Ma, X., Mathieu, L., Nason, S.L., Organtini, K., Oulhote, Y., Pociu, S., Godri Pollitt, K.J., Saiers, J., Thompson, D.C., Toal, B., Weiner, E.J., Whirledge, S., Zhang, Y., Vasiliou, V.*: Yale School of Public Health Symposium: An overview of the challenges and opportunities associated with per- and polyfluoroalkyl substances (PFAS). Science of The Total Environment. 778, 146192 (2021). https://doi.org/10.1016/j.scitotenv.2021.146192

36. Jain, D., Torres, R., Celli, R., **Koelmel, J.P.**, Charkoftaki, G., Vasiliou, V.*: Evolution of the liver biopsy and its future. Translational Gastroenterology and Hepatology. 6, (2021). https://doi.org/10.21037/tgh.2020.04.01

35. **Koelmel, J.P.**, Lin, E.Z., Nichols, A., Guo, P., Zhou, Y., Godri Pollitt, K.J.*: Head, Shoulders, Knees, and Toes: Placement of Wearable Passive Samplers Alters Exposure Profiles Observed. Environ. Sci. Technol. (2021). https://doi.org/10.1021/acs.est.0c05522

34. Doherty, B.T., **Koelmel, J.P.**, Lin, E.Z., Romano, M.E., Godri Pollitt, K.J.*: Use of Exposomic Methods Incorporating Sensors in Environmental Epidemiology. Curr Envir Health Rpt. (2021). https://doi.org/10.1007/s40572-021-00306-8

33. Nason, S.*, Lin, E., Eitzer, B.D., **Koelmel, J.P.**, Peccia, J.: Traffic, Drugs, Mental Health, and Disinfectants: Changes in Sewage Sludge Chemical Signatures During a COVID-19 Community Lockdown. (2021). https://doi.org/10.26434/chemrxiv.13562525.v1

32. **Koelmel, J.P.**, Lin, E.Z., Guo, P., Zhou, J., He, **J., Chen**, A., Gao, Y., Deng, F., Dong, H., Liu, Y., Cha, Y., Fang, J., Beecher, C., Shi, X., Tang, S., Godri Pollitt, K.J.*: Exploring the external exposome using wearable passive samplers - the China BAPE study. Environmental Pollution. 116228 (2020). https://doi.org/10.1016/j.envpol.2020.116228

31. Nason, S.L.*, **Koelmel, J.P.**, Zuverza-Mena, N., Stanley, C., Tamez, C., Bowden, J.A., Godri Pollitt, K.J.: Software Comparison for Nontargeted Analysis of PFAS in AFFF-Contaminated Soil. J. Am. Soc. Mass Spectrom. (2020). https://doi.org/10.1021/jasms.0c00261

30. **Koelmel, J.P.**, **Paige, M.K.**, **Aristizabal-Henao, J.J.**, **Robey, N.M.**, Nason, S.L., **Stelben, P.J.**, Li, Y., **Kroeger, N.M.**, Napolitano, M.P., Savvaides, T., Vasiliou, V., Rostkowski, P., Garrett, T.J., **Lin, E.**, Deigl, C., Jobst, K., Townsend, T.G., Godri Pollitt, K.J.*, Bowden, J.A.*: Toward Comprehensive Per- and Polyfluoroalkyl Substances Annotation Using FluoroMatch Software and Intelligent High-Resolution Tandem

Mass Spectrometry Acquisition. Anal. Chem. 92, 11186–11194 (2020). https://doi.org/10.1021/acs.analchem.0c01591

29. Kaur, S., Sarma, S.J., Marshall, B.L., Liu, Y., Kinkade, J.A., Bellamy, M.M., Mao, J., Helferich, W.G., Schenk, A.K., Bivens, N.J., Lei, Z., Sumner, L.W., Bowden, J.A., **Koelmel, J.P.**, Joshi, T., Rosenfeld, C.S.*: Developmental exposure of California mice to endocrine disrupting chemicals and potential effects on the microbiome-gut-brain axis at adulthood. Scientific Reports. 10, 10902 (2020). https://doi.org/10.1038/s41598-020-67709-9

28. Tsugawa, H.*, Ikeda, K., Takahashi, M., Satoh, A., Mori, Y., Uchino, H., Okahashi, N., Yamada, Y., Tada, I., Bonini, P., Higashi, Y., Okazaki, Y., Zhou, Z., Zhu, Z.-J., **Koelmel, J.P.**, Cajka, T., Fiehn, O., Saito, K., Arita, M., Arita, M.: A lipidome atlas in MS-DIAL 4. Nature Biotechnology. 1–5 (2020). https://doi.org/10.1038/s41587-020-0531-2

27. C.Z., Ulmer, **J.P., Koelmel.**, Cm, J., Tj, G., Jj, A.-H., Hw, V., J.A., Bowden.*: A Review of Efforts to Improve Lipid Stability during Sample Preparation and Standardization Efforts to Ensure Accuracy in the Reporting of Lipid Measurements. Lipids. (2020). https://doi.org/10.1002/lipd.12263

26. **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. https://doi.org/10.1007/s11306-020-01665-3

25. **Koelmel, J.P.***, Li, X., Stow, S.M., Sartain, M.J., Murali, A., Kemperman, R., Tsugawa, H., Takahashi, M., Vasiliou, V., Bowden, J.A., Yost, R.A., Garrett, T.J., Kitagawa, N.: Lipid Annotator: Towards Accurate Annotation in Non-Targeted Liquid Chromatography High-Resolution Tandem Mass Spectrometry (LC-HRMS/MS) Lipidomics Using A Rapid and User-Friendly Software. *Metabolites* **2020**, 10, 101. https://doi.org/10.3390/metabo10030101

24. 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.* **2020**, 19, 424–431. https://doi.org/10.1021/acs.jproteome.9b00605

23. **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* 2019 14, e0218690. https://doi.org/10.1371/journal.pone.0218690

22. **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* **2019**, *20* (1), 217. https://doi.org/10.1186/s12859-019-2803-8.

21. Jeanne Dit Fouque, K.; Ramirez, C. E.; Lewis, R. L.; **Koelmel, J. P.**; Garrett, T. J.; Yost, R. A.; Fernandez-Lima, F.* Effective Liquid Chromatography–Trapped Ion Mobility Spectrometry–Mass Spectrometry Separation of Isomeric Lipid Species. *Anal. Chem.* **2019**, *91* (8), 5021–5027. https://doi.org/10.1021/acs.analchem.8b04979.

20. **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.; … Bowden, J.A.* Lipidomics for Wildlife Disease Etiology and Biomarker Discovery: A Case Study of Pansteatitis Outbreak in South Africa. *Metabolomics* **2019**, *15* (3), 38. https://doi.org/10.1007/s11306-019-1490-9.

19. 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.* **2019**, *316* (3), E546–E556. https://doi.org/10.1152/ajpendo.00386.2018.

18. Kalavalapalli, S., Bril, F**., Koelmel, J.P.**, Abdo, K., Guingab, J., Andrews, P., Li, W.-Y., Jose, D., Yost, R.A., Frye, R.F., others: Mitochondria Dysfunction in Aging and Metabolic Diseases: Pioglitazone improves hepatic mitochondrial function in a mouse model of nonalcoholic steatohepatitis. *American Journal of Physiology-Endocrinology and Metabolism*. **2018**. 315, E163

17. 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**. https://doi.org/10.1152/ajpendo.00297.2018.

16. Gathungu, R. M.; Larrea, P.; SniatynskI, M. J.; Marur, V. R.; Bowden, J. A.; **Koelmel, J. P.**; Starke-Reed, P.; Hubbard, V. S.; Kristal, B. S.* Optimization of ESI-Source Parameters for Lipidomics Reduces Misannotation of In-Source Fragments as Precursor Ions. *Anal. Chem.* **2018**. https://doi.org/10.1021/acs.analchem.8b03436.

15. Kalavalapalli, S.; Bril, F.; **Koelmel, J. P.**; Abdo, K.; Guingab, J.; Andrews, P.; Li, W.-Y.; Jose, D.; Yost, R. A.; Frye, R. F.; et al. Pioglitazone Improves Hepatic Mitochondrial Function in a Mouse Model of Nonalcoholic Steatohepatitis. *Am. J. Physiol. Endocrinol. Metab.* **2018**. https://doi.org/10.1152/ajpendo.00023.2018.

14. Bowden, J. A.*; Ulmer, C. Z.; Jones, C. M.; **Koelmel, J. P.**; Yost, R. A. NIST Lipidomics Workflow Questionnaire: An Assessment of Community-Wide Methodologies and Perspectives. *Metabolomics* **2018**, *14* (5), 53. https://doi.org/10.1007/s11306-018-1340-1.

13. **Koelmel, J. P.**; Jones, C. M.; Ulmer, C. Z.; Garrett, T. J.; Yost, R. A.; Schock, T. B.; Bowden, J. A.* Examining Heat Treatment for Stabilization of the Lipidome. *Bioanalysis* **2018**, *10* (5), 291–305. https://doi.org/10.4155/bio-2017-0209.

12. Gill, E. L.; **Koelmel, J. P.**; Yost, R. A.; Okun, M. S.; Vedam-Mai, V.; Garrett, T. J. Mass Spectrometric Methodologies for Investigating the Metabolic Signatures of Parkinson's Disease: Current Progress and Future Perspectives. *Anal. Chem.* **2018**, *90* (5), 2979–2986. https://doi.org/10.1021/acs.analchem.7b04084.

11. **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* **2017**, *18* (1), 331. https://doi.org/10.1186/s12859-017-1744-3.

10. Ulmer, C. Z.; Ragland, J. M.; **Koelmel, J. P.**; Heckert, A.; Jones, C. M.; Garrett, T. J.; Yost, R. A.; Bowden, J. A.* LipidQC: Method Validation Tool for Visual Comparison to SRM 1950 Using NIST Interlaboratory Comparison Exercise Lipid Consensus Mean Estimate Values. *Anal. Chem.* **2017**, *89* (24), 13069–13073. https://doi.org/10.1021/acs.analchem.7b04042.

9. Bangma, J. T.; Reiner, J. L.; Botha, H.; Cantu, T. M.; Gouws, M. A.; Guillette, M. P.; **Koelmel, J. P.**; Luus-Powell, W. J.; Myburgh, J.; Rynders, O.; et al. Tissue Distribution of Perfluoroalkyl Acids and Health Status in Wild Mozambique Tilapia (Oreochromis Mossambicus) from Loskop Dam, Mpumalanga, South Africa. *J Environ Sci (China)* **2017**, *61*, 59–67. https://doi.org/10.1016/j.jes.2017.03.041.

8. 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**, *13* (11), 142. https://doi.org/10.1007/s11306-017-1280-1.

7. **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. *Biochim Biophys Acta Mol Cell Biol Lipids* **2017**, *1862* (8), 766–770. https://doi.org/10.1016/j.bbalip.2017.02.016.

6. **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. *J. Am. Soc. Mass Spectrom.* **2017**, *28* (5), 908–917. https://doi.org/10.1007/s13361-017-1608-0.

5. 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. *J Am Soc Mass Spectrom* **2017**, *28* (3), 562–565. https://doi.org/10.1007/s13361-016-1579-6.

4. Bowden, J. A.; Heckert, A.; Ulmer, C. Z.; Jones, C. M.; **Koelmel, J. P.**; Abdullah, L.; Ahonen, L.; Alnouti, Y.; Armando, A. M.; Asara, J. M.; … Bowden, J.A.* Harmonizing Lipidomics: NIST Interlaboratory Comparison Exercise for Lipidomics Using SRM 1950-Metabolites in Frozen Human Plasma. *J. Lipid Res.* **2017**, *58* (12), 2275–2288. https://doi.org/10.1194/jlr.M079012.

3. **Koelmel, J.**; Prasad, M. N. V.; Pershell, K. Bibliometric Analysis of Phytotechnologies for Remediation: Global Scenario of Research and Applications. *International Journal of Phytoremediation* **2015**, *17* (2), 145–153. https://doi.org/10.1080/15226514.2013.862207.

2. **Koelmel, J.**; 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. *Environ. Pollut.* **2013**, *174*, 222–228. https://doi.org/10.1016/j.envpol.2012.11.026.

1. **Koelmel, J.**; Amarasiriwardena, D. Imaging of Metal Bioaccumulation in Hay-Scented Fern (Dennstaedtia Punctilobula) Rhizomes Growing on Contaminated Soils by Laser Ablation ICP-MS. *Environ. Pollut.* **2012**, *168*, 62–70. https://doi.org/10.1016/j.envpol.2012.03.035.

Book Chapters

3. Ulmer, C. Z.; Patterson, R. E.; **Koelmel, J. P.**; Garrett, T. J.; Yost, R. A. A Robust Lipidomics Workflow for Mammalian Cells, Plasma, and Tissue Using Liquid-Chromatography High-Resolution Tandem Mass Spectrometry. In *Methods in Molecular Biology*; Springer: Clifton, N.J., 2017; Vol. 1609, pp 91–106.

2. **Koelmel, J.**; Sebastian, A.; Prasad, M. N. V. Chapter 26 - Synthetic Biology: An Emerging Field for Developing Economies. In *Bioremediation and Bioeconomy*; Prasad, M. N. V., Ed.; Elsevier, 2016; pp 665–685. https://doi.org/10.1016/B978-0-12-802830-8.00026-5.

1. **Koelmel, J.**; Prasad, M. N. V.; Velvizhi, G.; Butti, S. K.; Mohan, S. V. Chapter 15 - Metalliferous Waste in India and Knowledge Explosion in Metal Recovery Techniques and Processes for the Prevention of Pollution. In *Environmental Materials and Waste*; Prasad, M. N. V., Shih, K., Eds.; Academic Press, 2016; pp 339–390. https://doi.org/10.1016/B978-0-12-803837-6.00015-9.

Technical Reports

5. **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; Application Note 5994–0775en; Agilent Technologies (2019)

4. Ulmer, C.Z., Ragland, J.M., **Koelmel, J.P.**, Jones, C.M., Bowden, J.A.: LipidQC v 1.0. NIST: MML – Chemical Sciences Division (2017)

3. Ulmer, C.Z., Jones, C.M., **Koelmel, J.P.**, Ragland, J.M., Bowden, J.A.: Untargeted Data Processing Workflow for UHPLC-HRMS Metabolomic and Lipidomics Datasets. NIST: MML – Chemical Sciences Division (2017)

2. Ulmer, C.Z., Jones, C.M., **Koelmel, J.P.**, Bowden, J.A.: Lipid Identification Workflow for Untargeted UHPLC-HRMS/MS Applications. NIST: MML – Chemical Sciences Division (2017)

1. Ulmer, C.Z., **Koelmel, J.P.**, Ragland, J.M., Bowden, J.A.: LipidPioneer v0.9. NIST: MML – Chemical Sciences Division (2016)

Selected Presentations and Workshops (*invited talks)

31. ***Koelmel, J.P.**, FlouroMatch 2.0: Annotating thousands of PFAS with a few clicks. Agilent Webinar (2021).

30. ***Koelmel, J.P.**, Pollitt, K.: GC Orbitrap for Exposomics. Columbia Exposome Boot Camp (2020).

29. **Koelmel, J.P.**, Charkoftaki, G., Lin, E., Pollitt, K., Vasiliou, V., Bowden, J.A., Aristizabal, J.J., Stelben, P., Paige, M., Garrett, T.J.: A Comparison of Intelligent Data-Acquisition Methods for Exposomics and Lipidomics Applications. 65th Conference on Mass Spectrometry and Allied Topics (2020).

28. ***Koelmel, J.P.**, Tan, W.Y., Vasilou, V., Charkoftaki, G., Ni, Z., Federova, M., Bowden, J.A., Aristizabal-Henao, J.J., Guingab, J.D., Garrett, T.J., Williams, T.L., Penumetcha, M.. Millions of Possibilities: The Uncharted Waters of Redox Lipidomics. ELM Bioinformatics (2020).

27. ***Koelmel, J.P.**, Introduction to Lipidomics and Iterative exclusion, LipidPioneer, LipidMatch, LipidMatch Flow. Metabolomics Winter School - Southeast Center for Integrated Metabolomics (SECIM) & Metabolomics Consortium Coordinating Center (M3C). (Workshop, 2020)

26. **Koelmel, J.P.**, Chen, A., He, J., Aksenov, A., Lin, E., O'Brien, F., Zhou, J., Ganguly, K., Upadhyay, S., Veselkov, K., Vasiliou, V., Pollitt, K.: Automatically classifying airborne exposures using GC-HRMS of passive samplers. 2020 New York City Exposome Symposium: Measuring the Exposome Using Novel Methods and Big Data to Improve Human Health. (2020)

25. **Koelmel, J.P.**: Lipid Annotator: A Rapid, Accurate, and User-Friendly Software for Comprehensive LC-HRMS/MS Lipidomics. 67th ASMS Conference on Mass Spectrometry and Allied Topics. (2019)

24. ***Koelmel, J.P.**, Bowden, J.A., Nason, S., Lin, E., Vasiliou, V., Pollitt, K.: The Plethora of Perfluoros: Screening Thousands of Compounds using LC and GC HRMS/MS and FluoroMatch Software

23. **Koelmel, J.P.**: Informatics in Lipidomics: Developments and Considerations. 4th International Conference on Alcohol and Cancer. (2019)

22. ***Koelmel, J.P.**: Bioinformatic innovations for lipidomics. Pittcon 2019. (2019)

21. ***Koelmel, J.P.**: LipidMatch Flow: A high-throughput lipidomics open-source software covering the entire LC-HRMS/MS data-processing workflow. NIH Metabolomics Program Data Presentation Webinar Series. (2018)

20. ***Koelmel, J.P.**: Lipidomics Integration in Multi-omics Studies: Prospects and Challenges. ASMS Workshop: multi-omics interest group. 64th Conference on Mass Spectrometry and Allied Topics. San Diego, CA (2018)

19. ***Koelmel, J.P.**: Combining cutting edge lipidomics software with impactful applications. ASMS Workshop: Matchmaking session: Bridging the gap between computational biology and biology. 64th Conference on Mass Spectrometry and Allied Topics. San Diego, CA (2018)

18. **Koelmel, J. P.**; Li, Y.; Cochran, J. A.; Patt, A. C.; Kroeger, N. M.; Bowden, J. A.; Ulmer, C. Z.; Mathé, E.; Yost, R. A.; Garrett, T. J.: LipidMatch Flow: A User-Friendly Software Covering the Entire Lipidomics Workflow. Poster, 64th Conference on Mass Spectrometry and Allied Topics. San Diego, CA (2018)

17. ***Koelmel, J. P.**: An Open Source Tool Covering the Entire Lipidomics Workflow for LC-HRMS/MS Studies. 2018 SECIM Workshop and Symposium. Cancer and Genetics Research Complex, University of Florida, FL (2018)

16. ***Koelmel, J.P.**: Advancing Lipidomics using Novel Mass Spectrometric Data-Processing Strategies: Successes and Current Challenges. Agilent Technologies Invited Talk. Santa Clara, CA (2017)

15. **Koelmel, J.P.**: Examining Heat Treatment for Stabilization of the Lipidome. CPSA Metabolomics. University of Florida, FL (2017)

14. **Koelmel, J.P.**: An integrative approach for determining biomarkers and etiology of a disease leading to mass die offs of aquatic life in South Africa. CPSA USA. Philadelphia, PA (2017)

13. **Koelmel, J.P.**: LipidMatch Software: identification of lipids and their oxidation products using data-dependent and data-independent LC-MS/MS data. Poster, 64th Conference on Mass Spectrometry and Allied Topics. San Antonio, TX (2016)

12. ***Koelmel, J.P.**: Increasing the coverage and accuracy of lipid measurements, and applications in environmental science. Hollings Marine Laboratory Invited Talk. Charleston, SC (2016)

11. **Koelmel, J.P.**: Applying lipidomics for elucidating biomarkers and the role of environmental stressors leading to the pansteatitis outbreak in fish across South Africa. North American Chemical Residue Workshop. St. Pete Beach, FL (2016)

10. **Koelmel, J.P.**: Advances in lipidomics, and the case for lipidomics in environmental toxicology studies. The Biology and Ecotoxicology of the American Alligator, The 3rd Biennial Symposium. John F. Kennedy Space Center, FL (2016)

9. Torres, T.; Mitchell, A.; **Koelmel, J.P.**: Transforming Freshman Chemistry using Mini-Projects that Incorporate Engineering Context: The Graduate Teaching Assistant Perspective. ASEE SE Section Annual Conference. University of Florida (2015)

8. **Koelmel, J.P.**: Oxidized Lipidomics: Mechanisms, Products, and Libraries. Southeast Center for Metabolomics Lecture Series. University of Florida, FL (2015)

7. **Koelmel, J.P.**: Novel Strategies for Analysis of High-Resolution Data-Independent MS/MS Spectra for Rapid and Accurate Structural Confirmation of Lipids. 63rd Conference on Mass Spectrometry and Allied Topics. Poster, St. Louis, MO (2015)

6. **Koelmel, J.P.**: Lipidomics for Elucidating Biomarkers and Mechanisms of Perfluorooctanesulfonic acid (PFOS) Toxicity. ASMS Environmental Applications Interest Group Workshop. St. Louis, MO (2015)

5. **Koelmel, J.P.**: Comparison of MALDI-LTQ and Q-Exactive for Lipidomics; a case study on catfish plasma. Southeast Center for Metabolomics Lecture Series. Clinical and Translational Research Building, University of Florida, FL (2014)

4. **Koelmel, J.P.**; Bowden, J.A.; Garrett, T.J.; Guillette, L.G.: The Potential of Lipidomics for Elucidating Mechanisms of PFOS Toxicity. The Biology and Ecotoxicology of the American Alligator, The 2nd Biennial Symposium. John F. Kennedy Space Center, FL (2014)

3. **Koelmel, J.P.**: Chromium Contamination in India and the Potential for Phytoremediation and Bioremediation as Low-Cost Solutions. 2013 International Conference on the Biogeochemistry of Trace Elements. Athens, Georgia (2013)

2. **Koelmel, J.P.**: Modeling Chromium Emissions in India and Prospects for Bioremediation and Bioenergy in Contaminated Sites. Confederation of Indian Industries: Conference on Environmental Resource Conservation Reduce, Reuse and Recycle. , Hyderabad, India (2012)

1. **Koelmel, J.P.**: Biodiversity on Chromium Contaminated Sites in Tamil Nadu - A Bioremediation Tool-box. Second Indian Biodiversity Congress (IBC) and Expo. Indian Institute of Science, Bangalore, India (2012)

SOFTWARE (see innovativeomics.com for access to current software)

11. **Koelmel, J.P.**, Stelben, P., Paige, M., Li, Y., Bowden, J.A., Renei, E., Pollitt, K., Nason, S. FluoroMatch and FluoroMatch Flow. Languages: R, C#, and Java. Yale University, University of Florida, and Agilent Technologies, 2021.

10. **Koelmel, J.P.**, Intelligent Iterative Inclusion and Intelligent Iterative Exclusion. Langauge: R. Innovative Omics, 2021.

9. **Koelmel, J.P.**, Stelben, P., Paige, M., Pollitt, K. ChemCat. Language: R. Yale University, 2020.

8. Li, X., **Koelmel, J.P.**, Stow, S.M., Sartain, M., Murali, A., Kitagawa, N. Lipid Annotator. Language: C#, Agilent Technologies, Santa Clara, CA, 2019.

7. **Koelmel, J. P.**, Li, Y., Jason, C. A., Patt, A. C., Kroeger, N. M., Mathé, E., Garret, T. J. LipidMatch Flow. Language: C#, R. SECIM, University of Florida, 2019.

6. Patterson, R.E., Kirpich, A.S., **Koelmel, J.P.**, Morse, A.M., Ibarra, M., Moskalenko, O., Fear, J., Morse, A., McIntyre, L.M. Blank Feature Filtering (BFF). Language: Python, Galaxy. University of Florida, 2017.

5. Ulmer, C. Z., Ragland, J. M., **Koelmel, J. P.**, and Bowden, J. A. LipidQC. Language: Visual Basic, Excel. NIST, 2017.

4. **Koelmel, J. P.**, Cochran, J., Ulmer, C. Z., and Bowden, J. A. LipidMatch Normalizer. Language: R. University of Florida, 2017.

3. Ulmer, C. Z., **Koelmel, J. P.**, Ragland, J. M., and Bowden, J. A. LipidPioneer. Language: Visual Basic, Excel. NIST, 2017.

2. **Koelmel, J. P.**, Kroeger, N. M., and Cochran, J. LipidMatch. Language: R. University of Florida, 2017.

1. **Koelmel, J. P.**, and Kroeger, N. M. IE-Omics. Language: R. University of Florida, 2016.

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Research and Training Contracts (Innovative Omics Inc.)

PFAS software development, vendor integration, and publicizing, Agilent Technologies. (2021-2022)

Mentorship and Lipidomics Research, Southeast Center for Integrated Metabolomics. (2020-2021)

Lipidomics Software Training and Workflow Development, The Roskamp Institute. (2021-)

PFAS software training and Workflow Development, Cyclopure (2020)

Oxidized Lipidomics for Cooking Oils, Meera Penumetcha, University of Central Missouri (2018-2021)

Grants and Awards (Academic)

Applications and Core Technology Grant Recipient, Agilent Technologies Inc. (2020)
- Software development for PFAS annotation for non-targeted mass spectrometry data ($65,000)

Sanibel Student Travel Award, American Society for Mass Spectrometry (ASMS) (2019)
- Travel stipend for excellent contribution to the field of mass spectrometry

Applications and Core Technology Grant Recipient, Agilent Technologies Inc. (2017)
- Software development for lipidomics annotation for non-targeted mass spectrometry data ($25,000)

Steven A. Hofstadler Award, Clinical and Pharmaceutical Solutions for Analysis (CPSA) (2017)
- Awarded for outstanding contributions to the field through high-quality science

Graduate Student Mentoring Award, University of Florida, Division of Graduate Student Affairs (2017)
- Awarded for outstanding mentorship of undergraduates, only awarded to 6 out of 12,500 UF graduate students per year

NACRW Student Scholarship Award, North American Chemical Residue Workshop (2016)
- $500 travel stipend awarded to the top abstracts submitted to the conference, awarded for work related to trace metal contamination of river systems in South Africa

Office of Research Travel Award (2015)

College of Liberal Arts and Sciences Travel Award (2015)
- $400 and $300, respectively, for travel to South Africa

Graduate Student Council Travel Award (2015)
- $350 for travel to the American Society for Mass Spectrometry (ASMS) annual conference

Townes R. Leigh Prize, University of Florida, Graduate Standards Committee (2014)
- Awarded for exceptional achievement in course work, research, and teaching

Graduate School Fellowship, University of Florida, Department of Chemistry (2013-2017)
- Awarded to the top applicants applying to the Department of Chemistry

Nehru Fulbright Scholar, Institute of International Education (2012-2013)
- Awarded to research bioremediation techniques for chromium pollution in Tamil Nadu, India

Ingenuity Award, Hampshire College Community Campus Leadership and Activities (April 2011)
- Recommended by my peers for my dedication to making chemistry and statistics accessible to all students through my persistent work as a TA in Chemistry I, Chemistry II, and Statistics I

NSF REU Grantee, National Science Foundation (Summer 2010)
- Awarded to research factors for temporal variations in isoprene nitrates in Michigan

Young Naturalist Award, American Museum of Natural History (June 2007)

- Awarded for my independent research on lichens as indicators of vehicle pollution

Outstanding Leader Award, New York Urban Debate League (2006)

- Awarded for my work as a debate coach

EXPERIENCE IN TEACHING SCIENCE

Homeschool Science and Coding Instructor, Sarasota, FL (May 2020 – present)

- Lead course work in plant identification and gardening, the scientific method and statistics using fun applications, coding using Processing artistic computer programming language, PowerPoint, Excel, and general computer skills.

Research Mentor, Yale University, New Haven, CT (April 2019 – present)

- Mentored over 8 undergraduates, masters students, and PhD students as a Post Doc at Yale University. Lead teams of computer scientists for development of software in both biological and environmental mass spectrometry, and taught students how to design experiments, acquire data, and interpret data using the new mass spectrometers in the laboratory.

Undergraduate Research Mentor, University of Florida, Gainesville, FL (Spring 2014 – Fall 2017)

- Mentored Jordan Zeldin (Interdisciplinary biomedical sciences), Jason Cochran (computer science), Nicholas Kroeger (computer science), Michelle Palumbo (computer science), Nicholas Azcarate (statistics), and Berkley Olsen (biology) to work on interdisciplinary projects.
- Resulted in 7 publications with undergraduates as authors (one submitted and two in preparation), including two publications with undergraduates as co-first authors
- Encouraged undergraduates to present their work and attend conferences
- Three software written by undergraduates have been released and have associated publications

TA: Chemistry for Engineers, University of Florida, Gainesville, FL (Spring and Fall 2014)

- Attended weekly meetings and helped design a curriculum and rubric for a new class at UF
- Taught classes focused on applying chemical principles to engineering problems

TA: General Chemistry, University of Florida, Gainesville, FL (Fall 2013)

- Held study sessions for students

Science Teacher, Eden Village Camp, Putnam Valley, NY (July 2011)

- Designed curriculum and taught science (chemistry, anatomy, and ecology) to children ages 8 to 15
- Cared for and managed a bunk of thirteen 8 – 10 year olds

TA: Chemistry II, Hampshire College, Amherst, MA (Spring 2011)

- Made laboratory reagents, held study sessions, and had open office hours for students

TA: Statistics in R, Hampshire College, Amherst, MA (Fall 2010)

- Taught introductory classes in R, trained statistics tutors in R, and held study sessions

TA: Chemistry I, Hampshire College, Amherst, MA (Fall 2010)

- Made laboratory reagents, held study sessions, and had open office hours for students

Naturalist Camp Director, Dandelions Summer Camp, Temple, NH (Summer 2009)

- Designed and led day long ecology programs for children ages 8 – 13

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RELEVANT SKILLS

Instrument:

- Laser ablation inductively couple plasma mass spectrometry (LA-ICP-MS)
- Inductively coupled plasma-mass spectrometry (ICP-MS)
- Matrix Assisted Laser Desorption/Ionization (MALDI)
- High-Resolution Tandem Mass Spectrometry (HRMS/MS) (Waters, Thermo, Agilent)
- Liquid Chromatography methods (reverse and normal phase)
- Gas Chromatography Mass Spectrometry (GC-MS)

Fieldwork:

- Mapping out contamination and sampling sites (GIS, Google Earth)
- Hiring translators, conducting interviews, and ethnographic techniques
- Proper procedures for collection of plant, animal, soil, bacteria, and water samples for trace metal, genomics, and metabolomics analysis
- On-site blood preparation and measurements

Laboratory and Data-Processing skills:

- Acid digestion for trace metal analysis
- Quantitative trace metal analysis with external calibration for ICP-MS and LA-ICP-MS
- Extraction methods for lipidomic analysis
- Heat treatment using state of the art technology for sample preservation
- Developing and applying lipidomics and metabolomics workflows
- Imaging mass spectrometry acquisition
- Writing routines in R for automating data processing and statistical analysis
- Simple multivariate and univariate statistical methods

Mass Spectrometric Software:

- Thermo: Xcalibur, Compound Discoverer, LipidSearch
- Agilent: MPP, ID Browser, Qual Browser
- Peak picking: MZmine, XCMS, MS-DIAL
- Lipidomics: LipidSearch, Greazy, MS-DIAL, LipidBlast, LipidMatch, Lipid-Pro
- Bioinformatics: Metaboanalyst, Galaxy (SECIM metabolomics toolset)

Data Analysis Methods:

- Programming and data analysis in R and Excel

Interpersonal Skills

- Group project leader for undergraduate and graduate researchers
- Graphic design, oral presentations, and cartoon animations for public education
- Trained in communication, life coaching, counseling, and listening skills through:
    - Completing Principles and Practices of Transformative Coaching (PPTC) 6 month course (72 hours of direct training + over 70 hours of coursework)
    - Volunteering in numerous 3-day and 7-day workshops with Satvatove Institute
    - Designing curriculum and leading numerous 2-5 hour workshops on transformative communication, as well as offering 1-on-1 and couples coaching sessions

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jeremykoelmel@gmail.com

OTHER WORK AND VOLUNTEER EXPERIENCE

Post-Doctoral Research Fellow, Yale University, New Haven, CT (March 2019 – 2021)
- Developed a robust and user friendly lipidomics software for all data-processing needs of the core laboratory. Trained lab technicians on the use of various software and informatics tools. Was involved in research related to lipidomics and informatics resulting in a number of first author publications.

Communications Course Facilitator, New Haven, CT (2019 –)
- Organize and facilitate communication course for members of the community to learn to enter others worlds, express oneself assertively, and deal with emotionally charged situations

Vipassana Course Organizer, New Haven, CT (2019 –)
- Organize meditation courses for adults and teenagers to live a focused, balanced, and happy life
- Co-hosted weekly public meditation sits for members of the community
- Trained in conducting course for teens by the Vipassana association

Post-Doctoral Research Fellow, South East Center for Integrated Metabolomics, FL (March 2018 – March 2019)
- Developed a robust and user friendly lipidomics software for all data-processing needs of the core laboratory. Trained lab technicians on the use of various software and informatics tools. Was involved in research related to lipidomics and informatics resulting in a number of first author publications.

Personal Support Worker, Amherst, MA (2011 – 2013)
- Help a child with profound autism to advance in life skills, create social bonds, and remain safe

Improvisational Dance Teacher, Multiple Schools, MA and VT (2011 - 2012)
- Design curriculum and teach children improvisational dance, teach students in pre-K to High School programs, including deaf students and students with behavioral and mental disabilities

Environmental Chemistry Research Apprentice, Hampshire College, Amherst, MA (2011)
- Developed an analytical technique using in house standards for LA-ICP-MS for quantifying gold nanoparticles with different charged active sites in rice tissues
- Synthesized bimetallic silver nZVI

Residential Assistant, Hampshire College Residential Life, Amherst, MA (2009-2011)
- Helped mediate student conflicts, maintain community norms, and provide resources, counseling and space for students.
- Procided services to the foreign scholars, Tibetan monks, and international students housing and provided help in English, feeling at home in the new culture, and resources
- Created and led social, educational, and community service programs

Improvisational Bicycle Dance Troupe, New England (May 2011)
- Biked and camped around New England performing improvisational dance
- Taught dance across New England to elementary school children

Domestic Violence Shelter Volunteer, Safe Passage, Northampton, MA (2008-2010)
- Cared for children ages 1 - 16, led field trips, helped maintain grounds

Farm Intern, Herban Living Farm, Temple, NH (Summer 2009)
- Planted, nourished, and harvested crops, cared for livestock, helped run organic CSA

Habitat Restoration Assistant, Naturalist Professor's Private Property, Amherst, MA (Spring 2009 & 2011)
- Removed invasive species, sustained various habitat types

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Farm Volunteer and Employee, Hampshire College Farm, Amherst, MA (2007-2009)
- Planted, harvested, and packaged crops, set up irrigation

Canvasser, Clean Water Action, Northampton, MA (2007 – 2008)
- Educated communities on current environmental health issues
- Canvassed for letters to congressmen, donations, and membership

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REFERENCES

Dr. Richard A. Yost
University of Florida
ryost@aa.ufl.edu
(352) 392-0557
Ph.D. Research Advisor
2013 – 2017

Professor and Head, UF Analytical Chemistry Department

Professor, UF Pathology, Immunology, and Laboratory Medicine

Professor, UF School of Natural Resources and Environment

Professor, University of Utah Pathology and ARUP

Director, Southeast Center for Integrated Metabolomics

Dr. John A. Bowden
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Ph.D. Committee Member
Extensive Collaboration
2013 - Present

Research Chemist, National Institute of Standards and Technology

Dr. Timothy J. Garrett
University of Florida
tgarrett@ufl.edu
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Ph.D. Committee Member
Extensive Collaboration
2013 – Present

Associate Professor, UF Pathology, Immunology, and Laboratory Medicine

Dr. Dula Amarasiriwardena
Hampshire College
dula@hampshire.edu
(413) 559-5561
Undergraduate Research Advisor,
2007 – 2011

Professor of Chemistry

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Fulbright Mentor,
2012-2013

Professor – Environmental Biotechnology

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(954) 805-1427
Undergraduate Mentee
2015-2017

PhD Candidate, Computer Engineering