Jeremy P. Koelmel, PhD Chemistry

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CURRENT EMPLOYMENT

Associate Research Scientist (faculty position). 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/EMPLOYMENT

Yale University, New Haven, CT, Associate Research Scientist, 2024-Present

Innovative Omics, Sarasota, FL, CEO, 2019-Present

Yale University, New Haven, CT, Postdoctoral Associate, 2023-2024

Yale University, New Haven, CT, Postdoctoral Fellow, 2022-2023

Yale University, New Haven, CT, Research Associate, 2021-2022

Yale University, New Haven, CT, Postdoctoral Research Associate, 2019-2021

University of Florida, Gainesville, FL, Research Associate, 2017-2019

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

My research focuses on detecting hundreds to tens of thousands of contaminants simultaneously using a single platform consisting of high-resolution tandem mass spectrometry and associated techniques. Towards this end I have made great progress with the research group led by Krystal Pollitt, as well as with collaborations with Agilent technologies, and other academic and industrial partners around the world. 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 have been working with the EPA over the past 4 years 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 21 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

PUBLICATIONS

Manuscripts (Total Citations, google scholar: 4750+,
https://scholar.google.co.in/citations?user=jLbx6gcAAAAJ&hl=en)
Mentees for which I was the main mentor for this project are highlighted in blue
§denotes share first author
*denotes corresponding author

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Measuring the Exposome: A Practical Guide for Using Wearable Passive Samplers to Assess Environmental Influences. *Exposome* 2026, osag002.

74. Schiessel, D.; Chevallier, O.; **Kummer, M.**; Liu, S.; **Chang, P.**; Pyke, J.; Klein, C.; Rodowa, A. E.; Ragland, J. M.; Godri, D.; **Stelben, P.**; Williams, A.; Rennie, E. E.; Godri Pollitt, K. J.; **Koelmel, J. P.**
Approaching a 0 % False Positive Rate for PFAS Determination Leveraging Only MS1 Data. *Environ. Sci. Technol.* **2026**. https://doi.org/10.1021/acs.est.5c12047

73. **Koelmel, J. P.**; Ramos, P. S.; Costa, K. A.; Godri-Pollitt, K. J.; Kamen, D. L.; Bowden, J. A.
Lipidome Changes Indicate Oxidative Stress, Inflammation, and Specific Loss of Glycerophosphoserine Inflammatory Protection in Patients with Lupus. *J. Pharm. Biomed. Anal.* **2025**, 117302.

72. **Koelmel, J. P.**; Lin, E. Z.; **Chang, P.**; Johnson, E.; Stelben, P.; Liu, S.; Nishida, K.; Tsugawa, H.; Lin, A.; Newton, S.; et al. Shedding Light on PFAS Dark Matter Using a Novel GC-HRMS Approach. *Environ. Sci. Technol.* 2025, *59* (47), 25296–25308.

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68. Newton, Seth R; Bowden, John A; Charest, Nathaniel; Jackson, Stephen R; **Koelmel, Jeremy P**; Liberatore, Hannah K; **Lin, Ashley M**; Lowe, Charles N; Nieto, Sofia; Godri Pollitt, Krystal J Filling the Gaps in PFAS Detection: Integrating GC-MS Non-Targeted Analysis for Comprehensive Environmental Monitoring and Exposure Assessment. Environmental Science & Technology Letters (2025), 12 (2), 104-112

67. **Liu, Sheng**; Dukes, David A; **Koelmel, Jeremy P**; **Stelben, Paul**; Finch, Jasen; Okeme, Joseph; Lowe, Charles; Williams, Antony; Godri, David; Rennie, Emma E; Expanding PFAS Identification with Transformation Product Libraries: Nontargeted Analysis Reveals Biotransformation Products in Mice. Environmental Science & Technology (2024), 59 (1), 119-131

66. Lai, Yunjia; **Koelmel, Jeremy P**; Walker, Douglas I; Price, Elliott J; Papazian, Stefano; Manz, Katherine E; Castilla-Fernández, Delia; Bowden, John A; Nikiforov, Vladimir; David, Arthur; High-resolution mass spectrometry for human exposomics: Expanding chemical space coverage. Environmental Science & Technology (2024), 58 (29), 12784-12822

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64. **Koelmel, Jeremy P**; **Stelben, Paul**; Oranzi, Nicholas; **Kummer, Michael**; Godri, David; **Qi, Jiarong**; Rennie, Emma E; Lin, Elizabeth; Weil, David; Godri Pollitt, Krystal J. PolyMatch: Novel Libraries, Algorithms, and Visualizations for Discovering Polymers and Chemical Series. Journal of the American Society for Mass Spectrometry (2024), 35 (3), 413-420. https://www.doi.org/10.1021/jasms.3c00313

63. Upadhyay, Swapna; Rahman, Mizanur; Rinaldi, Selina; **Koelmel, Jeremy P**; Lin, Elizabeth Z; Mahesh, Padukudru Anand; Beckers, Johannes; Johanson, Gunnar; Pollitt, Krystal J Godri; Palmberg, Lena; Assessment of wood smoke induced pulmonary toxicity in normal-and chronic bronchitis-like bronchial and alveolar lung mucosa models at air–liquid interface. Respiratory Research (2024), 25 (1), 49

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59. Okeme, Joseph O; **Koelmel, Jeremy P**; Johnson, Emily; Lin, Elizabeth Z; Gao, Dong; Pollitt, Krystal J Godri. Wearable Passive Samplers for Assessing Environmental Exposure to Organic Chemicals: Current Approaches and Future Directions. Current Environmental Health Reports (2023). https://doi.org/10.1007/s40572-023-00392-w.

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analysis of dried blood spots. *Science of The Total Environment* (2023), 883. https://doi.org/10.1016/j.scitotenv.2023.163579.

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51. DeLay, K.; Lin, E. Z.; **Koelmel, J. P.**; Bornman, R.; Obida, M.; Chevrier, J.; Godri Pollitt, K. J. Personal Air Pollutant Exposure Monitoring in South African Children in the VHEMBE Birth Cohort. *Environment International* (2022), 170, 107524. https://doi.org/10.1016/j.envint.2022.107524.

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49. **Koelmel, J. P.**; **Tan, W. Y.**; Li, Y.; Bowden, J. A.; Ahmadireskety, A**.; Patt, A. C.**; Orlicky, D. J.; Mathé, E.; **Kroeger, N. M.**; Thompson, D. C.; **Cochran, J. A.**; Golla, J. P.; Kandyliari, A.; **Chen, Y.**; Charkoftaki, G.; Guingab-Cagmat, J. D.; Tsugawa, H.; Arora, A.; Veselkov, K.; Kato, S.; Otoki, Y.; Nakagawa, K.; Yost, R. A.; Garrett, T. J.*; Vasiliou, V.* Lipidomics and Redox Lipidomics Indicate Early Stage Alcohol-Induced Liver Damage. *Hepatology Communications* (2022), 6 (3), 513–525. https://doi.org/10.1002/hep4.1825.

48. Nason, S. L.*; Lin, E.; Eitzer, B.; **Koelmel, J.**; Peccia, J. Changes in Sewage Sludge Chemical Signatures During a COVID-19 Community Lockdown, Part 1: Traffic, Drugs, Mental Health, and Disinfectants. *Environmental Toxicology and Chemistry* (2022), 41 (5), 1179–1192. https://doi.org/10.1002/etc.5217.

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54. Savvaides, T.; **Koelmel, J. P.**; Zhou, Y.; Lin, E. Z.; Stelben, P.; Aristizabal-Henao, J. J.; Bowden, J. A.; Godri Pollitt, K. J.* Prevalence and Implications of Per- and Polyfluoroalkyl Substances (PFAS) in Settled Dust. *Curr Envir Health* Rpt (2021), 8 (4), 323–335. https://doi.org/10.1007/s40572-021-00326-4.

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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. (2021).

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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

8. **Jeremy Koelmel**, Krystal Godri Pollitt, Michael Kummer, Stephan Baumann and Olivier Chevallier. Expanding PFAS Coverage in Nontargeted Analysis Using Data-Independent Analysis. Agilent Application Note, Accepted (2025)

7. **Koelmel, Jeremy P**; Stelben, Paul; Lin, Elizabeth; Godri Pollitt, Krystal J; Rennie, Parry, Emily; Pyke, James. Non-Target PFAS Analysis in Dried Blood Spots Using the Agilent 6546 LC/Q-TOF with Profinder and FluoroMatch. Agilent Application Note (2024) https://www.agilent.com/cs/library/applications/an-non-target-pfas-dried-blood-6546-lc-q-tof-5994-7023en-agilent.pdf

6. **Jeremy Koelmel**. Workflows for Non-Targeted Analysis of PFAS in Biological Matrices. Executive Summary, LCGC Sponsored Content, 2024. https://www.chromatographyonline.com/view/workflows-for-non-targeted-analysis-of-pfas-in-biological-matrices

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)

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Selected Presentations and Workshops (*invited talks)

106. Siyu Li; **Jeremy P. Koelmel**. Improving Detection of Per- and Polyfluoroalkyl Substances (PFAS) in Non-Targeted Analysis Through Systematic Evaluation of HRMS Acquisition Modes. ASMS (2026).

105. Mark Sartain; Julie Horner-Buxton; **Jeremy P. Koelmel**. Lipid Insight Unblocked: Integrating Nontargeted LC/MS Chemometrics With Automated Lipid Annotation. ASMS (2026).

104. **Jeremy P. Koelmel**; Fanny Chu; Randolph Singh; Sophie Thuault-Restituito; Abigail Melican; Thomas O. Metz; Krystal J. Godri Pollitt. Exposomics Survey Reveals Community Wide Non-Targeted Analysis Workflows in Proteomics, Lipidomics, Metabolomics, and Xenobiotics Analysis. ASMS (2026).

103. David Schiessel; **Jeremy P. Koelmel**; Olivier Chevallier; David Godri; Randolph R. Singh; Thomas O. Metz; Emma Rennie; Cairo Ortiz; Parker Chang; Sheng Liu; Krystal J. Godri Pollitt. Evaluation of MS/MS Library Match Similarity Metrics and Integration into a New All-In-One Non-Targeted Software Platform for Increasing Exposome Coverage. ASMS (2026).

102. Sheher Mohsin; Parker Chang; Yanan Chen; Olivier Chevallier; Erin Baker; MaKayla Foster; Kara Joseph; Sarah Stow; Rachel Smolinski; Lauren Royer; Emma Rennie; Michael Kummer; Paul Stelben; David Schiessel; Carrie McDonough; Krystal J. Godri Pollitt; **Jeremy P. Koelmel**. Leveraging Ion Mobility for PFAS Non-Targeted Analysis Using FluoroMatch IM 2.0 and a CCS Atlas. ASMS (2026).

101. Christine M. Fisher (O'Donnell); Brian Ng; **Jeremy P. Koelmel**. Prioritization of MS2 Selection Based on Precursor Mass Defect for Non-Targeted Analysis of Per- and Polyfluoroalkyl Substances. ASMS (2026).

100. Parker Chang; **Jeremy P. Koelmel**; Cairo Ortiz; Sheng Liu; Joseph M. Braun; Katherine E. Manz; Aimin Chen; Bruce P. Lanphear; Kimberly Yolton; Krystal J. Godri Pollitt.
Identifying Hundreds of PFAS in Dust Using Multimodal Mass Spectrometry Approaches: An Understudied Matrix with Potential Human Health Impact. ASMS (2026).

99. *Jeremy P. Koelmel**. NEXUS International Survey. BP4NTA Monthly Webinar (2026)

98. **Jeremy P. Koelmel.** Workshop: Non-Targeted and Targeted PFAS Analysis Using LC-HRMS/MS. SETAC (2025).

97. **Jeremy P. Koelmel.** The FluoroMatch Multimodal PFAS Atlas: High-Resolution Libraries Covering Gas Chromatography, Liquid Chromatography, and Ion Mobility. SETAC (2025).

96. **Jeremy P. Koelmel**. De Novo PFAS Annotation and Classification Using Highly Accurate Formula Prediction and Kaufmann Algorithms Embedded in FluoroMatch Suite. ASMS (2025).

95. **Jeremy P. Koelmel**, John Bowden. Workshop: Unveiling Thousands of PFAS Exposures: Interpreting Mass Spectrometry Data for Unknown Discovery. ISES / ISEE (2025).

94. **Jeremy P. Koelmel**. Assessing Airborne PFAS Personal Exposure Profiles Using Wearable and Stationary Passive Sampling Technology and a Novel GC-HRMS Workflow. ISES / ISEE (2025).

93. **Jeremy P. Koelmel**, Krystal Godri Pollitt. Community Wide Perspectives, Methodologies, and Applications in Exposomics: Results from the Network for Exposomics in the U.S. (NEXUS) Center for Exposome Research Coordination Survey. ISES / ISEE Joint Annual Meeting, Atlanta, GA (2025).

92. **Jeremy P. Koelmel**, Krystal Godri Pollitt. FluoroMatch: A Comprehensive Solution for Non-Targeted PFAS. iSLS13 (2025)

91. **Jeremy P Koelmel**. Live Software Demos: Agilent Suites (multiple days, 8-10pm). ASMS (2024)

90. Alan A. McKenzie-Coe, Thomas Lubinsky**, Jeremy Koelmel**, Emma E. Rennie, David Weil, Sarah Stowe, Paul Stelben, Krystal Pollitt, David Godri, Frederick G. Strathmann, Daniel DeBord. Faster Analysis for Forever Chemicals: Accelerating PFAS Analysis with UPLC-HRIM-MS. ASMS (2024)

89. Sheng Liu, **Jeremy P. Koelmel**, David Schiessel, Michael Kummer, David Godri, Elizabeth Z. Lin, Emma E. Rennie, Krystal Godri Pollitt. Targeted and non-targeted analyses of per- and polyfluorinated alkyl substances (PFAS) in dried blood spots of newborns in California. ASMS (2024)

88. **Jeremy Koelmel**; Elizabeth Z. Lin; Emily Johnson; Paul Stelben; Sheng Liu; Kozo Nishida; Hiroshi Tsugawa; Ashley Lin; Yakun Zhou; Vladimir Nikiforo; Alexander Aksenov; Joseph Okeme; John Bowden; Krystal Godri Pollitt. Enhanced Coverage of Volatile and Semi-Volatile PFAS Using Experimental and Predicted GC-HRMS PCI and EI Libraries. ASMS (2024)

87. **Jeremy Koelmel**; John Bowden; Juan Henao. 1-day Workshop: Lipidomic Workflows: An Introduction. ASMS (2024)

86. David Schiessel*; **Jeremy Koelmel**; Michael Kummer; David Godri; Sheng Liu; Elizabeth Z. Lin; John Bowden; Olivier Chevallier; Camden G. Camacho; Emma E. Rennie; Krystal Godri Pollitt. Leveraging the MS1 Dimension and Formula Prediction in Non-Targeted Analysis of PFAS using New FluoroMatch Algorithms: Assessing Confidence and Coverage**,** ASMS (2024) https://www.agilent.com/cs/library/posters/public/po-fluoromatch-asms-2024-tp113-en-agilent.pdf

85. **Jeremy Koelmel**; David A Weil; Emma E. Rennie*; Paul Stelben; Nicholas Oranzi; Michael Kummer; David Godri; Jiarong Qi; Elizabeth Z. Lin; Krystal J. Godri Pollitt; Non-targeted analysis, interactive visualization, and online sharing of interactive LC-HRMS/MS data of polymers using a comprehensive software PolyMatch Suite, ASMS (2024) https://www.agilent.com/cs/library/posters/public/po-lc-hrms-ms-polymatch-asms-2024-mp216-en-agilent.pdf

84. **Jeremy Koelmel**. Workflows for Non-Targeted Analysis of PFAS in Biological Matrices. RA45408.4717939815 Agilent Webinar (2024)

83**. Jeremy Koelmel**. FluoroMatch Suite: New Software Advances for Non-Targeted Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in LC-HRMS and Ion Mobility. Agilent Breakfast Seminar (2024)

82. Liu, Sheng; **Koelmel, Jeremy**; Schiessel, David; Lin, Elizabeth Ziying; Kummer, Michael; Brooks, Bernard; Godri, David; Fortner, John; Morimoto, Libby; Ma, Xiaomei; Godri Pollitt, Krystal. Exploring PFAS Exposures In Utero: Streamlining Non-Targeted Analysis of PFAS in Neonatal Dried Blood Spots. SETAC (2024)

81. **Jeremy P. Koelmel**, Michael Kummer, David Schiessel, Bernard Brooks, David Godri, Ansgar Korf, Robin Schmid, John A Bowden, Olivier Chevallier, Christian Klein, Emma E. Rennie, Krystal Godri Pollitt. Moving Towards a Comprehensive Open-Source Software and Data-Visualization Platform for General Non-Targeted Analysis using LC-HRMS/MS, SETAC 2024

80. Stephan Baumann, **Jeremy P Koelmel**, Michael Kummer. Expanding Per- and Polyfluoroalkyl Substances Coverage in Nontargeted Analysis Using Data-Independent Analysis and IonDecon. SETAC – Seville (2024)

79. **Jeremy P. Koelmel**, Paul Stelben, Michael Kummer, Bernard Brooks, Sheng Liu, Carrie A. McDonough, David Godri, Jiarong Qi, Elizabeth Z. Lin, Antony J. Williams, Nandarini Abril, John A. Bowden, Ralph Hindle, Kathy Hunt, David Weil, Sarah Stow, Emily Parry, Jacqueline Bangma, Emma E Rennie, Krystal J. Godri Pollitt. FluoroMatch Suite Software: Advancing Non-Targeted Analysis for the Comprehensive Detection and Identification of PFAS and Polymers. SETAC North American Annual Conference (2023)

78. **Jeremy P. Koelmel**, John A. Bowden. Non-Targeted PFAS Analysis Using GC and LC-HRMS/MS. SETAC Workshop, SETAC North American Annual Conference (2023)

77. *__Jeremy P Koelmel__. Unravelling the PFAS puzzle with Comprehensive Targeted & Untargeted Workflows FluoroMatch Suite: Comprehensive Non-Targeted Software for LC-HRMS/MS PFAS Data Analysis. Agilent Morning Seminar (2023)

76. *__Jeremy P Koelmel__. FluoroMatch Suite: Addressing the need for Visual Confirmation in Non-Targeted Software Platforms. ASMS Environmental Applications Interest Group (2023)

75. **Jeremy Koelmel**, Michael Kummer, Ralph Hindle, Kathy Hunt, Stephan Baumann, Krystal Pollitt, Emma Rennie. Creating Deconvoluted Open-Source Files from Data-Independent Analysis Files using IonDecon. ASMS (2023)

74. Michael Kummer; Nandarani Abril; Emily Parry; Sheng Liu; Carrie A Mcdonough; David Dukes; David Godri; Elizabeth Z. Lin; Emma E Rennie; **Jeremy Koelmel**; Krystal J Godri Pollitt. FluoroMatch 3.0 – Automated PFAS Non-Targeted Analysis and Visualizations Applied to Mammalian Biofluids. ASMS (2023)

73. **Jeremy P Koelmel**, Paul Stelben, Bernard Brooks, Jung Suh, Mark J. Sartain, Timothy J. Garrett, John A. Bowden, Emma E. Rennie, Krystal Pollitt. All-in-one Data-Processing and Interactive Visualizations of Lipid LC-HRMS/MS Data using LipidMatch 4.0. ASMS (2023)

72. ***Koelmel, J.P.** An Actionable Annotation Scoring Framework for GC-HRMS Targeted Analysis, Suspect Screening, and Non-Targeted Analysis. Thermo Fisher Morning Seminar, ASMS (2023)

71. Bowden, J.A., **Koelmel, J.P.**, and Aristizabal-Henao, J.J. An Introduction to Lipidomic Workflows. ASMS Workshops (2023)

70. *__Jeremy P Koelmel__, Jacqueline Bangma. FluoroMatch: Developments and Applications for Source Characterization by the EPA. FluoroMatch 1st Users Meeting. (2023)

69. *__Jeremy P Koelmel__, FluoroMatch and Friends: NTA PFAS Software for Ion Mobility, GC-HRMS PCI and EI, LC-HRMS/MS, All-Ions, and more! BP4NTA Monthly Meeting. (2023)

68. **Jeremy P Koelmel**, Emma E Rennie, Michael Kummer, Bernard Brooks, Sheng Liu, Carrie A McDonough, Emily Parry, David Godri, Jacqueline Bangma, Nandarini Abril, John A Bowden, Krystal J Godri Pollitt. Comprehensive Coverage of Both Known and Unknown PFAS in Ocean, Leachate, and Lake Foam using Non-Targeted Analysis and FluoroMatch 3.0. SETAC Europe 33rd Annual Meeting (2023)

67. Bowden, J.A., Koelmel, J.P., and Aristizabal-Henao, J.J. An Introduction to Lipidomic Workflows. ASMS Workshops (2022)

66. **Koelmel, J.P.**, Weil, D., Stelben, P., Godri, D., Qi, J., Rennie, E.E., Lin, E.Z., Bowden, J.A., McDonough, C.A., Post, D., Godri Pollitt, K.J. Novel Algorithms and Visualizations for Discovering Polymers and Chemical Series in Industrial and Environmental Applications. ASMS (2022)

65. **Koelmel, J.P.**, Environmental Exposures and Cancer: Novel Software for Screening Thousands of Per- and Polyfluoroalkyl Substances (PFAS) in Biological Matrices. CPC Fellows Meeting (2022)

64. *__Koelmel, J.P.__, Uncommonly Screened PFAS are Everywhere; Answering the Need for Non-Targeted PFAS Analysis with FluoroMatch, Delaware Valley Mass Spectrometry Discussion Group (2022)

63. **Koelmel, J.P.**, Stelben, P., McDonough, C.A., Godri, D., Qi, J., Lin, E.Z., Williams, A.J., Bowden, J.A., Rennie, E.E., Godri Pollitt, K.J. Comprehensive Annotation and Validation of PFAS and PFAS transformation Products Using FluoroMatch Software and Interactive LC-HRMS/MS Visualizations, SETAC NTA (2022)

62. **Koelmel, J.P.**, Stelben, P., McDonough, C.A., Aristizabal-Henao, J.J., Bowden, J.A., Godri Pollitt, K.J. FluoroMatch: The First Software for Processing and Visualizing Non-Targeted PFAS Datasets, Agilent University Relations Fair (2022)

61. **Koelmel, J.P.**, Stelben, P., McDonough, C.A., Rennie, E.E., Boweden, J.A., and Pollitt, K.J., Non-targeted PFAS analysis: Challenges and Successes using FluoroMatch Software, Agilent Post-ASMS webinar (2021)

60. Pollitt, K.J., **Koelmel, J.P.**, Stelben, P., Nason, S., Lin, E., Rennie, E.E., Pyke, J., Bowden, J.A. Challenges and Progress in Software Development for Non-Targeted PFAS Analysis, AGU (2021)

59. Stelben, P., **Koelmel, J.P.**, McDonough, C.A, Dukes, D.A., Henao, J.J., Nason, S.L., Li, Y., Sternberg, S., Lin, E., Beckmann, M., Williams, A.J., Draper, J., Finch, J., Deigl, C., Rennie, E.E., Bowden, J.A., Pollitt, K.J., FluoroMatch: A Non-Targeted Approach to Per- and Polyfluoroalkyl Substances (PFAS). SETAC (2021)

58. **Koelmel, J.P.**, Lin, E.Z., Guo, P., Stelben, P., Zhou, J., Delay, K., Williams, A.J., Zhou, Y., Bornman, R., Obida, M., Chevrier, J., Shi, X., Tang, S., Pollitt, K.J., Exploring Personal Chemical Exposure Profiles of Vulnerable Populations in Emerging Economies using State of the Art Passive Sampling, Instrumentation, and Software. SETAC (2021)

57. Stelben, P., **Koelmel, J.P.**, McDonough, C.A., Dukes, D.A., Aristizabal-Henao, J.J., Nason, S., Li, Y., Sternberg, S., Lin, E., Beckmann, M., Williams, A.J., Draper, J., Finch, J., Deigl, C., Rennie, E.E., Bowden, J.A., and Godri Pollitt, K.J. The First Comprehensive Open-Source Software Dedicated to the Non-Targeted Analysis of Per- and Polyfluoroalkyl Substances for GC and LC-HRMS. ASMS (2021).

56. **Koelmel, J.P.**, Aristizabal-Henao, J.J., Ni, Z., Federova, M., Kato, S., Otoki, Y., Nakagawa, K., Lin, E.Z., Godri Pollitt, K.J., Guingab, J.D., Garrett, T.J., Williams, T.L., Stingl, U., Bowden, J.A., Vasiliou, V., and Penumetcha, M. Software Solutions and Diverse Applications of Redox Lipidomics – Detecting Universal Markers of Stress. ASMS (2021).

55. Johnson E, Lin EZ, Okeme J, Stelben P, **Koelmel JP**, Godri Pollitt KJ. Capturing Personal Exposures to Airborne PFAS using Wearable Passive Samplers. FLUOROS Global 2021 Annual Conference. Oral Presentation, Providence, RI. October 2021.

54. Lin EZ, Nason SL, Zhong A, **Koelmel JP**, Godri Pollitt KJ. Trace analysis of per- and polyfluorinated alkyl substances in dried blood spots and whole blood. FLUOROS Global 2021 Annual Conference. Poster, Providence, RI. October 2021.

53. Zhou Y, **Koelmel JP**, Lin EZ, Wang C, Hou M, Shi Y, Tang S, Godri Pollitt KJ. Targeted Analysis of PFAS in Household Dust in North China. FLUOROS Global 2021 Annual Conference. Poster, Providence, RI. October 2021.

52. Lin EZ, Nichols A, Zhou Z, **Koelmel JP**, Godri Pollitt KJ. Characterizing the external exposome using passive air samplers – comparison of chemical exposures using different wearable form factors. International Society of Exposure Science (ISES). Oral Presentation, Virtual Meeting. August 2021.

51. Lin EZ, Guo P, Xiao J, Hagan C, **Koelmel JP**, Tseng W-L, Liew Z, Godri Pollitt KJ.The impact of COVID-19 stay-at-home orders on personal chemical exposures. International Society of Exposure Science (ISES). Poster, Virtual Meeting. August 2021.

50. DeLay K, Lin EZ, **Koelmel JP**, Bornman R, Obida M, Chevrier J, Godri Pollitt KJ. Personal air pollutant exposure monitoring in South African children participating in the VHEMBE study. International Society of Exposure Science (ISES). Oral Presentation, Virtual Meeting. August 2021.

49. Stelben, P., **Koelmel, J.P.**, 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., Deigl, C., Rennie, E.E., Bowden, J.A., and Godri Pollitt, K.J. FluoroMatch: A Comprehensive Software for Non-Targeted PFAS Analysis. ISEE (2021).

48. **Koelmel, J.P.**, Lin, E.Z., Guo, P., Stelben, P., Zhou, J., DeLay, K., Williams, A.J., Zhou, Y., Bornman, R., Obida, M., Chevrier, J., Shi, X., Tang, S., and Godri Pollitt, K.J. Personal external exposomes from around the world. ISEE (2021).

47. Pollitt, K., and **Koelmel, J.P.**, 50 chemical exposures of concern discovered using wearable passive samplers and gas chromatography high-resolution mass spectrometry in South African children. ISEE (2021).

46. ***Koelmel, J.P.**, Stelben, P., Pollitt, K., and Bowden, J.A., Identification of Non-Targeted PFAS using FluoroMatch – Progress and Limitations. Waters Virtual Seminar (2021).

45. ***Pollitt, K.**, **Koelmel, J.P.**, GC-Orbitrap and Sensors to Capture the Exposome. Columbia Exposome Bootcamp (2021).

44. ***Koelmel, J.P.**, Stelben, P., Rennie, E., Pollitt, K., and Bowden, J.A., FluoroMatch 2.0 Software – Realizations from Automating the PFAS Non-Targeted Workflow. BP4NTA July Meeting (2021).

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

42. Tan WY, **Koelmel JP**, Li Y, Bowden JA, Ahmadireskety A, Patt AC, Orlicky DJ, Mathé E, Kroeger NM, Cochran JA, Golla JP, Kandyliari A, Chen Y, Charkoftaki G, Godri Pollitt KJ, Cagmat JG Tsugawa H, Arora A, Veselkov K, Yost RA, Thompson DC, Garrett TJ, Vasilou V. Lipidomics and redox lipidomics indicate early-stage alcohol-induced liver damage. 16th Annual Metabolomics 2020 Conference. Poster, Virtual Meeting. October 2020.

41. Lin EZ, Nichols A, Zhou Y, **Koelmel JP**, Godri Pollitt KJ. Contrasting personal chemical exposures using different wearable form factors. American Chemical Society (ACS) Spring Meeting. Virtual Meeting. Invited Oral Presentation. April 2021

40. Nason SL, **Koelmel JP**, Paige M, Aristizabal JJ, Stelben P, Bowden JA, Godri Pollitt KJ. Analysis of PFAS contaminated soil from Loring Airforce Base using iterative exclusion and FluoroMatch software. Society for Environmental Toxicology and Chemistry (SETAC) SciCon European Annual Conference. Oral Presentation. Virtual Meeting, May 2020.

39. Ganguly K, Thimraj TA, Nordström A, Ramström M, Lin EZ, O'Brien F, **Koelmel JP**, Ernstgård L, Johanson G, Godri Pollitt KJ, Palmberg L, Upadhyay S. Flavor, nicotine content and lung region matter: Alarm anti-proteases and anti-microbial defensins are important for electronic cigarette related pulmonary response. American Thoracic Society (ATS). Oral Presentation. Virtual Meeting. May 2020.

38. Upadhyay S, Rinaldi S, Thimraj TA, Lin EZ, O'Brien F, **Koelmel JP**, Ernstgard L, Johanson G, PA M, Godri Pollitt KJ, Palmberg L, Ganguly K. Assessment of Biomass Smoke Induced Pulmonary Response and the Protective Effect of Magnolol Using Physiologically Relevant Normal- and Chronic Bronchitis-like Bronchial Mucosa Models. American Thoracic Society (ATS). Poster. Virtual Meeting. May 2020.

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

36. **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).

35. ***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).

34. ***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)

33. **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)

32. **Koelmel JP**, Chen A, Aksenov, A, Lin EZ, O'Brien F, Zhou J, Ganguly K, Upadhyay S, Veselkov K, Godri Pollitt KJ. Automatically classifying airborne exposures using gas chromatography high resolution mass spectrometry of passive samplers, neural networks, and EPA compound databases. American Society for Mass Spectrometry Sanibel Conference: Unravelling the Exposome. Captiva Island, FL. January 2020.

31. Godri Pollitt KJ, **Koelmel JP**, Lin EZ, He J, Chen A, Aksenov A, Ganguly K, Upadhyay S, Chevrier J, Song T, Shi X. ChemCat Software – Automated Determination of Compound Source and Toxicity from GC-HRMS and LC-HRMS acquisition. American Society for Mass Spectrometry Sanibel Conference: Unravelling the Exposome. Captiva Island, FL. January 2020.

30. **Koelmel JP**, Lin EZ, He J, Chen A, Aksenov A, Tang S, Shi X, Godri Pollitt KJ. New informatics techniques for studying the exposome in large scale studies. NYC Exposome Symposium. New York, NY. March 2020.

29. Godri Pollitt KJ, Jobst K, Lin EZ, **Koelmel JP**, Cahill LS, Sled J. Top-down exposomics of persistent and bioaccumulative organics. Society of Environmental Toxicology and Chemistry (SETAC). Toronto, Canada. Speaker. November 2019.

28. Bowden JA, **Koelmel JP**, Lin EZ, Jobst K, DeStefano N, Godri Pollitt KJ. Toward Comprehensive PFAS Annotation using a Novel Software FluoroMatch for LC-HRMS/MS Data. SETAC. Toronto, Canada Poster. November 2019

27. **Koelmel JP**, Bowden JA, Lin EZ, Vasiliou V, Jobst K, Godri Pollitt KJ. Untargeted Annotation of PFAS using a novel software for gas chromatography positive chemical ionization high resolution tandem mass spectrometry. SETAC. Toronto, Canada Poster. November 2019.

26. Lin EZ, **Koelmel JP**, Seethapathy S, Godri Pollitt KJ. A wearable polydimethylsiloxane-based passive air pollutant sampling device: Development of calibration constants. SETAC. Toronto, Canada. Speaker. November 2019.

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

13. **Koelmel, J.P.**, Kummer, M., Godri, D., Stelben, P., Paige, M., Li, Y., Bowden, J.A., Renei, E., Pollitt, K. PolyMatch Suite. Languages: R, C#, Java, and PowerBI. Yale University and Agilent Technologies, 2024-current.

12. **Koelmel, J.P.**, Kummer, M., Godri, D., Stelben, P., Paige, M., Li, Y., Bowden, J.A., Renei, E., Pollitt, K. FluoroMatch Suite. Languages: R, C#, Java, and PowerBI. Yale University, University of Florida, and Agilent Technologies, 2021-current.

11. **Koelmel, J. P.**, Kroeger, N. M., Li, Y., Jason, C. A., Patt, A. C., Kroeger, N. M., Mathé, E., Garret, T. J. LipidMatch Suite. Language: C#, R, PowerBI. University of Florida & Yale University 2017-current.

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

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.

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

PATENTS

U.S. Patent 63/074,705 "Wearable Air Pollutant Monitoring Device" Provisional application filed September 4, 2020.
U.S. Patent 63/074,705 "Wearable Air Pollutant Monitoring Device" Non-Provisional filed September 3, 2021.

Professional Service

Journals

Reviewer, *Analytical Chemistry* (American Chemical Society, IF=8.0) (2016)
Reviewer, *Cell Systems* (Cell Press, IF=11.1) (2017)
Reviewer, *Analytical Chemistry* (American Chemical Society, IF=8.0) (2018)
Reviewer, *PLOS ONE* (PLOS, IF=3.7) (2019)
Reviewer, *Analytical Chemistry* (American Chemical Society, IF=8.0) (2019)
Reviewer, *Biomolecules* (MDPI, IF=5.5) (2020)
Reviewer, *Environmental Toxicology* (Wiley-Blackwell, IF=4.2) (2020)
Reviewer, *Nutrients* (MDPI, IF=5.7) (2020)
Reviewer, *Metabolites* ((MDPI, IF= 5.6) (2020)
Reviewer, *PLOS ONE* (PLOS, IF=3.7) (2020)
Reviewer, *PLOS ONE* (PLOS, IF=3.7) (2020)

Reviewer, *PLOS ONE* (PLOS, IF=3.7) (2020)
Reviewer, *Analytical Chemistry* (American Chemical Society, IF=8.0) (2021)
Reviewer, *Global Change Biology* (Wiley-Blackwell, IF= 11.6) (2021)
Reviewer, *Metabolites* (MDPI, IF= 5.6) (2021)
Reviewer, *Analytical Chemistry* (American Chemical Society, IF=8.0) (2021)
Reviewer, *Analytical Chemistry* (American Chemical Society, IF=8.0) (2021)
Reviewer, *Journal of the American Society for Mass Spectrometry* (ACS Publications, IF=3.2) (2021)
Reviewer, *Journal of the American Society for Mass Spectrometry* (ACS Publications, IF=3.2) (2021)
Reviewer, *Nature Communications* (Springer Nature, IF=16.6) (2022)
Reviewer, *Nature Methods* (Springer Nature, IF=48.0) (2022)
Reviewer, *Chemosphere* (Elsevier, IF=8.9) (2022)
Reviewer, *Journal of Proteome Research* (American Chemical Society, IF=5.3) (2022)
Reviewer, *Environmental science & technology letters* (American Chemical Society, IF=10.9) (2022)
Reviewer, *Environmental science & technology letters* (American Chemical Society, IF=10.9) (2022)
Reviewer, *Environmental Science & Technology* (American Chemical Society, IF=11.4) (2022)
Reviewer, *Nature Communications* (Springer Nature, IF=16.6) (2023)
Reviewer, *Journal of Exposure Science & Environmental Epidemiology* (Springer Nature, IF=6.371) (2023)

Organizations

Co-President, BP4NTA PFAS Sub-Committee. (2023-present)
ASMS (member) 2017-present
SETAC (member) 2021-present

Media

None

Grants and Awards (Academic)

Oracle for Research Project Award, Oracle award for substantial cloud credits for any research projects related to PFAS cloud computing and storage (2023)

Agilent's ASMS Steve Berger Travel Award Today, targeted to ambitious and promising researchers, including scientists and professors. ASMS (2023)

Best Oral Presentation, 17th Annual Workshop on Emerging High-Resolution
Mass Spectrometry and LC-MS/MS Applications in Environmental Analysis and Food Safety (2021)

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

Volunteer 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

Jeremy P. Koelmel
jeremy.koelmel@yale.edu

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

OTHER WORK AND VOLUNTEER EXPERIENCE

High School / Elementary Volunteer Science Teacher, Sarasota, FL (2023 – present)
- Taught all topics of High School Chemistry to 6 homeschool students
- Led students on project based-learning experiences covering scientific studies on climate change and water quality culminating in manuscripts and scientific presentations at well known conferences

Trainings, Global (2019 – present)
- Provide trainings on LipidMatch, FluoroMatch, and PolyMatch

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, Southeast 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

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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