# Anachem
# 2026 Symposium

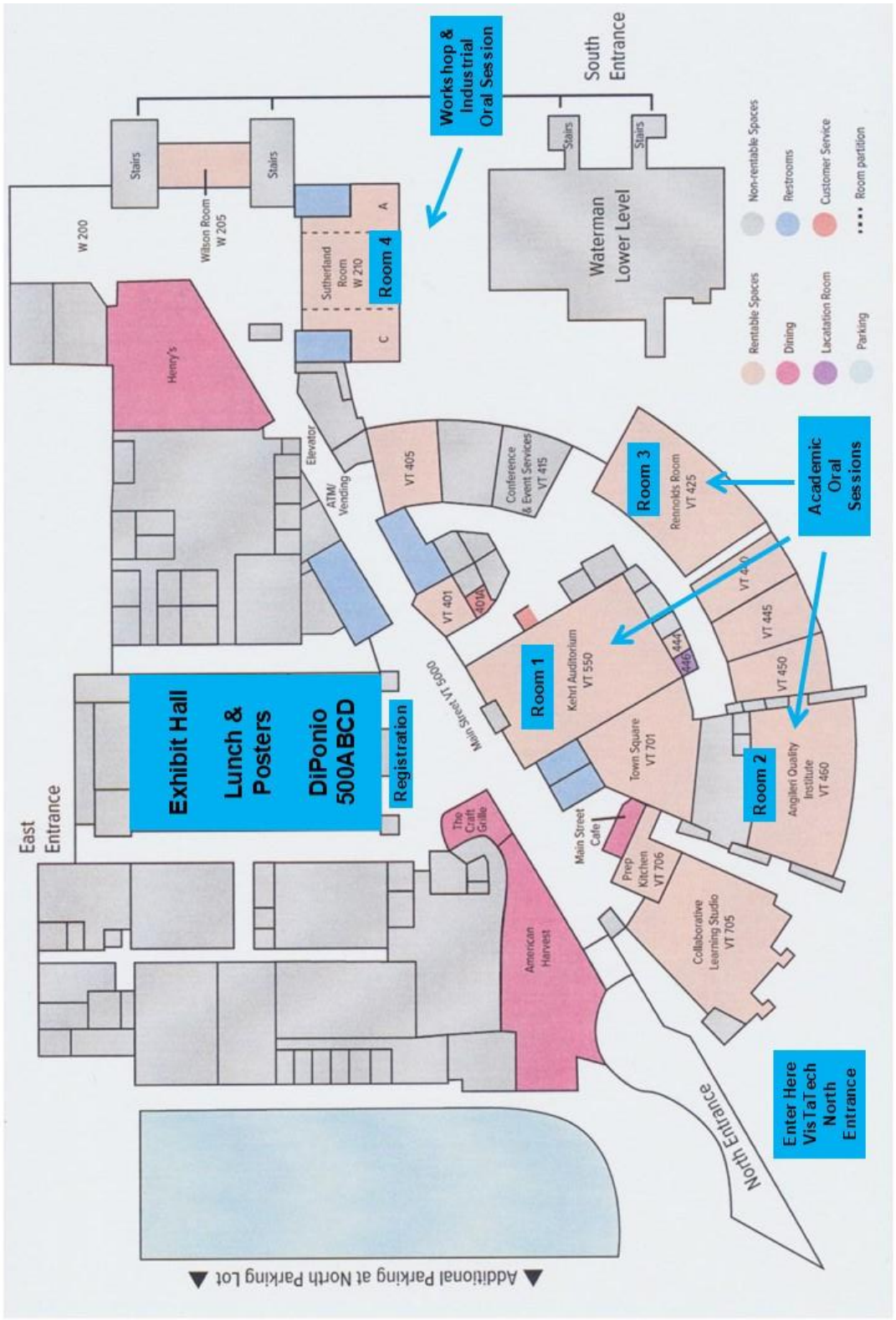
Anachem

Association of Analytical Chemists • Founded 1941

2026

VisTaTech Center
Schoolcraft College, Livonia, Michigan
November 5, 2026

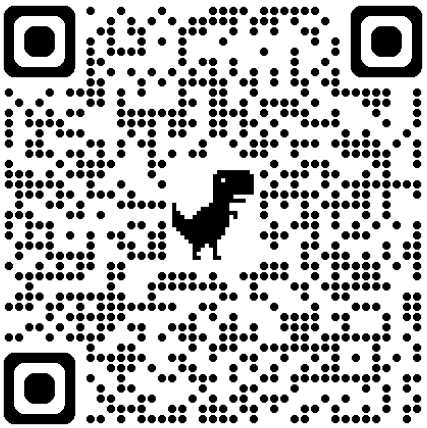
# SYMPOSIUM MAP AT SCHOOLCRAFT COLLEGE VISTATECH CENTER



# TECHNICAL PROGRAM - AT A GLANCE

| | Room 1<br>VT550 | Room 2<br>VT460 | Room 3<br>VT425 | Room 4<br>W210B |
|---|---|---|---|---|
| **Morning Session 8:30 – 10:30 AM** | **Anachem Award Session** | **Advances in Academic Research I** | **Anachem Perspectives** | **Educational Workshop** |
| **Plenary Session 11:30 AM – 12:30 PM** | **Kelsey D. Cook** | | | |
| **Afternoon Session 1:30 – 3:30 PM** | **Advances in Academic Research II** | **Advances in Academic Research III** | **Advances in Academic Research IV** | **Educational Workshop** |
| **Poster Session 3:30 – 5:00 PM Exhibit Hall DP500ABCD** | | | | |

Use the following QR-code to access a pdf version of the full program, which also includes abstracts and detailed contact information for the exhibitors.



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Use the following QR-code to complete an attendee survey.

# OUR PLENARY SPEAKER

## KELSEY D. COOK, Ph.D.

## 2026 ANACHEM AWARD RECIPIENT



## Kelsey D. Cook

**University of Tennessee, Knoxville (Professor Emeritus)**
**National Science Foundation (Retired)**

Kelsey Cook is a native of Denver Colorado, where he earned a BA (Magna cum Laude) in Chemistry from Colorado College (1974). He pursued a PhD in analytical chemistry with Jim Taylor at the University of Wisconsin – Madison (1978), investigating hydrogen bonding interactions using a supersonic molecular beam/photoionization mass spectrometer. He commenced his independent academic career at the University of Illinois – Champaign/Urbana in 1978 (where he was a Fellow in the Center for Advanced Studies), and moved to the University of Tennessee – Knoxville in 1984, where he collaborated extensively with colleagues at nearby Oak Ridge National Laboratory. In Illinois and Tennessee, he directed thesis research of 17 PhD and 9 MS students, studying research on mass spectrometric ionization mechanisms, with applications in process, polymer, and bioanalytical chemistry. This work resulted in 85 publications in respected journals, including *Analytical Chemistry*, *Proceedings of the National Academy of Sciences*, *Journal of the American Chemical Society*, and *Journal of the American Society for Mass Spectrometry*.

In Tennessee, he co-founded the East Tennessee Mass Spectrometry Discussion Group, co-chaired the 1999 Southeast Regional ACS Meeting, and directed the NSF Measurement and Control Engineering Center and an NSF Research Site for Educators in Chemistry. He also served as chair of the local section of the American Chemical Society (ACS), treasurer of the American Society for Mass Spectrometry (ASMS), and co-chair of the Council for Chemical Research's Action Network on Research Collaboration. He is a member Phi Beta Kappa and Sigma Xi; a 50-year member of ACS and ASMS; and a Fellow of the American Association for the Advancement of Science. He served as a founding Associate Editor of the ASMS Journal (1989 – 2016).

He began a second career at the National Science Foundation in 2006, serving first a 2-year term as a rotator in the Analytical and Surface Chemistry program (Division of Chemistry), then returning as a permanent Federal employee in 2009 to lead the Chemical Measurement and Imaging (CMI) program. At NSF, he served details as a Senior Policy Analyst at the White House Office of Science and Technology Policy (2011-12); a Staff Associate in the Office of the Assistant Director for Mathematical and Physical Sciences (2012-13); and Acting Section Head for International Science and Engineering (2013-14). In the year of Dr. Cook's retirement (2024), the CMI active award portfolio totaled over $90 million, of which he had direct responsibility for nearly $36 million and 85 awards (including the NeXUS laser at Ohio State), and managed new expenditures totaling over $20 million, including over $3 million in co-funding received from other programs across the Foundation. He received special recognition at NSF for efforts in leading and coordinating a new cross-cutting science initiative in biotechnology; dedication and unyielding perseverance that led to the successful inauguration of the CHE Mid-scale Program; efforts relevant to inter- and intra-agency collaboration; and for exceptional service on the Council for Financial Assistance Reform.

# ANACHEM AWARD

The Anachem Award was established in 1953 and is presented annually to an outstanding analytical chemist for teaching, research, administration or other activity which has advanced the art and science of the field. The Award was presented as a part of the Anachem Conference through 1972. From 1973 to 2022, the Anachem Award was presented at the National FACSS SciX meeting as a part of a special symposium arranged and given by former students and colleagues honoring the recipient. Since 2024, the Anachem Award has been presented at the annual Anachem Symposium. At each Symposium, the recipient delivers the Plenary Address, and an Award Session is held in honor of the recipient.

# CALL FOR NOMINATIONS for the 2027 ANACHEM AWARD

Members of the Anachem community are invited to nominate individuals for the 2027 Anachem Award. Please visit the Anachem website awards page for complete eligibility, submission, and award-selection information.

## https://www.anachem.org/awards

Deadline for nominations is January 15, 2027

# ANACHEM AWARD 1953-2026

| | | | |
|---|---|---|---|
| 1953 | Hobart H. Willard | 1990 | Janet Osteryoung |
| 1954 | M. G. Mellon | 1991 | Ben S. Freiser |
| 1955 | No Awardee | 1992 | Milos V. Novotny |
| 1956 | William Fredrick | 1993 | Richard Nyquist |
| 1957 | Philip J. Elving | 1994 | Joseph A. Caruso |
| 1958 | Charles Gambrill | 1995 | George G. Stafford |
| 1959 | G. Frederick Smith | 1996 | James Jorgenson |
| 1960 | Harry A. Bright | 1997 | Michael Morris |
| 1961 | I. M. Kolthoff | 1998 | Lloyd Snyder |
| 1962 | Paul K Winter | 1999 | Steve Stein |
| 1963 | AA. Benedetti-Pichler | 2000 | Robert S. Houk |
| 1964 | Lawrence Hallett | 2001 | Charles C. Sweeley |
| 1965 | John Hague | 2002 | Bruce Chase |
| 1966 | Harvey Diehl | 2003 | Catherine Fenselau |
| 1967 | Ralph G. Smith | 2004 | Walter Jennings |
| 1968 | Eugene Sawicki | 2005 | Mary J. Wirth |
| 1969 | Sidney Siggia | 2006 | Richard Sacks |
| 1970 | Vernon Stenger | 2007 | Isiah Warner |
| 1971 | Velmer Fassel | 2008 | Scott McLuckey |
| 1972 | Charles Reilly | 2009 | E. Neil Lewis |
| 1973 | Rosalyn Yallow | 2010 | Marc Porter |
| 1974 | John Mitchell Jr. | 2011 | Robert B. Cody |
| 1975 | David F. Boltz | 2012 | Peter R. Griffiths |
| 1976 | John Vandenbelt | 2013 | Norman J. Dovichi |
| 1977 | Richard Hahn | 2014 | David E. Clemmer |
| 1978 | Jeannette Grasselli | 2015 | Jonathan V. Sweedler |
| 1979 | J. J. Kirkland | 2016 | Paul Cremer |
| 1980 | James Winefordner | 2017 | Jennifer Brodbelt |
| 1981 | Walter McCrone | 2018 | Susan Lunte |
| 1982 | James Shoolery | 2019 | Robert T. Kennedy |
| 1983 | Roger Bates | 2020 | Gary J. Blanchard |
| 1984 | Gary Hieftje | 2021 | Mark E. Meyerhoff |
| 1985 | Fred M. McLafferty | 2022 | Joseph A. Loo |
| 1986 | Henry Freiser | 2024 | Facundo M. Fernandez |
| 1987 | Howard Malmstadt | 2025 | Mary T. Rodgers |
| 1988 | Walter Slavin | **2026** | **Kelsey D. Cook** |
| 1989 | Harry L. Pardue | | |

# Anachem Symposium Student Awards

Awards will be given to students for excellence in oral and poster presentations. A panel of judges will be on hand to evaluate the presentations.

**Best Student Oral Presentations - *Sponsored by Anachem and GFM LLC.***

A $100 prize will be awarded to the best oral presentation by a graduate student in each Academic Research session:

Advances in Academic Research I
Advances in Academic Research II
Advances in Academic Research III
Advances in Academic Research IV

**Best Graduate Student Posters - *Sponsored by SCIEX and SHIMADZU.***

A $100 prize will be awarded given to the four best posters presented by a graduate student.

**Best Undergraduate Student Posters - *Sponsored by JASCO.***

A $100 prize will be awarded to the two best posters presented by an undergraduate student.




# Exhibitors Hall and Raffle Ticket Drawing

**Win one of three $25 Amazon gift cards.**
**Increase your chances of winning by visiting the exhibitors.**

1) Upon registration at the desk, you will get a pair of matching tickets. Place one of the tickets in the "lottery bucket" in the exhibit hall. Keep the matching ticket for the drawings.
2) Obtain additional tickets by visiting exhibitors. They will give you a matched pair of tickets after a visit (please, only one pair per exhibitor). Place one of the matched pair in the lottery bucket and keep the other one for the drawings.

**Winning tickets will be drawn during lunch and the poster session/social hour.**

## Winners must be present to win. Good Luck!

# TECHNICAL PROGRAM

**8:30 – 10:30 AM** **MORNING SESSIONS –**

**ROOM 1 (VISTATECH 550)**
**ROOM 2 (VISTATECH 460)**
**ROOM 3 (VISTATECH 425)**
**ROOM 4 (SUTHERLAND, W210B)**

## ANACHEM AWARD SESSION HONORING KELSEY D. COOK

*Moderators: Mary T. Rodgers, Wayne State University, Detroit, MI*
*and Paul W. Bohn, University of Notre Dame, Notre Dame, IN*

Room 1 (VistaTech 550)

**8:30 AM: Hierarchically-Organized Electrochemical-Photonic Nanostructures for Studies of Single Entities - Molecules, Particles, and Cells**
*Paul W. Bohn*
*Department of Chemistry & Biochemistry, University of Notre Dame, Notre Dame, IN 46556*, *Department of Chemical & Biomolecular Engineering, University of Notre Dame, Notre Dame, IN 46556*

**9:00 AM: NSF NeXUS: A New Model for Accessing the Frontiers of Ultrafast Science**
*L. Robert Baker*
*The Ohio State University, Columbus, OH 43210*

**9:30 AM: Nanobubble Enhanced Electrospray Ionization Mass Spectrometry**
*Andre R Venter, George Joseph, Bincy Binny*
*Department of Chemistry, Western Michigan University, Kalamazoo, MI 49008*

**10:00 AM: Chromatographic Approaches to Improving Identification and Estimation of Number of Compounds present in the Metabolome and Industrial Samples**
*Robert T. Kennedy*
*Department of Chemistry, University of Michigan, Ann Arbor, MI 48109*

**ADVANCES IN ACADEMIC RESEARCH I**
*Moderator: Marwa Abdel Latif, University of Detroit, Mercy Detroit, MI*
*Judge: Kate Lanigan, University of Detroit Mercy, Detroit, MI*
Room 2 (VistaTech 460)

**8:30 AM: Characterization of Insulin Degradation Products Using Thermal Gel Electrophoresis Coupled to Particle Motion Tracking**
*John A. Tetteh, Thomas H. Linz*
*Department of Chemistry, Wayne State University, Detroit, MI 48202*

**8:50 AM: Creating Scalable Multichannel Boron Doped Diamond Microelectrodes for Neurochemical Measurement**
*James R. Siegenthaler[1,2], Niko Siratskiy[1], Pramod Gupta[1], Luke Suter[1], Bhavna Gupta[3], Mason L. Perillo[4], Michael F. Becker,[1] Erin K. Purcell[2,3,4], and Wen Li[1,2,4]*
*[1]Fraunhofer USA Center Midwest, Coatings and Diamond Technologies Division, East Lansing, MI 48824; [2]Department of Electrical and Computer Engineering, Michigan State University, East Lansing, MI 48824; [3] Neuroscience Program, Michigan State University, East Lansing, MI 48824; [4]Department of Biomedical Engineering and Institute for Quantitative Health Science and Engineering, East Lansing, MI 48824*

**9:10 AM: Integrated Bottom-Up and Top-Down CE-MS Reveals Kinase-Specific Phosphorylation and Proteoform Remodeling of Tau441**
*Reyhane Tabatabaeian Nimavard, Jorge A. Colón Rosado, Seyed Amirhossein Sadeghi, Yifan Yue, Fei Fang, Guijie Zhu, Guangyao Gao, Lance Thorp, and Liangliang Sun*
*Department of Chemistry, Michigan State University, East Lansing, MI 48824*

**9:30 AM: Developing a Framework for the Structural Characterization of RNAs Using Analytical Ultracentrifugation**
*Alec Garasimowicz[1,2], Ethan Dixon[1], Martin O'Steen[1], Sarah Keane[1,2]*
*[1]Department of Chemistry, University of Michigan, Ann Arbor, MI 48109, [2]Department of Biophysics, University of Michigan, Ann Arbor, MI 48109*

**9:50 AM: Utilization of a Chlorine Oxidation Flow Reactor for the Discovery of Novel Chlorinated Compounds**
*Gergana M. Milkova[1], Claire M. Thomson[1,2], Kathryn D. Kulju[1], Daun Jeong[1,3], Andrew R. Jensen[1,4], Graham O. Frazier[1,5], Nicole Woodall[1], Jordan E. Krechmer[6,7], Brian M. Lerner[6], Paul M. Zimmerman[1], Andrew T. Lambe[6,8], Kerri A. Pratt[1]*
*[1]Department of Chemistry, University of Michigan, Ann Arbor MI 48109*

**10:10 AM: Quantifying Electrochemically Accessible Primary Amines on Ammonia Plasma-Treated Boron-Doped Diamond Electrodes**
*Ruben Levy-Guiance[1], Pramod K. Gupta[1], Aaron I. Jacobs[1], Rebecca Anthony[1,2], James Siegenthaler[1,3]*
*[1]Fraunhofer USA Center Midwest, Coatings and Diamond Technologies Division, East Lansing, MI 48824;[2]Department of Mechanical Engineering, Michigan; State University, East Lansing, MI 48824; [3]Department of Electrical and Computer Engineering, Michigan State University, East Lansing, MI 48824*

**ANACHEM PERSPECTIVES:**

**Where it All Started: How Anachem Shaped Our Careers**

*Moderator: Matthew J. Fhaner, University of Michigan, Flint, MI*

Room 3 (VistaTech 425)

**Abstract:**
Regional conferences play a vital role in launching scientific careers by providing students with early opportunities to present their work, build professional networks, and gain confidence as communicators. For many local analytical chemists, ANACHEM offered a first chance to present research beyond their research team and home institution.

This session will share personal reflections on how participation in regional conferences fostered professional connections and career growth. Through these different perspectives, we aim to emphasize the importance of regional scientific meetings for early-career scientists to become the next generation of analytical chemists.

**8:30 AM: A Curiosity-Driven Approach to Research in an Academic Setting**
*Colin F. Poole*
*Department of Chemistry, Wayne State University, Detroit, MI 48202*

**9:00 AM: Opening Doors Through Anachem: From Graduate School to Industry**
*David A. Bolliet*
*Analytical R&D Department, Kalsec, Kalamazoo, MI 49006*

**9:30 AM: More Than the Science: How Communication Skills Create Career Opportunities**
*Rena Pomaville*
*Tsunagari Services, Inc, Brighton, MI 48116*

**10:00 AM: Learning on the Job and in Scientific Communities: How Building Networks Can Lead to the Unexpected**
Donna Seibert
*Expreris/Pfizer Consultant, Groton, CT 06340*

**EDUCATIONAL WORKSHOP**
*Presenter: Ryan Smith, Thermo Fisher Scientific, USA*

Room 4 (Sutherland Room, W210B)

**8:30 – 10:30 AM: From Fundamentals to Applications: Practical FT-IR, FT-NIR and IR Microscopy**



**Who Should Attend:**
This session is designed for scientists and laboratory professionals who are new to FT-IR or FT-NIR spectroscopy as well as experienced spectroscopists interested in expanding their understanding of alternative sampling techniques, IR microscopy, and complementary infrared analytical approaches.

**Abstract:**
Infrared spectroscopy offers a versatile range of analytical approaches for material identification, characterization, and quantitative analysis. This session will introduce the fundamentals of FT-IR and FT-NIR spectroscopy while focusing on practical considerations for selecting the appropriate technique and sampling approach for different analytical challenges. Attendees will explore common FT-IR sampling techniques and representative applications, along with the use of IR microscopy for the analysis of small particles, defects, contaminants, and other microscale samples. The session will also introduce FT-NIR spectroscopy, compare common NIR sampling approaches, and highlight applications where NIR can provide rapid, non-destructive analytical measurements. Through practical examples, attendees will gain a better understanding of the capabilities of FT-IR, FT-NIR, and IR microscopy and how to select the appropriate technique for their analytical needs.

**Topics**
- Fundamentals of infrared spectroscopy
- FT-IR sampling techniques and selection considerations
- Practical FT-IR applications
- IR microscopy techniques and applications
- Fundamentals of near-infrared spectroscopy
- FT-NIR sampling techniques and selection considerations
- Practical FT-NIR applications (laboratory and process analytical)
- Selecting the appropriate IR technique for different analytical challenges

**Biography:**
Ryan Smith is a Senior Applications Scientist at Thermo Fisher Scientific specializing in FT-IR and FT-NIR spectroscopy. He earned his Ph.D. in Chemistry from the University of Iowa, where his research focused on the use of terahertz time-domain spectroscopy for quantitative vapor analysis. Ryan has extensive experience developing qualitative and quantitative methods using near-infrared, mid-infrared, and Raman spectroscopy, with experience spanning R&D, applications development, and technical sales support.

| | |
|---|---|
| **10:30 – 11:20 AM** | **BREAK – EXHIBIT HALL (DIPONIO, 500ABCD)** |
| **11:30 AM – 12:30 PM** | **PLENARY LECTURE – ROOM 1 (VistaTech 550)** |

## PLENARY LECTURE BY THE 2026 ANACHEM AWARD RECIPIENT

# KELSEY D. COOK

*University of Tennessee, Knoxville (Emeritus); National Science Foundation (Retired)*

*Moderators:*

*Stephen C. Gibson, US Environmental Protection Agency, Ann Arbor, MI and Bill Boggess, University of Notre Dame, Notre Dame, IN*

Room 1 (VistaTech 550)

**11:30 AM: My Careers in Science: From Lincoln High to the White House**
*Kelsey D. Cook, University of Tennessee, Knoxville, Knoxville, TN (Emeritus); National Science Foundation, Alexandria, VA (Retired).*

| | |
|---|---|
| **12:30 – 1:30 PM** | **LUNCH – EXHIBIT HALL (DIPONIO, 500ABCD)** |
| **1:30-3:30 PM** | **AFTERNOON SESSIONS – ROOMS 1 –4** |

**ADVANCES IN ACADEMIC RESEARCH II**
*Moderator: Dragan Isailovic, University of Toledo, Toledo, OH*
*Judge: Mary T. Rodgers, Wayne State University, Detroit, MI*

Room 1 (VistaTech 550)

**1:30 PM: Immobilized Metal Affinity Beads for Recombinant Protein Analysis by Desorption Electrospray Ionization Mass Spectrometry**
*Christopher Taylor, Andre Venter*
*Department of Chemistry, Western Michigan University, Kalamazoo, MI, 49008*

**1:50 PM: Capillary Zone Electrophoresis-Mass Spectrometry Is Ready for Reproducible Multi-level Proteomics**
*Guijie Zhu[1], Yifan Yue[1], Jorge A Colón Rosado[1], Guangyao Gao[1], Xiaowen Liu[2], Liangliang Sun[1]; [1]Department of Chemistry, Michigan State University, East Lansing, MI 48824; [2]Deming Department of Medicine, Tulane University School of Medicine, New Orleans, LA 70112*

**2:10 PM: Development Towards a Multilayer Microfluidic Paper Analytical Device for the Early Prediction of Severe Acute Pancreatitis**
*Ruth Speidel[1], Peter Lee[2], Sophie Miller[1], Alyssa Perez[1], Samuel Huttner[1], Goergios Papachristou[2], Abraham Badu-Tawiah[1]*
*[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [2]Division of Gastroenterology, Hepatology, and Nutrition, Department of Internal Medicine, The Ohio State University Wexner Medical Center, Columbus, OH*

**2:30 PM: Biphasic Reactivity Enables Tunable Electrolyte and Heavy Metal Detection in Droplet Microfluidics**
*Camila Gonzalez Curbelo, Ayush Chitrakar, and Ryan C. Bailey*
*Department of Chemistry, University of Michigan, Ann Arbor, MI 48109*

**2:50 PM: Multivariate Analysis of Volatile and Semi-volatile Organic Compounds in Water by Vacuum Assisted Headspace Solid-Phase Microextraction**
*Temitope Alonge,[1,2] Alja Contala,[1,2] Emanuela Gionfriddo,[3] and Jon R. Kirchhoff[1,2]*
*[1]Department of Chemistry and Biochemistry, The University of Toledo, Toledo, OH, 43606, [2]Dr. Nina McClelland Laboratory for Water Chemistry and Environmental Analysis, Department of Chemistry and Biochemistry, The University of Toledo, Toledo, OH, 43606, [3]Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY, 14260*

**3:10 PM: Electrochemical Immunosensors for Non-Invasive Monitoring of Lung Cancer and Heart Failure**
*Erfan Omid Najafabadi, Greg M. Swain*
*Department of Chemistry, Michigan State University, East Lansing, MI 48824*

**ADVANCES IN ACADEMIC RESEARCH III**
*Moderator: Thomas Linz, Wayne State University, Detroit, MI*
*Judge: Ruth Ann Armitage, Eastern Michigan University, Ypsilanti, MI*
Room 2 (VistaTech 460)

**1:30 PM: Ambient Ionization Mass Spectrometry for Detection of RNA Biomarkers and Disease Diagnostics**
*Anju Sheregar[1], Rachel M. Robertson[1,2], Ayesha Seth[1], Keerthana Ravi[1], Adom Amparbeng[1], Venkat Gopalan[1,2], Abraham Badu-Tawiah[1]*
*[1]Department of Chemistry and Biochemistry, [2]Center for RNA Biology, The Ohio State University, Columbus, OH 43210*

**1:50 PM: Structural and Energetic Effects of Nucleobase Methylation on Guanosine Nucleosides: IRMPD, ER-CID, and Theoretical Studies**
*Bijoy Krishna Roy[1], N. M. R. Frieler[1], Giel Berden[2], M. T. Rodgers[1]*
*[1]Department of Chemistry, Wayne State University, Detroit, MI 48202, [2]Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Toernooiveld 7, 6525 ED, Nijmegen, The Netherlands*

**2:10 PM: Investigation of Halogen Oxidation of Toluene using a Novel Oxidation Flow Reactor Coupled to a Reagent Ion Switching Chemical Ionization Time-of-Flight Mass Spectrometer (CI-TOF-MS)**
*Anya C. Romig[1], Andrew T. Lambe[2], Kerri A. Pratt,[1]*
*[1]Department of Chemistry, University of Michigan, Ann Arbor, MI 48109; [2]Now at Entegris Inc., Bedford, MA 01821*

**2:30 PM: Single-sample Calibration Based on Experimental Multiple Isotopologues and Charge-state Ion Ratios for Quantitative LC–MS/MS Analysis of Cyanotoxins**
*Yohan C. Y. Sudusingha, Dragan Isailovic*
*Department of Chemistry and Biochemistry, University of Toledo, Toledo, OH 43606*

**2:50 PM: Electropolymerized *p*-Aminobenzoic Acid on Boron-Doped Nanocrystalline Diamond for Label-Free Electrochemical Detection of PfHRP-2**
*Pramod K. Gupta[1], Ruben Levy[1], Aaron I. Jacobs[1], James R. Siegenthaler[1,2]*
*[1]Coatings and Diamond Technologies Division, Fraunhofer USA Center Midwest, East Lansing, MI 48824; [2]Department of Electrical and Computer Engineering, Michigan State University, East Lansing, MI 48824*

**3:10 PM: Multi-omic Evaluations of Nanodiscs Incorporating Blood Coagulation Membrane Proteins**
*Anusha Vajrala, Hanyu Zheng, Michael Armbruster, Brandon Ruotolo, Ryan C. Bailey*
*Department of Chemistry, University of Michigan, Ann Arbor, MI 48104*

**ADVANCES IN ACADEMIC RESEARCH IV**
*Moderator: Colin F. Poole, Wayne State University (Emeritus), Detroit MI*
*Judge: Kendra Evans, University of Detroit Mercy, Detroit, MI*

Room 3 (VistaTech 425)

**1:30 PM: Novel Gas Chromatography - Chemical Ionization Mass Spectrometry Measurements of Volatile Organic Compounds in an Arctic Oilfield**
*Anthony J. Rovinski[1], Andrew R. Jensen[1,2], Frozan Tahiry[1], Daun Jeong[1,3], Nicole Woodall[1], Kathryn D. Kulju[1], Jordan E. Krechmer[4,5], Brian M. Lerner[4], Megan S. Claflin[4], Andrew T. Lambe[4,6], Kerri A. Pratt[1] [1]Department of Chemistry, University of Michigan, Ann Arbor, MI 48109; [2]Now at Department of Chemistry and Biochemistry, Kalamazoo College, Kalamazoo, MI 49006; [3]Now at NOAA Chemical Sciences Laboratory, Boulder, CO 80305; [4]Aerodyne Research, Inc, Billerica, MA 01821; [5]Now at Osmo Labs, PBC, Somerville, MA; [6]Now at Entegris Inc., Bedford, MA 01730*

**1:50 PM: Resonance-Enhanced, Label-Free Detection in Free Solution using Droplet Microfluidic Gratings**
*Hannah H. Morris, Lindsay J. Heagle, Diana C. Weiland, Ryan C. Bailey*
*Department of Chemistry, University of Michigan, Ann Arbor, MI 48197*

**2:10 PM: Correlating Internal miRNA and External Protein from Individual Small Extracellular Vesicles with Digital-Quantitative-PCR**
*Rebecca K. Partee, Brice C. Vanness, Thomas H. Linz,*
*Department of Chemistry, Wayne State University, Detroit, MI 48202*

**2:30 PM: Cyclic Voltammetric Studies of Boron-Doped Diamond Microelectrodes**
*Grace E. Leahey, Greg M. Swain*
*Department of Chemistry, Michigan State University, East Lansing, MI 48824*

**2:50 PM: Fluorescence-Based Photothermal Infrared Spectroscopy Methods for the Single-Particle Detection of Aerosolized Microplastics and Nanoplastics**
*Randi Libin-Straub, Wilson Chen, Abbygail M. Ayala, Andrew P. Ault*
*Department of Chemistry, University of Michigan, Ann Arbor, MI 48109*

**3:10 PM: Optimization of Digestion Protocols for Comprehensive Profiling of the Elemental Composition of Mount Etna Lava Ash.**
*Oluwaseun I. Akindumila[1,2], , Alja Čontala[1,2], Catherine Lu[3], Emanuela Gionfriddo[3], and Jon R. Kirchhoff[1,2]. [1]Department of Chemistry and Biochemistry, The University of Toledo, Toledo, OH, 43606, [2]Dr. Nina McClelland Laboratory for Water Chemistry and Environmental Analysis, Department of Chemistry and Biochemistry, The University of Toledo, Toledo, OH, 43606, [3]Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY 14260*

**EDUCATIONAL WORKSHOP**
*Presenter: Matt Gabel, Thermo Fisher Scientific, USA.*

Room 4 (Sutherland Room, W210B)

**1:30 – 3:30 PM: From Fundamentals to Applications: Practical Raman Spectroscopy and Microscopy**



**Who Should Attend:**
This session is designed for scientists and laboratory professionals who are new to Raman spectroscopy and microscopy, as well as experienced Raman users interested in expanding their understanding of confocal microscopy, Raman imaging, and alternative approaches to microscopic material characterization.

**Abstract:**
Raman spectroscopy is a powerful, non-destructive analytical technique for material identification, characterization, and microscopic analysis. This session will introduce the fundamentals of Raman spectroscopy while focusing on practical considerations for applying Raman microscopy to a variety of analytical challenges. Attendees will explore the principles of dispersive and confocal Raman microscopy, including how instrumental and experimental parameters influence spectral and spatial information. The session will also highlight Raman imaging and representative applications demonstrating how chemical and spatial information can be combined to characterize complex samples and materials. Through practical examples, attendees will gain a better understanding of the capabilities of Raman spectroscopy and microscopy, and how modern instrumentation and software can be used to efficiently collect, visualize, and interpret Raman data.

**Topics**
- Fundamentals of Raman spectroscopy
- Principles of dispersive and confocal Raman microscopy
- Practical considerations for Raman measurements
- Raman imaging and chemical visualization
- Applying Raman microscopy to material identification and characterization
- Representative Raman microscopy applications
- Modern Raman instrumentation and software (laboratory and process analytical)

**Biography:**
Matt is a Raman Applications Scientist at Thermo Fisher Scientific specializing in Raman spectroscopy and microscopy. He earned his Ph.D. in Physics from Washington State University, where his research focused on the ferroelectric properties of two-dimensional semiconductor materials. His expertise in vibrational spectroscopy expanding during his time as a visiting researcher at Pacific Northwest National Laboratory, where he investigated semiconductor materials using tip-enhanced Raman spectroscopy. His experience provides a strong foundation in applying advanced Raman techniques to materials characterization and microscopic analysis.

**3:30-5:00 PM POSTER SESSION – EXHIBIT HALL (DIPONIO, 500ABCD)**

# POSTER SESSION

# EXHIBITORS

# WINE AND CHEESE RECEPTION

# AWARDS PRESENTATIONS

**BEST STUDENT ORAL PRESENTATIONS**

**BEST GRADUATE STUDENT POSTER PRESENTATIONS**

**BEST UNDERGRADUATE STUDENT POSTER PRESENTATIONS**

# RAFFLE WINNERS

# ABSTRACTS

## Anachem Award Session Honoring Kelsey D. Cook

***University of Tennessee, Knoxville (Professor Emeritus); National Science Foundation (Retired)***

*Moderator: Paul W. Bohn, University of Notre Dame, Notre Dame, IN*

Room 1 (VistaTech 550)

### Hierarchically-Organized Electrochemical-Photonic Nanostructures for Studies of Single Entities - Molecules, Particles, and Cells

*Paul W. Bohn*

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Structurally regular nanopore arrays containing independently-controllable annular band nanoelectrodes are capable of manipulating optical field distributions and electrochemical potential in a single integrated nanoscale architecture. The special characteristics of these nanopore electrode arrays (NEAs) make it possible to address small collections of matter down to the single entity (molecule, particle, biological cell) level using spectroelectrochemistry. These capabilities are enabled by a transparent substructure that permits optical access to the interior of the nanopore, thus effectively trapping radiation in an ultrasmall volume inside the nanopore and permitting optical interrogation of the entities contained therein. The capabilities of NEAs can be extended by adding a self-organized block copolymer (BCP) layer capable of pH- and voltage-controlled transport gating, thus realizing hierarchically-organized BCP@NEA structures capable of high-sensitivity electrochemical characterization of single entities. Recent experiments have utilized these strategies to investigate the behavior of single enzymes (glutathione reductase, aldehyde dehydrogenase), single extracellular vesicles, and single copies of the pathogenic Gram-negative bacterium *Pseudomonas aeruginosa*. Importantly, these hierarchically-organized architectures make it possible to interrogate large parallel arrays of single entities simultaneously, so that population averages can be obtained while simultaneously capturing rare events that are normally missed in ensemble-average measurements.

### NSF NeXUS: A New Model for Accessing the Frontiers of Ultrafast Science

*L. Robert Baker*

*The Ohio State University, Columbus, OH*

At this award symposium in honor of Kelsey Cook, I will describe the frontier of ultrafast science and how this field is benefiting from the significant NSF investment in the National eXtreme Ultrafast Science Facility (NeXUS) where I serve as director. As the first Program Officer overseeing this Mid-scale Research Infrastructure project, Kelsey laid much of the groundwork for this NSF-sponsored, open-access user facility. At the heart of NeXUS is a new technology for high repetition rate, kilowatt-class lasers, and NeXUS is the first facility to translate this technology to the US. The combination of attosecond pulses, soft x-ray photon energies, and high repetition rate in a laboratory setting is enabling measurements that currently cannot be made anywhere

else in the world. Scientific challenges being addressed by this facility include the ability to efficiently capture and store sunlight using artificial systems mimicking the precision of natural photosynthesis and the ability to master information transport on the atomic scale to create new quantum information technologies. Accordingly, NeXUS meets a critical need in the US research landscape by providing an unprecedented view into the electron dynamics that underlay quantum information and energy conversion technologies, making this facility an invaluable national resource and a focal point for interdisciplinary collaboration in ultrafast science.

**Nanobubble Enhanced Electrospray Ionization Mass Spectrometry**

*Andre R Venter, George Joseph, Bincy Binny*
*Department of Chemistry, Western Michigan University, Kalamazoo, MI 49008*

Nanobubbles enriched solvent systems are easy to prepare and a powerful additive to improve analytical chemistry workflows for sample preparation, analysis, and microdroplet reactions. The use of nanobubble enriched solvent systems are demonstrated for electrospray ionization (ESI-MS), desorption-ESI (DESI), and nanospray-DESI (nanoDESI). Nanobubble-enriched solvent systems significantly enhance analyte ion signals and signal-to-noise (S/N) ratios for all studied analytes in both positive and negative ion modes. Ion suppression is also reduced for a two-component model system containing Rhodamine and caffeine. By simultaneously lowering LODs and increasing the limits of linearity, substantial increases in linear dynamic range are affected. Protein molecules unfold when nanobubbles are added to spray solvent systems reminiscent of electrothermal supercharging. This is demonstrated for cytochrome c, myoglobin, and ubiquitin, all of which also displayed substantial signal enhancement in their higher charge state ions. Chemical reactions, already accelerated in microdroplets, are further enhanced with the addition of nanobubbles, as reagent carriers, but also by catalytic interfacial effects. Carbon capture applications of accelerated chemical reactions will be highlighted. The effect sizes not only depend on solvent system but also on method of nanobubble generation. Nanobubbles produced by the novel flow regime switching method using a Tesla valve provided the largest increase in intensities, flowed by pressure cycling. Sonication did not cause protein unfolding, and also delivered lower signal enhancements compared to the other methods.

**Chromatographic Approaches to Improving Identification and Estimation of Number of Compounds present in the Metabolome and Industrial Samples**

*Robert T. Kennedy*
*Department of Chemistry, University of Michigan, Ann Arbor, MI 48109*

LC-MS methods have been critical for advancing metabolomics. A persistent finding has been that while many features, i.e. signals at a given m/z and retention time, are detected in complex samples using untargeted LC-MS, a relatively small number of metabolites are identified. For example, it is not uncommon to detect over $10^4$ features and identify only 200-500 compounds from MS/MS spectra. Further, often known significant compounds are not identified in the data sets. One reason for this is inability to acquire high quality MS/MS spectra. We have shown that combining several simple techniques like preconcentration, extended gradient times, iterative analysis, and multidimensional fractionation can dramatically increase the number of identified compounds. Using these approaches we identified over 2000 metabolites in plasma. A second issue is that many features are degenerate, i.e. they are the sample compound detected as different isotopes, adducts, or in-source decay. We have developed a lack of fit metric, which fits chromatographic features at a given retention time to identify degeneracies. This method is based on the concept that the same compound will give the same chromatographic peak shape

regardless of what species is detected in the mass spectrometer. Using this approach, we show dramatic reduction in the number of unknown (unannotated) features in biological samples. The same approach also reduced the number of unknowns in an analysis of contaminants in a polymer sample.

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## ANACHEM PLENARY LECTURE BY 2026 ANACHEM AWARD RECIPIENT KELSEY D. COOK

*Moderator: Stephen C. Gibson, US Environmental Protection Agency, Ann Arbor, MI*

Room 1 (VistaTech 550)

**"My Careers in Science: From Lincoln High to the White House"**

*Kelsey D. Cook*

*Department of Chemistry, University of Tennessee, Knoxville, TN (Emeritus); National Science Foundation, Arlington, VA (Retired)*

Born near the middle of the Baby Boom, the 2026 Anachem Awardee was subjected to a range of influences in following a slightly eccentric career path, uniformly guided by valuing contribution – his "north star." A Google search on characteristics of Boomers hits some labels dead on, such as "Workaholics & Career-Focused", "Company Loyalty", "Independent & Resilient", and "Altruism and Legacy". Others are less applicable to the 2026 Awardee, such as "Competitive & Goal-Oriented" and "Cultural Shapers". This presentation will acknowledge the people and highlight some of the perspectives and insights they provided that shaped a relatively unconventional career path for a very conventional person. It is hoped that some of these insights may help instill courage and resilience for some of the youngsters among you to follow both your heart and your "north star," and may help the presenter's contemporaries to realize that change remains an option.

## Advances in Academic Research I

*Moderator: Marwa Abdel Latif, University of Detroit Mercy, Detroit, MI*

Room 2 (VistaTech 460)

### Characterization of Insulin Degradation Products Using Thermal Gel Electrophoresis Coupled to Particle Motion Tracking

*John A. Tetteh, Thomas H. Linz*
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Insulin can undergo conformational changes and degradation during manufacturing, storage, and sample preparation, potentially compromising its biological activity and therapeutic performance. This study presents a label-free analytical platform combining thermal gel electrophoresis (TGE) with particle motion tracking (PMT) to characterize insulin degradation products based on their electrophoretic behavior. Native insulin stored under different pH conditions and chemically-reduced insulin were spiked into Pluronic thermal gel containing 200 nm fluorescent beads. Samples were loaded into a temperature-controlled, single-channel microfluidic device. Upon application of an electric potential, soluble insulin species concentrated into migrating bands that induced motion of the insoluble beads. We employed a sensitive MATLAB-based image analysis to track the bead motion in the microfluidic channel. Frame-to-frame image changes and particle displacement were determined using phase-correlation and particle-tracking procedures. The resulting time-dependent motions indirectly measured changes in the local gel environment caused by migrating insulin species. Differences in peak position, height, width, and integrated area provided measurable signatures distinguishing native, pH-stressed, and reduced insulin samples. These findings demonstrate the potential of TGE–PMT for detecting insulin heterogeneity without covalent fluorescent labeling. With further optimization and validation against established separation methods, this low-volume and cost-effective platform could support insulin stability testing, biopharmaceutical quality assessment, and characterization of structurally heterogeneous peptides and proteins.

### Creating Scalable Multichannel Boron Doped Diamond Microelectrodes for Neurochemical Measurement

*James R. Siegenthaler[1,2], Niko Siratskiy[1], Pramod Gupta[1], Luke Suter[1], Bhavna Gupta[3], Mason L. Perillo[4], Michael F. Becker[1], Erin K. Purcell[2,3,4], and Wen Li[1,2,4]*
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Neurodegenerative diseases such as Parkinson's and Alzheimer's affect millions of people globally. One challenging aspect for microelectrodes for neurotransmitter measurements is that they are hand-fabricated individually, a tedious and highly variable process. To overcome this, we report on our efforts to use boron-doped diamond (BDD) electrodes for neurochemical measurements using fast-scan cyclic voltammetry (FSCV) as an alternative material for long-term chemical measurement. BDD is a versatile material that has been shown to have excellent biocompatibility, a wide working potential window in aqueous solutions, and has been shown to

be an excellent material to study electrochemical systems. Through wafer processing batches of identical electrodes can be produced reproducibly in a production process. We fabricated freestanding BDD microelectrodes insulated with polycrystalline insulating diamond, creating 8 channel single-shank Michigan-style microelectrodes. We characterized the impedance and electrochemical response of the electrodes using slow cyclic voltammetry and studied the effect of surface termination on electrode response. We studied how etching the BDD surface can increase the electroactive area and how the response changes for neurotransmitter measurement. We then characterized the electrode response to several common neurotransmitters, including dopamine, serotonin, and hydrogen peroxide, using FSCV, showcasing the linear dynamic range, detection limit, and noise of these electrodes. Using all-diamond electrodes for neurotransmitter analysis is advantageous as it is the gateway towards customized wafer batch fabrication of microelectrodes, decreasing both errors generated in the traditional hand fabrication methods and building towards a scalable batch method for electrode array technologies.

**Integrated Bottom-Up and Top-Down CE-MS Reveals Kinase-Specific Phosphorylation and Proteoform Remodeling of Tau441**

*Reyhane Tabatabaeian Nimavard, Jorge A. Colón Rosado, Seyed Amirhossein Sadeghi, Yifan Yue, Fei Fang, Guijie Zhu, Guangyao Gao, Lance Thorp, and Liangliang Sun*
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Tau is an intrinsically disordered microtubule-associated protein whose abnormal phosphorylation and truncation are hallmarks of Alzheimer's disease. To characterize kinase-dependent remodeling of tau across both peptide and intact-proteoform levels, we integrated bottom-up capillary zone electrophoresis (CZE)-MS/MS and nanoRPLC-MS/MS with top-down CZE-MS/MS. Recombinant human 2N4R tau was analyzed as an untreated control and after separate in vitro incubation with GSK3β, DYRK1A, or TTBK1. Bottom-up analysis localized phosphorylation sites, whereas top-down analysis characterized intact and truncated proteoforms; proteoforms were grouped by identical first/last residues and a 2 Da mass window. Bottom-up MS identified 65 phosphosites in kinase-treated 2N4R tau, including 31 sites shared across kinase conditions, together with kinase-selective phosphorylation signatures. CZE and nanoRPLC provided complementary phosphopeptide coverage, improving characterization of highly modified tau regions. Top-down MS revealed extensive proteoform heterogeneity, including condition-dependent overlap, diverse truncation architectures, and representative high-confidence truncated proteoforms. Together, these data show that kinase treatment remodels tau across both site-level phosphorylation patterns and proteoform architecture. The integrated workflow links localized PTMs with intact-proteoform context, providing a more complete view of kinase-dependent tau remodeling than either bottom-up or top-down analysis alone. This work highlights the utility of complementary CE-MS and LC-MS separations for characterizing complex phosphoproteoform mixtures relevant to Alzheimer's disease.

**Developing a Framework for the Structural Characterization of RNAs Using Analytical Ultracentrifugation**

*Alec Garasimowicz[1,2], Ethan Dixon[1], Martin O'Steen[1], Sarah Keane[1,2]*
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RNAs are prime drivers of numerous processes in the cell. There has been growing evidence that RNAs adopt multiple distinct conformations and form higher order assemblies that direct different biological outputs. Therefore, it is becoming increasingly important to study the structures and conformational rearrangements of RNAs, but traditional structural biology techniques often struggle in RNA characterization. Analytical ultracentrifugation (AUC) is capable of visualizing macromolecular structure in a solution state. Traditionally, AUC is used to extract parameters that denote solution-phase structure, such as sedimentation, and diffusion. Additional parameters like partial specific volume and anisotropy of a molecule can also be determined, but only if one of the two is known. The partial specific volume for RNA, unlike proteins, varies greatly between different molecules and different folded states, making it a powerful measurement for visualizing RNA structural dynamics. Determining this parameter can be difficult however, and researchers often opt for estimates when performing AUC analysis, leading to inaccurate measurements. To address this, we leveraged advanced computational techniques to develop a new method for determining accurate apparent partial specific volume and anisotropy values in tandem. Using this method, we tracked the folding of tRNA when exposed to magnesium and calculated a literature accurate $K_d$, something which is difficult to do when measuring sedimentation alone. This method opens the possibility of studying many other dynamic structural biological systems in-solution using AUC.

**Utilization of a Chlorine Oxidation Flow Reactor for the Discovery of Novel Chlorinated Compounds**

*Gergana M. Milkova[1], Claire M. Thomson[1,2], Kathryn D. Kulju[1], Daun Jeong[1,3], Andrew R. Jensen[1,4], Graham O. Frazier[1,5], Nicole Woodall[1], Jordan E. Krechmer[6,7], Brian M. Lerner[6], Paul M. Zimmerman[1], Andrew T. Lambe[6,8], Kerri A. Pratt[1]*
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Chlorine radicals (Cl) are important atmospheric oxidants that can react with unsaturated volatile organic compounds (VOCs) via electrophilic addition, rapidly forming chlorinated VOCs (Cl-VOCs). Although Cl-VOCs are associated with adverse health effects, their identities and formation pathways remain poorly understood. To investigate the potential of ambient air to form Cl-VOCs, chlorine oxidation flow reactor (Cl-OFR) was coupled to an iodide chemical ionization high-resolution time-of-flight mass spectrometer ($I^-$-CI-HR-ToF-MS) during the Arctic ChLORine OXidation (Arctic CLOROX) field campaign at Oliktok Point, Alaska. The CLOROX campaign was also conducted near approximately 4,000 active well sites, providing an abundant source of VOCs. This was also the first field deployment of the prototype Cl-OFR, a ~13 L cylindrical PTFE chamber with radially mounted UVC lamps to photolyze oxalyl chloride and generate high concentrations of Cl within the chamber. Ambient air and oxalyl chloride were continuously introduced in the Cl-OFR, where high concentrations of Cl oxidized reactive atmospheric gases

to form Cl-VOCs. From the initial examination, six Cl-VOCs were tentatively identified, only three of which, to our knowledge, have previously been observed in the atmosphere. Work is ongoing to identify additional Cl-VOCs during the Cl-OFR experiments, as well as in the ambient atmosphere. These findings demonstrate the potential of *in-situ* ambient VOC precursors to form Cl-VOCs and highlight the utility of the Cl-OFR as a discovery tool for identifying previously unknown Cl-VOCs in the highly complex atmosphere.

**Quantifying Electrochemically Accessible Primary Amines on Ammonia Plasma-Treated Boron-Doped Diamond Electrodes**

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Boron-doped nanocrystalline diamond (B-NCD) is an attractive platform for electrochemical biosensors, but its chemical inertness makes the covalent attachment of bioreceptors difficult. Here, hydrogen-terminated B-NCD was aminated in a solvent-free ammonia plasma at different powers and $NH_3$ flow rates. The resulting surfaces were characterized by contact angle measurements, X-ray photoelectron spectroscopy and amine-selective fluorescent labeling. The density of amines available for covalent coupling was then determined in situ from the voltammetric charge of coupled ferrocenecarboxylic acid and compared with the absolute nitrogen coverage obtained by XPS. As a demonstration, antibodies against the malaria antigen pfHRP-II were immobilized on electrodes prepared under the optimal conditions, and the electrochemical response scaled with antigen concentration over the range (1pg/mL to 1000pg/mL). The sensor retained its 98% response after 20 cyclic voltammetry cycles and 87% after 30 days of storage. These findings represent a key next step into wafer scalable, robust, diamond-based electrodes for biosensing diagnostic sensors.

## ANALYTICAL PERSPECTIVES:
## Where it All Started: Anachem Shaped Our Careers

*Moderator: Matthew J. Fhaner, University of Michigan, Flint, MI*

Room 3 (VistaTech 425)

### A Curiosity-Driven Approach to Research in an Academic Setting

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The beginnings of an adventure rarely signal what the end will look like. My adventure started as a young assistant professor reading scattered reports in the physical chemistry literature of a new type of solvent, ethylammonium nitrate, that today we would call a room temperature ionic liquid. It was claimed to have properties like water. Contemporary chromatographic studies at that time were focused on kinetics and column performance and stability. I contributed to these studies while intrigued by how one might predict and control chromatographic selectivity. Progress was inhibited by the general use of impure polymeric stationary phases and ionic liquids seemed to potentially offer a more direct approach given their simple structure. Several questions, however, needed to be answered. What parameters could be explored to generate a more structurally diverse set of ionic liquids? Because all ionic liquids are cohesive, are they adsorbents or solvents? What was wrong with the system of McReynolds phase constants that consistently misrepresented the commonsense solvation properties of ionic liquids? Addressing these issues led the author to a multi-year collaboration with Michael Abraham at University College London on the development of the solvation parameter model. Today, this model is the main tool used to understand and predict chromatographic retention, to characterize biphasic systems, and to estimate the physicochemical properties of compounds.

### Opening Doors Through Anachem: From Graduate School to Industry

*David A. Bolliet*
*Analytical R&D Department, Kalsec, Kalamazoo, MI 49006*

Regional scientific conferences often provide the first opportunity for students to engage with the broader analytical chemistry community. As a graduate student at Wayne State University, ANACHEM served as that introduction, offering a chance to present research, interact with scientists from academia and industry, meet and engage with instrument manufacturer representatives, and gain exposure to career paths beyond the traditional academic setting. More importantly, it demonstrated the broad applicability of analytical chemistry to real-world problems across diverse industries. Participation in ANACHEM revealed opportunities to apply analytical chemistry in fields that this presenter had not previously considered, including the food and ingredient industry. Conversations with practicing scientists highlighted how analytical techniques could be used to support product development, quality assurance, authenticity testing, and regulatory compliance, while also fostering professional connections that helped broaden career perspectives. This presentation will reflect on the journey from graduate research at Wayne State University to a career in the food industry and the role ANACHEM played in shaping that path. Examples of analytical chemistry applications in the food industry will be discussed, illustrating how fundamental analytical techniques are used to solve practical challenges, support innovation, and ensure product quality. The presentation will underscore the lasting value of regional

conferences in expanding professional horizons and helping young scientists discover unexpected career opportunities.

**More Than the Science: How Communication Skills Create Career Opportunities**

*Rena Pomaville*
*Tsunagari Services, Inc, Brighton, MI 48116*

Technical expertise is essential for success in analytical chemistry, but the ability to communicate ideas effectively often determines how far those ideas travel and what opportunities follow. Regional scientific meetings such as Anachem provide much more than a venue for presenting technical work. They offer valuable opportunities to develop presentation skills, build confidence, establish professional relationships, and learn how to communicate complex concepts to diverse audiences. This presentation will share personal experiences and lessons learned about the role of communication in professional growth. From presenting research and networking with peers to advocating for projects and influencing decision-makers, the ability to effectively "sell" both yourself and your ideas is a critical skill that is rarely taught in the laboratory. Strong communication skills not only amplify the impact of good science but also create pathways to leadership opportunities, meaningful professional connections, and long-term career success.

**Learning on the Job and in Scientific Communities: How Building Networks Can Lead to the Unexpected**

*Donna Seibert*
*Expreris/Pfizer Consultant, Groton, CT 06340*

Small regional conferences provide opportunities to not only present student work but also exposure to potential applications and industries where student work may be valuable. Contacts made at conferences can be valuable for moving a specific project forward and can also develop into long and meaningful working relationships. This talk will focus on aspects of the pharmaceutical industry that are typically learned on the job as opposed to in an academic setting and weaves in how contacts made outside the workplace have led to some of the most meaningful and far-reaching projects of my career. I'll also touch briefly on the importance of science advocacy--keeping science in the conversation despite the overwhelming amount of information we face on a daily basis.

## Advances in Academic Research II

*Moderator: Thomas Linz, Wayne State University, Detroit, MI*

Room 1 (VistaTech 550)

### Immobilized Metal Affinity Beads for Recombinant Protein Analysis by Desorption Electrospray Ionization Mass Spectrometry

*Christopher Taylor, Andre Venter*
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We previously reported on metal affinity surfaces for recombinant protein analysis by ESI- and DESI-MS. The low binding capacity (femtomoles per $mm^2$) of the chelated nickel modified glass slides limited the mass range of proteins that could be analyzed. Here we improve on the low specific binding capacity of smooth glass surfaces by affixing 30 μm diameter spherical metal affinity magnetic beads to the surface after protein capture. Close packing of the spherical beads provides surfaces with a high binding capacity on the order of nanomoles per $mm^2$, while their magnetic properties provide a highly efficient analytical workflow. This approach allows for a simplified and efficient purification of histidine-tagged recombinant proteins directly from complex mixtures. We demonstrate this approach by purifying known concentrations of recombinant S-adenosylhomocysteine (His-SAHN) nucleosidase and lactate oxidase (His-LOx) from cellular lysate. We show that these proteins retain their activity once captured on the beads by screening their enzymatic reactions. Doing so, we observe the conversion of S-adenosyl homocysteine to adenine and a ribose product from captured His-SAHN and lactate to pyruvate from captured His-LOx. Subsequently, protein release for analysis is facilitated by acidified desorption solvents containing typical concentrations of formic acid (0.2%), lowering local pH and disrupting interactions between chelated nickel and the recombinant proteins' histidine tag.

### Capillary Zone Electrophoresis-Mass Spectrometry Is Ready for Reproducible Multi-level Proteomics

*Guijie Zhu[1], Yifan Yue[1], Jorge A Colón Rosado[1], Guangyao Gao[1], Xiaowen Liu[2], Liangliang Sun[1], [1]Department of Chemistry, Michigan State University, East Lansing, MI 48824, [2]Deming Department of Medicine, Tulane University School of Medicine, New Orleans, LA 70112*

Capillary zone electrophoresis–mass spectrometry (CZE-MS) has been proposed as a powerful analytical tool for bottom-up, top-down, and native proteomics (multi-level proteomics) for decades, enabling the analysis of complex biological samples at the levels of peptides, proteoforms, and complexoforms, respectively. However, its broad adoption has been impeded by limited robustness and reproducibility. Here, we systematically evaluate the reproducibility of CZE-MS across over 170 runs (over 170 h of instrument time), spanning peptides, intact proteoforms, and native protein complexes from biological samples of substantially different complexities, including *Escherichia coli* (*E. coli*), HeLa cells, and human plasma. Across 67 bottom-up proteomics (BUP) runs of HeLa cell digests, the numbers of identified peptides, protein groups, and peptide-spectrum matches (PSMs) showed RSDs below 9%, while the migration times of 400 selected peptides had RSDs below 10%. Peptide intensities were highly reproducible across runs, with a mean pairwise Pearson's r of 0.94 ± 0.04 (mean ± SD). Across 26 top-down proteomics (TDP) runs of an *E. coli* cell lysate, the numbers of identified proteoforms, proteins, and proteoform-spectrum matches and the migration times of 195 selected proteoforms showed RSDs below 10%, with a mean pairwise Pearson's r of 0.97 ± 0.02 for proteoform intensities.

Reproducible performance was further demonstrated across 29 TDP runs of the substantially more complex HeLa cell lysate, with identification-number RSDs of approximately 20%. Native CZE-MS enabled the detection of hundreds of complexoforms with molecular masses up to 800 kDa from complex biological samples while consuming only nanogram amounts of protein material. Representative complexoforms were consistently detected across repeated analyses of *E. coli*, HeLa fraction, and human plasma. The migration times of four representative *E. coli* complexoforms showed RSDs below 10% across 11 MS1-only runs, while those of two representative human plasma complexoforms showed RSDs below 4% across 12 MS1-only runs further supporting reproducible native CZE-MS separation. Collectively, these results demonstrate sustained reproducible performance of CZE-MS across multiple levels of proteomic analysis and support its readiness for broad application in multi-level proteomics.

**Development Towards a Multilayer Microfluidic Paper Analytical Device for the Early Prediction of Severe Acute Pancreatitis**

*Ruth Speidel[1], Peter Lee[2], Sophie Miller[1], Alyssa Perez[1], Samuel Huttner[1], Goergios Papachristou[2], Abraham Badu-Tawiah[1]*

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Acute Pancreatitis (AP) is one of the most common gastrointestinal hospitalizations in the United States. Globally, the incidence has been increasing by more than 3% annually. In approximately 20% of cases the patients will develop severe AP (SAP) defined by the presence of persistent organ failure (POF, organ failure lasting longer than 48 hours). Many clinical scoring models that are used to predict POF in patients lack sensitivity and/or specificity in early diagnosis. Recently, it has been shown that a 5-cytokine panel can outperform current clinical methods for predicting SAP patients in the early phases; however, we lack a method that can easily measure the cytokines at bedside. Herein, we have developed a multilayer paper analytical device (μPAD) for the measurement of cytokines using automated paper-based immunoassays paired with ionic probes that can be detected by mass spectrometry (MS). The ionic probe is easily cleaved at high pH and offers a low molecular weight mass tag that can be analyzed via paper spray ionization. Data will be presented on the optimization of immunoassay and the shelf life of the microfluidic device. As well as the design process for the microfluidic device, calibration curves, and clinical validation using over 100 AP patients. The development of this device has the advantage of measuring cytokines directly from patient samples with no pre-treatment which reduces the turnaround time for diagnosis.

**Biphasic Reactivity Enables Tunable Electrolyte and Heavy Metal Detection in Droplet Microfluidics**

*Camila Gonzalez Curbelo, Ayush Chitrakar, and Ryan C. Bailey*
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We present a droplet microfluidics platform for the quantitation of electrolyte and heavy metal ions via selective transport of the analyte across the biphasic interface and demonstrate this response can be chemically tuned to favor desirable concentration regimes. The biphasic nature of droplet microfluidics makes it an enabling sensing platform for analyte ions via liquid-liquid extraction. The microfluidic ion-selective optode (“droptode”) has emerged as a promising platform for the fluorescence-based quantification of biologically relevant ions via selective analyte extraction at the oil-aqueous interface of segmented microdroplets. Droptodes uniquely employ the ion-

selective sensing chemistry within the oil phase, functioning as a matrix-isolated detection zone. Droplets are generated in High-Purity Perfluoroalkoxy (HPFA) tubing via a commercial T-junction. Our recent work demonstrates the analyte concentration regime can be tuned through systematic modulation of the ion-selective oil composition, including the reagent stoichiometry and polarity of the oil solvent. The droptode has been contextualized for its promising suitability as a diagnostic tool given its semi-continuous measurements only necessitate sub-µL samples, making it timely and minimally invasive for patients. However, extension of the droptode toward the detection of non-electrolyte ions, more specifically toxic heavy metals for drinking water assessment, has not yet been demonstrated. Here we also present the first cadmium-selective microfluidic droptode using a complementary biphasic reactivity-based sensing strategy based on a fluorogenic quinoline chelator. Furthermore, modulation of ion-exchanger identity, may enhance analyte extraction, representing another dynamic-range tuning strategy.

**Multivariate Analysis of Volatile and Semi-volatile Organic Compounds in Water by Vacuum Assisted Headspace Solid-Phase Microextraction**

*Temitope Alonge,[1,2] Alja Contala,[1,2] Emanuela Gionfriddo,[3] and Jon R. Kirchhoff.[1,2]*
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Vacuum-assisted headspace solid-phase microextraction (Vac-HS-SPME) is an underexploited analytical technique that further advances traditional headspace solid-phase microextraction (HS-SPME) by reducing pressure in the headspace. This allows for the efficient extraction of semi-volatile and less volatile compounds at shorter timeframes and significantly milder temperatures to preserve the sample properties and avoid decomposition. Because it is an SPME method, optimization of extraction parameters such as incubation time, extraction time, sample volume, agitator speed and extraction/incubation temperature are important for effective extraction. This project investigated these parameters simultaneously for the extraction of twenty organic compounds in water using multivariate analysis methods. Unlike traditional univariate (One-Factor-at-a-Time) approach for optimization that allows the examination of effects of one variable at a time and keeps the others constant at a particular optimization condition, multivariate analysis simultaneously evaluates and optimizes multiple extraction parameters. The results show that incubation time and agitator speed are non-significant at the 95% confidence interval, while extraction time, sample volume, and extraction/incubation temperature were significant. The significant parameters were further optimized for both traditional HS-SPME and Vac-HS-SPME. Vac-HS-SPME showed higher extraction efficiency for the sum of all targeted peak areas. The optimized extraction conditions for Vac-HS-SPME for the selected analytes were 5 mL sample volume, 45 °C incubation and extraction temperature, and 40min extraction time. The use of experimental design reduced the number of experiments required, identifying significant and interacting factors and ensuring reliable conclusions.

**Electrochemical Immunosensors for Non-Invasive Monitoring of Lung Cancer and Heart Failure**

*Erfan Omid Najafabadi, Greg M. Swain*
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Cancer diagnosis and treatment monitoring often rely on methods that are costly, time-consuming, and not always suitable for frequent point-of-care testing. In addition, some cancer therapies can lead to cardiotoxicity and cardiac dysfunction, creating a need to monitor both cancer progression and cardiovascular health during treatment. Programmed Death-Ligand 1 (PD-L1) is an important biomarker associated with several cancers, including lung cancer, while N-terminal pro-B-type natriuretic peptide (NT-proBNP) is widely used as a biomarker of cardiac stress and heart failure. This work focuses on the development of electrochemical immunosensors for sensitive detection of PD-L1 and NT-proBNP, with the long-term goal of enabling rapid, low-cost, and point-of-care biomarker analysis. Boron-doped diamond (BDD) electrodes are being investigated as the electrochemical transducer because of their low background current, wide potential window, chemical stability, and resistance to fouling. These properties make BDD attractive for sensitive biomarker detection in complex biological samples. Electrochemical detection also offers simple instrumentation, low sample-volume requirements, high sensitivity, and potential portability. These features are especially attractive for analysis of non-invasive biological samples, such as exhaled breath condensate, which may reduce dependence on repeated blood collection and enable more frequent monitoring. The overall objective is to develop and optimize electrochemical immunoassays for clinically relevant detection of PD-L1 and NT-proBNP and ultimately apply these assays to non-invasive samples for routine cancer and cardiac monitoring.

## Advances in Academic Research III

*Moderator: Dragan Isailovic, University of Toledo, Toledo, OH*

Room 2 (VistaTech 460)

### Ambient Ionization Mass Spectrometry for Detection of RNA Biomarkers and Disease Diagnostics

*Anju Sheregar[1], Rachel M. Robertson[1,2], Ayesha Seth[1], Keerthana Ravi[1], Adom Amparbeng[1], Venkat Gopalan[1,2], Abraham Badu-Tawiah[1]*

*[1]Department of Chemistry and Biochemistry, [2]Center for RNA Biology, The Ohio State University, Columbus, OH 43210*

Dysregulation of RNA metabolism is associated with many diseases – RNA expression is altered before the onset of disease symptoms. Cell-free RNA is common in many bodily fluids, such as blood, saliva, and urine; therefore, these fluids can be used in non-invasive tests for disease diagnosis. To this end, we leverage a mass spectrometry-based platform to detect specific RNAs. Our method provides a unique pipeline in amplifying the analytical signal through our dendrimer-based signal amplification strategy. Here, *in-vitro* proof-of-concept model was designed using a biotin-streptavidin assay to pull-down the target RNA (n-Tr20 variant engineered with extensions at both termini). Specifically, the tRNA was incubated with a DNA oligo complementary to its 3' extension. A biotinylated DNA oligo that binds the overhang was then used to capture the tRNA on streptavidin beads. Once captured, the tRNA is ready for interrogation with a second DNA probe that is complementary to the tRNA 's 5' extension. In parallel with the pull-down assay development, we developed a detection conjugate by attaching an in-house-synthesized ionic probe to a dendrimer, which in turn was attached to a DNA oligo that is complementary to the tRNA's 5' extension. The ionic probe is hydrolyzed by alkali to release the diagnostic mass tag. Our results show high sensitivity and multiplexing capabilities through validation experiments – bio-specificity, cross-reactivity, and multiplexing. We will also discuss the translation into a paper-based platform for its implications in assay cost, turnaround time, and point-of-care diagnostics.

### Structural and Energetic Effects of Nucleobase Methylation on Guanosine Nucleosides: IRMPD, ER-CID, and Theoretical Studies

*Bijoy Krishna Roy[1], N. M. R. Frieler[1], Giel Berden[2], M. T. Rodgers[1]*

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1-Methylguanosine ($m^1$Guo) and 7-methylguanosine ($m^7$Guo) are naturally occurring methylated analogues of the canonical RNA nucleoside guanosine (Guo). These modifications are found in biologically important RNA systems. In particular, methylation at different nitrogen sites is expected to produce distinct effects on the electronic structure and intrinsic stability of guanosine. Characterization of these effects at the molecular level can provide greater insight into how site-specific methylation modulates nucleoside structure and stability and, ultimately, contributes to the structural and functional properties of modified RNA. In this study, the effects of N1- and N7-methylation on the structure, preferred sites of protonation, and glycosidic bond stability of guanosine are investigated through comparative analyses of $m^1$Guo, $m^7$Guo, and canonical Guo, where guanosine serves as the unmodified control system. Energy-resolved collision-induced

dissociation (ER-CID) experiments, coupled with survival yield analyses, are employed to evaluate the effects of methylation on the stability of the N-glycosidic bond and associated dissociation behavior. Wavelength-resolved infrared multiple photon dissociation (IRMPD) action spectroscopy experiments are employed to characterize the structures and intramolecular interactions of the experimentally populated ions. Density functional theory (DFT) calculations are performed to identify stable low-energy conformations available to Guo and its N1- and N7-methylated analogues, determine their relative stabilities, and predict their infrared spectra. Experimentally populated structures are assigned through comparison of the measured IRMPD spectra with IR spectra predicted from calculations. DFT calculations are also employed to characterize the energetic and mechanistic pathways associated with N-glycosidic bond cleavage. The combined experimental and theoretical results provide a direct comparison of the effects of methylation at the N1 and N7 positions of guanine and establish how the location of methyl substitution influences the conformational landscape, protonation, and intrinsic glycosidic bond stability of guanosine nucleosides.

**Investigation of Halogen Oxidation of Toluene using a Novel Oxidation Flow Reactor Coupled to a Reagent Ion Switching Chemical Ionization Time-of-Flight Mass Spectrometer (CI-TOF-MS)**

*Anya C. Romig[1], Andrew T. Lambe[2], Kerri A. Pratt,[1]*
*[1]Department of Chemistry, University of Michigan, Ann Arbor, MI 48109; [2]Now at Entegris Inc., Bedford, MA 01821*

Atmospheric oxidation of volatile organic compounds (VOCs) results in the formation of oxygenated VOCs (OVOCs), both of which have implications for climate, air quality, and human health. OVOCs can further react to form highly oxygenated multigenerational products, yet formation pathways and product identities, which are oxidant-dependent, remain poorly understood. While hydroxyl radicals (OH) are the most abundant globally, chlorine radicals (Cl) are more reactive than OH for most VOCs. Bromine radical (Br) oxidation may also play a key role. Yet, halogen oxidation of VOCs is relatively understudied. Because atmospheric oxidation is complex and driven by multiple oxidants, this highlights a knowledge gap in our understanding of VOC oxidation. Here, we present a novel, double oxidation flow reactor (OFR) set-up, using toluene as the VOC precursor, and both Cl and Br as the primary oxidants. We utilized toluene, a common combustion emission product, due to well-characterized reaction mechanisms with OH, and to a lesser extent, Cl. We also conducted two single OFR experiments to investigate: (1) Cl oxidation of toluene and (2) Br oxidation of benzaldehyde, a toluene oxidation product. We identify early and multigenerational OVOCs in all three OFR experiments using a novel chemical ionization high resolution time-of-flight mass spectrometer (CI-TOF-MS) with reagent ion switching between $H_3O^+$ and $NH_4^+$ to probe a wider suite of molecules. We observe preferential formation of $C_{6-7}$ products and identify unique $C_{4-5}$ product formation for Br oxidation of benzaldehyde. Our results highlight differing oxidant pathways, and demonstrate the value of probing complex, multi-oxidant systems.

**Single-sample Calibration Based on Experimental Multiple Isotopologues and Charge-state Ion Ratios for Quantitative LC–MS/MS Analysis of Cyanotoxins**

*Yohan C. Y. Sudusingha, Dragan Isailovic*
*Department of Chemistry and Biochemistry, University of Toledo, Toledo, OH 43606*

Rapid and accurate quantification of cyanotoxins in freshwater during harmful algal blooms (HABs) is critical for public health protection. This study introduces a multiple-isotopologue and

charge-state reaction monitoring (MICRM) strategy to generate calibration levels from a single standard solution for quantitative LC–MS/MS analysis of cyanotoxins. Microcystin-LR (MC-LR), one of the most prevalent microcystins in freshwater, was used as the primary model analyte. Six selected precursor-to-product ion transitions (two from the doubly charged MC-LR precursor and four from the singly charged precursor) and their summed response were used to develop single-sample calibration based on the experimental MICRM ion ratio (SSC-MICRM). A seven-point SSC-MICRM was constructed using a 10 µg/L MC-LR standard solution and compared with a traditional multiple-sample calibration (MSC) prepared in MC-free lake water. The SSC-MICRM method was validated in terms of accuracy, precision, linearity, sensitivity, matrix effects, LOD, and LOQ, and compared with traditional MSC for both low- and high-concentration ranges (0.05-600 µg/L). This strategy was further validated using microcystin-YR (MC-YR) and anabaenopeptin-B (AP-B), confirming its applicability for cyanotoxins that produce multiple charge ions during electrospray ionization. Concentrations of MC-LR, MC-YR, and AP-B measured in Lake Erie water samples collected during HABs showed strong agreement with traditional MSC results. Overall, the present SSC strategy, based on the simultaneous use of isotopologues and charge-state transitions, provides an accurate, high-throughput, and cost-effective alternative to conventional LC-MS/MS calibration while maintaining quantitative performance across environmentally relevant concentration ranges.

**Electropolymerized *p*-Aminobenzoic Acid on Boron-Doped Nanocrystalline Diamond for Label-Free Electrochemical Detection of PfHRP-2**

*Pramod K. Gupta[1], Ruben Levy[1], Aaron I. Jacobs[1], James R. Siegenthaler[1,2]*
*[1]Coatings and Diamond Technologies Division, Fraunhofer USA Center Midwest, East Lansing, MI 48824; [2]Department of Electrical and Computer Engineering, Michigan State University, East Lansing, MI 48824*

Reliable point-of-care malaria testing requires sensitive detection of Plasmodium falciparum histidine-rich protein 2 (PfHRP-2). We describe a label-free electrochemical immunosensor for PfHRP-2 built on boron-doped nanocrystalline diamond (B-NCD), a transducer that combines near-metallic conductivity with a wide working potential window, low background current, and chemical durability. Antibody attachment was enabled by electropolymerizing p-aminobenzoic acid (p-ABA) directly on the electrode, producing a thin carboxyl-terminated film without diazonium coupling or harsh surface pretreatment. During deposition, the first cyclic voltammetry scan showed the oxidation peak of the p-ABA monomer, and currents then fell progressively with each cycle as the growing film restricted charge transfer. Higher interfacial impedance and a weaker differential pulse voltammetry (DPV) response compared with bare B-NCD confirmed film formation. Surface carboxyl groups were activated with EDC/NHS and covalently coupled to anti-PfHRP-2 antibodies. The DPV peak current dropped at every step of the build, polymer deposition, antibody immobilization, and antigen capture, giving a clear signature of successive surface modification. Calibration was linear from 1 pg/mL to 1 µg/mL PfHRP-2, with a detection limit close to 3 pg/mL. The sensor also detected PfHRP-2 in spiked serum, indicating that nonspecific adsorption remains modest in complex matrices. Electropolymerized B-NCD therefore offers a stable, sensitive interface for malaria antigen detection and a workable basis for point-of-care devices.

**Multi-omic Evaluations of Nanodiscs Incorporating Blood Coagulation Membrane Proteins**

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*Department of Chemistry, University of Michigan, Ann Arbor, MI 48104*

Membrane proteins such as tissue factor (TF) play a significant role in the initiation of the extrinsic blood coagulation cascade. Such proteins rely heavily on specific lipid environments for functional activity. Specifically, during external injury phosphatidylserine (PS) lipids are flipped onto the outer membrane, contributing to the decryption of TF. Membrane protein-lipid interactions, such as the synergistic relationships between TF and PS, are difficult to study due to the loss of function of membrane proteins outside their native environment. Hence, in this work, we utilize nanodiscs as membrane mimetics to study the lipid-protein interactions of this biological system. Nanodiscs are desirable mimetics due to their stability against aggregation and their purification simplicity; here, we assembled nanodiscs by modulating lipid compositions and incorporating recombinant coagulation cascade membrane proteins. Following protein incorporation, lipid extraction and tandem mass spectrometry were performed to profile lipid species and assess how protein incorporation may influence lipid enrichment. Comparative analyses of empty versus protein loaded discs can provide information about preferential lipid-protein interactions. This study integrates nanodisc technology with lipidomic analysis to probe lipid dependent membrane protein environments and can provide new insights into the role of changing lipid composition in coagulation protein behavior.

## Advances in Academic Research IV

*Moderator: Colin F. Poole, Wayne State University (Emeritus), Detroit, MI*

Room 3 (VistaTech 425)

### Novel Gas Chromatography - Chemical Ionization Mass Spectrometry Measurements of Volatile Organic Compounds in an Arctic Oilfield

*Anthony J. Rovinski[1], Andrew R. Jensen[1,2], Frozan Tahiry[1], Daun Jeong[1,3], Nicole Woodall[1], Kathryn D. Kulju[1], Jordan E. Krechmer[4,5], Brian M. Lerner[4], Megan S. Claflin[4], Andrew T. Lambe[4,6], Kerri A. Pratt[1]*

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Rapid Arctic warming and declining sea ice are expected to increase Arctic resource extraction, including oil and gas operations, which can contribute to local air pollution and alter the atmospheric radiation budget. Oil and gas operations are widespread throughout the region and known to emit thousands of different volatile organic compounds (VOCs), but their identities in the Arctic are poorly constrained. Emitted VOCs can react to form ozone, a greenhouse gas and criteria pollutant, and they can contribute to the formation of secondary organic aerosol with implications for human health and the climate. Alkylbenzenes, a class of aromatic VOCs, are of particular interest as many are classified as hazardous air pollutants yet remain understudied. This work focuses on $C_{10}$ alkylbenzenes (isomers of $C_{10}H_{14}$), a subset of aromatic VOCs that are rarely measured in the atmosphere due to analytical challenges. Therefore, *in-situ* measurements of $C_{10}$ alkylbenzenes in the air were conducted through the first Arctic field deployment of a novel fast gas chromatograph coupled with a mixed reagent ion $NO^+$/ $O_2^+$ chemical ionization high-resolution time-of-flight mass spectrometer coupled during the 2020 Arctic ChLORine OXidation (CLOROX) field campaign at Oliktok Point, Alaska, within the active North Slope of Alaska oilfields. Of the 22 possible $C_{10}$ alkylbenzene isomers, eight were measured in the field, five of which have not been previously reported in Arctic measurements. The sources and distributions of the measured $C_{10}$ alkylbenzene isomers will be discussed.

### Resonance-Enhanced, Label-Free Detection in Free Solution using Droplet Microfluidic Gratings

*Hannah H. Morris, Lindsay J. Heagle, Diana C. Weiland, Ryan C. Bailey*
*Chemistry Department, University of Michigan, Ann Arbor, MI 48197*

Droplet microfluidics is a powerful analytical technique that enables high-sensitivity detection, separation, and reaction of discrete nano to picoliter droplets. Recent work has demonstrated label-free, multi-parametric analysis of droplet content by treating the droplet train as a transmission-based diffraction phase grating capable of quantifying refractive index (RI). To further advance this platform, RI modulation by resonant absorption, established by the Kramers-Kronig (KK) relation, must be explored. The KK relation is a bidirectional mathematical framework that links optical absorption and dispersion, establishing an intrinsic connection between the real and imaginary components of RI. Multiwavelength measurements of the halochromic dye bromocresol green have been performed to probe resonance-driven RI changes across varying pH conditions. Considerable quantifiable changes in signal response are observed at different

wavelengths, which is consistent with absorption-induced effects on the real RI. This work aims to validate experimental results by developing a theoretical model that applies the KK relation to compute real RI variations from experimentally acquired absorption spectra. Demonstrating the KK relation using this microfluidic platform establishes its potential for label-free, resonance-enhanced chemical sensing where its integration into high-throughput workflows could provide a rapid and customizable method for extracting spectroscopic information from low-abundance samples.

**Fluorescence-Based Photothermal Infrared Spectroscopy Methods for the Single-Particle Detection of Aerosolized Microplastics and Nanoplastics**

*Randi Libin-Straub, Wilson Chen, Abbygail M. Ayala, Andrew P. Ault*
*Department of Chemistry, University of Michigan, Ann Arbor, MI 48109*

Detecting and identifying microplastics and nanoplastics (MNPs), especially those with diameters less than 10 μm, is essential for understanding their environmental and health impacts. Microplastic (MP) studies have largely focused on MPs with diameters greater than 10 μm, particularly those aimed at identifying MNPs via single-particle vibrational spectroscopy. However, there are key limitations, including the potential for fluorescence to overwhelm the signal in Raman microspectroscopy and the poor spatial resolution of traditional infrared (IR) spectroscopy. Optical photothermal infrared spectroscopy (O-PTIR) addresses these issues by using both visible and infrared light to detect photothermally-induced changes to a sample's refractive index. By using a counterpropagating configuration, O-PTIR spatial resolution has been improved to measure particles less than 400 nm in diameter. Two recently developed fluorescence-based techniques can use MNP autofluorescence in tandem with photothermal vibrational spectroscopy. The first, fluorescence-guided O-PTIR (FL-O-PTIR), uses fluorescence to select particles for IR analysis, increasing throughput, especially in complex environmental mixtures. The second method, widefield fluorescence-detected photothermal IR (FL-PTIR), simultaneously collects the spectra of all points within a field of view. The absorption of IR light causes changes in the fluorescence intensity, which are measured to produce a hyperspectral IR image. This study marks the first time fluorescence-based PTIR methods identified aerosolized MNP particles, including polyethylene, polypropylene, and polystyrene, as well as atmospheric proxies. These results demonstrate the efficacy of these techniques for identifying atmospheric MNPs in complex mixtures while addressing the need for methods to identify sub-micron plastics in the atmosphere and broader environment.

**Cyclic Voltammetric Studies of Boron-Doped Diamond Microelectrodes**

*Grace E. Leahey, Greg M. Swain*
*Chemistry Department, Michigan State University, East Lansing, MI 48824*

Boron-doped diamond (BDD) as an electrode material has become both well-known and used for a variety of electrochemical applications. Unlike materials like glassy carbon, BDD does not require polishing, has a large potential window, produces low background currents, and is stable long term, making them an attractive electrode material. BDD electrodes can be fabricated on both a macro and microelectrode scale. These microelectrodes have advantages to the typical macroelectrode, including enhanced mass transport. This is due to the small diffusion layer across the surface which allows steady state limiting currents to be achieved. BDD microelectrodes have been applied to *in vitro* electrochemical sensing in gastrointestinal tissue, as well as *in vivo* detection of neurotransmitters like dopamine. Understanding the mechanical and electrochemical properties of these microelectrodes will provide necessary information on

their use in electrochemical biosensing applications. Therefore, several BDD microelectrodes were grown using chemical vapor deposition (CVD) and characterized using both Raman spectroscopy and scanning electron microscopy (SEM). The reproducibility of these microelectrodes was assessed for microelectrodes grown under the same conditions via cyclic voltammetry. Well-known redox probes, both inner and outer sphere, as well as potential biological interferents were studied. Inner sphere redox systems, like $Fe(CN)_6^{-3/-4}$, provide information on the cleanliness of the surface and electron transfer kinetics. Outer sphere redox systems, like $Ru(NH_3)_6^{+2/+3}$, are surface insensitive and can provide information on the resistivity of the electrode. Taken together, a full picture of the electrode's properties can be ascertained.

**Correlating Internal miRNA and External Protein from Individual Small Extracellular Vesicles with Digital-Quantitative-PCR**

*Rebecca K. Partee, Brice C. Vanness, Thomas H. Linz,*
*Department of Chemistry, Wayne State University, Detroit, MI 48202*

Small extracellular vesicles (sEVs) are lipid-bound nanoparticles containing bioactive molecules such as proteins and nucleic acids which are secreted from cells as messengers. sEVs are promising targets for early-disease detection, because they travel via accessible biofluids and provide vital information on the identity of the parent cell. However, sEVs are highly heterogenous, and sEVs from the same cell often differ in internal and external composition. The goal of this work was to correlate internal miRNAs and external protein targets from individual sEVs using digital-quantitative-PCR (dqPCR). Over- and under-expression of specific biomarkers within sEV populations can indicate for specific illnesses within the parent cell, making correlational data vital. The miRNA Let-7a and the membrane protein CD-81 were selected as model targets. Master mix composition and thermocycling conditions were optimized to promote efficient reverse transcription-free amplification of Let-7a simultaneously with immuno-PCR detection of CD-81. sEVs were isolated from cell culture media before being captured via anti-CD-63 onto magnetic beads and labelled via an anti-CD-81 immuno-PCR tag. Incubation conditions were optimized to maximize sEV capture and labelling before analysis using dqPCR. The dPCR dimension, the presence of Let-7a and CD-81 was established, while the qPCR dimension determined the copy numbers of said biomolecules. By analyzing both dimensions, the presence and copy number of both Let-7a and CD-81 were correlated to single CD-63+ sEVs. These results open a promising avenue for early disease detection using correlational information from individual sEVs.

**Optimization of Digestion Protocols for Comprehensive Profiling of the Elemental Composition of Mount Etna Lava Ash.**

*Oluwaseun I. Akindumila[1,2], Alja Čontala[1,2], Catherine Lu[3], Emanuela Gionfriddo[3], Jon R. Kirchhoff[1,2]. [1]Department of Chemistry and Biochemistry, The University of Toledo, Toledo, OH 43606, [2]Dr. Nina McClelland Laboratory for Water Chemistry and Environmental Analysis, Department of Chemistry and Biochemistry, The University of Toledo, Toledo, OH 43606, [3]Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY 14260*

Volcanic eruptions are persistent environmental events that release substantial quantities of gases and particulate matter enriched with potentially hazardous materials. According to the Smithsonian Institution Global Volcanism Program, at least 50 volcanic eruptions have been reported annually from 1960 to 2025. Lava can contain major, trace, and rare earth elements (REEs) that may be transported into surrounding soils and water systems, creating potential environmental and human health concerns. However, accurate elemental analysis of silicate-rich

volcanic matrices remains analytically challenging. This study investigates the development of a safer and more environmentally sustainable hydrofluoric acid (HF)-free digestion process for determination of trace metals and REEs in lava samples. EPA solid-sample digestion protocols, aqua regia digestion, microwave-assisted digestion, and ultrasonic pretreatment were systematically evaluated to improve matrix dissolution while reducing acid consumption and avoiding HF. Optical microscopy was used to visualize lava samples before and after digestion. Thermogravimetric analysis and dry ashing were used to determine the percentage of organic matter in the samples. Energy-dispersive X-ray spectroscopy (EDS) was used for preliminary element identification before and after digestion. Notably, elements detected in the undigested samples were absent following digestion under optimized conditions, indicating effective dissolution of the elements. The resulting digests were analyzed by inductively coupled plasma–tandem mass spectrometry (ICP-MS/MS) for a comprehensive analysis of the elemental composition of the lava. Overall, the developed HF-free approach demonstrates potential for safer and more sustainable multi-element analysis of volcanic materials.

# Poster Session

Exhibit Hall (DiPonio 500ABCD)

# Undergraduate Posters

**(UG1)**
**Characterization of a Custom Atmospheric Chamber with Secondary Organic Aerosol Formation**

*Justin M. French[1], Joseph N. Berberich[2], Rachel E. O'Brien[1]*
*[1]Department of Civil and Environmental Engineering, University of Michigan, Ann Arbor, MI 48109, [2]Department of Chemistry, University of Michigan, Ann Arbor, MI 48109*

Volatile organic compounds (VOCs) are found in many household products like cleaning sprays due to their pleasant aromas. However, once they are emitted into the air, they may eventually undergo oxidation and form secondary organic aerosol (SOA) particles, which could have undesirable health impacts. Human health outcomes from aerosol exposure depend on the physical and chemical properties of aerosol particles. For example, smaller particles can reach lower regions of the lungs and deposit, and more oxidized particles may be more reactive and thus harmful. A detailed analysis of aerosol particle composition and size during SOA formation and aging begets the need for an atmospheric chamber. To conduct such experiments, we develop a 0.25 $m^3$ PTFE chamber, with capabilities for inorganic seed aerosol introduction as well as VOC and ozone injection. To characterize the chamber, we examine secondary organic aerosol formation from multiple different organic compounds– including the terpenes α-pinene and (-)-limonene. We employ an online aerosol mass spectrophotometer (AMS) to look at aerosol composition in the chamber in real-time, comparing its mass spectra to those from literature using cosine similarity scores. In addition, we use a new visualization and analysis tool based on delta analysis to compare functional group makeup across these different standards. This work serves as a foundation for an analytical platform to enable a better understanding of the potential health risks from indoor exposure to many common household products.

**(UG2)**
**Investigating the Effects of Field Sample Conditions and Metal Content on Bacteriophage Presence**

*Maxwell L. Williams[1], Audra Auston[2], Emma Volk[2], Rebecca Tonietto[2], Maeve McLaughlin[2], Matthew J. Fhaner[1], [1]Department of Green Chemistry and Biochemistry, University of Michigan-Flint, Flint, MI 48502; [2]Department of Biology, University of Michigan-Flint, Flint, MI 48502*

The role of bacteriophage (phage) in bacterial ecosystems and their impact on larger environments is highly varied by location and species. This makes establishing patterns and consistent predictive strategy for finding phage more difficult. For this reason, it is important to catalogue new species of bacteriophage along with the environmental conditions from which they are collected in an effort to better understand the mechanisms of phage at micro- and macroscale. Various field soil samples were collected and analyzed for both phage and heavy metal analysis. Soil samples were digested and heavy metals were determined via ICP-OES. Metal

concentrations were then indexed to “high” and “low” relative values and compared against the presence, or lack thereof, of phage. Preliminary findings suggest that the relationship between soil conditions and phage availability could serve as a predictive metric for the environment-phage relationship.

**(UG3)**

**UHPLC-DAD-MS For the Identification of Dyes in Blue, Green, and Purple Yarns from WK-12/382 Textiles**

*Sam Branscum[1], Ann Peters[2], and Ruth Ann Armitage[1]*

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*[2]University of Pennsylvania Museum of Archaeology and Anthropology, Philadelphia, PA 19104*

The Necropolis of Wari Kayan, located on the Paracas Peninsula in southern Peru, is a site with many well-preserved textiles. The textiles, dating to around 2000 years ago, are made up of many different colors including blues, greens and purples that were prepared from indigo-bearing plants. The other colors, red and yellow, come from a variety of other plant sources, most of which are not well understood. This project seeks to characterize the many different colors associated with indigo in textiles from the Wari Kayan bundle 12/382. UHPLC-DAD-MS gives a comprehensive analysis of all the components extracted, in this case, in DMSO, the only solvent appropriate for indigoids. These findings contribute to the overall understanding of the dye plants chosen by the ancient Andeans to prepare their colorful textiles for their funerary bundles.

**(UG4)**

**Characterizing Functional Group Evolution in Biomass Burning Organic Aerosols Using Delta Analysis**

*Hyunji (Willow) Hwang[1], Yeasul (Janie) Kim[1], Jesse Kroll[2], Chris Lim[2], Chris Cappa[3], Rachel O’Brien[1]*

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Biomass burning organic aerosol (BBOA) is a major contributor to atmospheric particulate matter that can influence air quality and climate. However, predicting the atmospheric impact remains challenging because the particles contain thousands of different organic compounds and are subject to photochemical aging processes. Previous studies suggest that these aging processes can change the composition of BBOA and thus the particles’ behavior and interactions with the surrounding environment. Despite increasing wildfire emissions, the effect of atmospheric aging on the chemical evolution of BBOA is poorly understood. Aerosol Mass Spectrometry (AMS) provides insights into organic aerosol composition; however extensive electron-ionization fragmentation complicates direct determination of functional group distributions. In this study, we investigated changes in functional group distributions following aging experiments during the Fire Influence on Regional and Global Environments Experiment (FIREX) 2016. We used delta functional group analysis, which provides quantitative estimates of functional group fractions from high resolution AMS mass spectra. In FIREX, fresh emissions from multiple biomass fuels were subjected to controlled photochemical aging in an environmental chamber. The initial functional group distributions and the changes that occurred during aging were characterized across different burns to evaluate the effects of fuel type and combustion conditions. We also examined the AMS mass spectra of oxidized aromatic standards to gain context for assigning functional groups to certain delta values. The characterization of functional group distributions will improve

our understanding of biomass burning organic aerosol aging and support more accurate predictions of the particles' atmospheric impact.

**(UG5)**

**Effect of Controlled Electrolysis Treatment at Elevated Temperatures on Primary and Secondary Oxidation Products in Edible Oils**

*Katelin J. Fields, Matthew J. Fhaner*
*Department of Green Chemistry and Biochemistry, University of Michigan-Flint, Flint, MI 48502*

Oxidation remains the ever-present challenge in the processing, storage, transportation, and use of edible oils. To this end, researchers are continuously seeking innovative approaches to minimize fatty acid oxidation in edible oils, especially those high in unsaturated fatty acids such as oleic, linoleic, and linolenic acids. To date, the primary strategy for minimization fatty acid oxidation is through the use of chemical antioxidant species which sacrifice their own electrons to inhibit lipid autooxidation. In this study, we investigate a novel antioxidant technological approach, through an applied electrolysis voltage. Three commonly used edible oils in industrial, food service, and home kitchens were selected for investigation. Canola, vegetable (100% soybean), and coconut oils stripped of any natural or added antioxidants, heated to 180 °C, and a controlled electrolysis was applied for 8-hours at -0.6 V, 0.0 V, and 0.6V versus a saturated silver-silver/chloride reference electrode. Aliquots were removed at 1-hour intervals and treatment, and control samples were analyzed for primary (peroxides) and secondary (conjugated dienes) oxidation products. While there were select data points that yielded statistical differences, overall, the peroxide values and conjugated diene values suggest that all treatments evaluated had no effect on the rate of lipid oxidation compared to control samples. Future work will utilize LC-MS analysis to determine fatty acid profile and oxylipin concentrations between treatment and control samples to better characterize the potential impacts controlled electrolysis treatment may have on lipid oxidation processes.

**(UG6)**

**Development of a 128-Channel Potentiostat for Chemical Sensing**

*Luca L. Moll[1], Henki Xhepa[2], Christine McBeth[3], James R. Siegenthaler[1,4]*
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Electrochemical sensing is currently at a critical inflection point, driven by simultaneous advancements in novel sensor materials and accessible, high-performance hardware. Custom miniaturized systems can now achieve sensitivities and accuracies comparable to commercial benchtop instruments at a fraction of the cost. This democratization enables point-of-need field measurements, facilitating real-time environmental monitoring for heavy metals and rapid diagnostic screening for infectious diseases such as HIV. This work presents the development of a simultaneously sampling 16 channel potentiostat that is scalable to 128 channels using multiplexing. The system supports standard analytical techniques, including Cyclic Voltammetry (CV), Differential Pulse Voltammetry (DPV), and Square Wave Voltammetry (SWV). The project details the integration of a custom analog front-end optimized for precise voltage control and low-noise current measurement, alongside a modified microcontroller-based data acquisition architecture using a Raspberry Pi 5 for synchronized signal processing, controlled via a custom graphical user interface (GUI) for real-time data visualization. Key design objectives focused on

minimizing analog noise, ensuring strict channel-to-channel consistency, and maximizing sample throughput. Finally, the system's analytical capabilities are characterized and validated in a laboratory setting through the integration of diamond-based electrodes, demonstrating its viability as a robust, low-cost platform that enables the rapid, cost-effective detection and quantification of low-concentration analytes directly at the point of need.

**(UG7)**

**Nanobubble Formations by Optimizing Internal Tesla Valve Geometry**

*Sam J. Langsdorf, Andre R. Venter*
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Nanobubbles are buoyant, and unlike microbubbles, remain stable in solution for days or weeks. Nanobubbles increase the solvent-air interface surface area and facilitate analyte transport to droplet surfaces. In addition, nanobubbles can act as surface cleaning agents through microstreaming and cavitation effects, removing bound contaminants and improving analyte accessibility. Batch preparation of nanobubbles is already possible by cycling water though a Tesla Valve with two syringes on either end. This research intends to use a blueprint from “Fabrication of Microfluidic Tesla Valve Employing Femtosecond Bursts”. The current models were optimized by changing the length to diameter ratio and using manual flow speed control. Here we report on more detailed optimization of the device by adjusting four different variables of the internal geometry of a Tesla valve. The variables studied include the turbulent length (*l* ), the width of the channel (W), the leaving angle (α), and the return angle (β), comprising all of the variables that affect the internal geometry of the Tesla Valve. The different Tesla valve designs are evaluated by nanoparticle tracking analysis for their ability to efficiently generate nanobubbles under controlled flow conditions.

**(UG8)**

**Analysis of Phenyl Mercapturic Acid as a Biomarker for Benzene Exposure**

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Benzene is a widespread environmental contaminant linked to serious adverse health effects, creating a need for sensitive and reliable methods to monitor human exposure. This study focuses on the development and evaluation of an LC–MS/MS method for the analysis of the urinary benzene metabolites pre-phenylmercapturic acid (pre-PhMA) and phenylmercapturic acid (PhMA) to assess low-level benzene exposure in urine samples collected during pregnancy. Using tandem mass spectrometry, the compounds are separated chromatographically and quantified using selective mass transitions and appropriate internal standards. Preliminary data from 231 samples suggest that using PhMA alone for quantification does not accurately represent exposure. Nearly all samples that previously showed low amounts of PhMA resulted in having prominent amounts of pre-PhMA present. Because pre-PhMA can undergo dehydration to form PhMA, accurate quantification requires careful consideration of the relationship between the two metabolites. The goal of this work is to improve the reliability of benzene biomonitoring by characterizing and quantifying both metabolites, evaluating how their individual and combined measurements represent low-level benzene exposure, and investigating the association between low-level exposure and adverse pregnancy outcomes.

**(UG9)**

**Single Particle Analysis of Sub-micron Microplastics via Fluorescence Optical Photothermal Infrared Spectroscopy (FL-O-PTIR)**

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Microplastics and nanoplastics (MNPs) are synthetic or semi-synthetic organic polymers, ranging in size from 1 mm to 5 μm and less than 5 μm, respectively. MNPs that accumulate and persist throughout the atmosphere have been linked to worsening respiratory diseases. These particles exist primarily in the lower size regimes. Consequently, one major issue researchers face when attempting to identify single particle MNPs is the spatial limitations of vibrational spectroscopy techniques at the micron scale. For example, Raman spectroscopy provides spectral information down to 1 μm. However, fluorescence can overwhelm the Raman signal making it difficult to obtain useful data. Fourier transform infrared spectroscopy (FT-IR) is not impacted by fluorescence, but is limited by a size threshold of approximately 10 μm. Optical photothermal infrared spectroscopy (O-PTIR) uses IR light to induce localized thermal expansion of a particle and a visible wavelength probe laser to measure the resulting change in refractive index. The recent implementation of counterpropagating light sources allows O-PTIR to characterize particles as small as 400 nm while simultaneously collecting Raman spectra. Fluorescence guided O-PTIR (FL-O-PTIR) further improves on this technique using fluorescence-based image differentiation to allow for more efficient particle selection, increasing throughput, particularly in complex mixtures. For this project, MNP, atmospheric, and fluorescent standards were impacted onto calcium fluoride substrates to demonstrate the efficacy of the FL-O-PTIR technique. Particle sizes were confirmed using environmental scanning electron microscopy (E-SEM); elemental composition was characterized using energy-dispersive X-ray spectroscopy (EDX).

**(UG10)**

**Structural and Energetic Effects of C2′ Methylation to Protonated Cytidine and Uridine Nucleosides: IRMPD, ER-CID, and Theoretical Studies**

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Nucleosides are among the foundational molecules that form the basis of all life. Nucleoside modifications occur naturally though a variety of mechanisms and can also be introduced via chemical synthesis. The canonical DNA and RNA nucleosides are composed of a nitrogenous base covalently bonded to a 2′-deoxyribose or ribose sugar moiety. Modifications can occur or be synthesized at select positions of the nucleobase and virtually every position of the sugar moiety, but occur most commonly at the 2′-position. C2′-methylcytidine and C2′-methyluridine are examples of synthetic nucleoside analogues that have pharmaceutical applications as antiviral drugs. This work examines the effects of C2′methylation on the structure and glycosidic bond stability of the protonated forms of these nucleoside analogues via complementary tandem mass spectrometry experiments and computational chemistry approaches. Results for C2′-methylcytidine and C2′-methyluridine are compared to findings for canonical cytidine and uridine and their O2′-methylated analogues, O2′-methylcytidine and O2′-methyluridine, to straightforwardly elucidate the effects of C2′methylation and to compare the influences of methylation at the 2′-hydroxy oxygen vs. the 2′-carbon atoms. Two types of tandem mass

spectrometry approaches are employed that differ only in the means by which the ions are activated. Infrared multiple photon dissociation (IRMPD) action spectroscopy experiments examine the wavelength dependence of the IR photodissociation of these systems and provide structural information. Energy-resolved collision-induced dissociation experiments combined with survival yield analyses provide a measure of the relative glycosidic bond stability. Our computational workflow begins with a molecular mechanics simulated annealing protocol to rapidly identify viable candidate structures of the nucleosides, which are then subjected to high-level geometry optimization using density functional theory methods. The structures that manifest in the experiments are determined by comparing the measured IRMPD spectra to the IR spectra predicted for the stable low-energy conformations found. Mapping of the glycosidic bond cleavage pathways provides mechanistic details and theoretical estimates for the activation energies for glycosidic bond cleavage. Comparison of the trends in the relative glycosidic bond stabilities measured and predicted are used to elucidate the influence of these modifications on glycosidic bond stability.

**(UG11)**

**Metabolomic and Viability Characterization of PDH1-Deletion Yeast Under Metabolic Challenge**

*Lindsay Chung[1,2], Shreyana S. Keeta[1,2], Nour W. Hamdan[1,2], Christine Shim[1], Hyunmyung Shin[1], Noelle Shakouri[1,2], Nicole A. Najor[2], and Kendra R. Evans[1], [1]Department of Chemistry and Biochemistry, University of Detroit Mercy, Detroit, MI 48221, [2]Department of Biology, University of Detroit Mercy, Detroit, MI 48221*

Putative 2-methylcitrate dehydratase (Pdh1) is a mitochondrial protein involved in propionate metabolism in *Saccharomyces cerevisiae*. The yeast *PDH1* gene is orthologous to the human gene *ACOD1*, which encodes a reported regulator of immunometabolism during inflammation and infection. However, the metabolic and physiological consequences of *PDH1* deletion remain incompletely characterized. To investigate Pdh1 function, we combined liquid chromatography–mass spectrometry (LC–MS)-based metabolomics with a resazurin reduction assay comparing *PDH1*-deletion yeast, BY4741 wild-type (WT) yeast, and *GUT1*-deletion yeast. *GUT1* encodes glycerol kinase, which converts glycerol to glycerol-3-phosphate and is required for efficient glycerol utilization. Therefore, *GUT1*-deletion yeast provides a useful comparison strain for evaluating metabolic activity and viability during exposure to glycerol. For metabolomic analysis, intracellular and extracellular metabolites were extracted from cultures harvested during mid-logarithmic growth and analyzed using reversed-phase chromatography coupled to time-of-flight mass spectrometry in positive-ionization mode. Untargeted feature detection, alignment, and univariate and multivariate statistical analyses were used to identify differential metabolic features, followed by putative annotation through accurate-mass matching to literature databases. Preliminary results suggest that *PDH1* deletion produces multiple metabolic effects. Cellular metabolic activity and viability were also assessed using resazurin, which viable cells reduce to fluorescent resorufin. After correction for baseline fluorescence, significant differences in viability in phosphate-buffered saline (PBS) were observed between *PDH1*-deletion and WT yeast and between *PDH1*- and *GUT1*-deletion yeast. Future studies will expose these strains to glycerol as a metabolic challenge and evaluate strain-dependent changes in viability. Together, these complementary approaches will clarify how *PDH1* deletion alters yeast metabolism and viability under metabolically challenging conditions.

# Graduate Posters

**(G1)**
**Understanding Yellow Dyes in Ancient Peruvian Textiles Using UHPLC-DAD-MS AND DART-MS**

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This research focuses on the analysis of yellow dyes in textiles from archaeological contexts in Peru. Some of the objects are part of the Soldi Collection, and originate from the Ica River Valley near Ocucaje, whereas others are from the Necropolis of Wari Kayan further to the north on the Paracas Peninsula. The textiles date to as early as 2000 years ago and as late as the Inca period. Yellow dyes have been and continue to be the most complex dyes to identify due to their chemistry, which has many overlapping isomers, particularly for the flavonoids. The aim here is to characterize the yellow dyes to see how they change through time and across geographic regions, as well as to determine how they were produced and where their source plant materials may have originated. Rapid screening of samples by DART-MS provides some information, while UHPLC-DAD-MS gives a more comprehensive analysis of all the extracted components. These findings will contribute to the understanding of the technology, culture, and trading patterns of these ancient Peruvian craftspeople and expand upon earlier research on yellow dyes on archeological textiles.

**(G2)**
**Combining Nano-RPLC and CZE-MS/MS for Deeper Histone Proteoform Coverage**

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Bovine histone standard protein mixture is dissolved into nLC-compatible buffer and subjected to offline, 60-minute nanoflow RPLC fractionation. The six fractions are then analyzed via CZE-MS/MS, and the TopPIC suite used for database proteoform identification. The identifications are compared to bovine standard also analyzed exclusively via the CZE-MS/MS with no previous fractionation and exclusively nLC-MS/MS using the same settings/gradient for the individual separation methods as in the combined workflow. The workflow will also be employed to two CRC cell lines (480/620) in attempts to increase sample proteoform coverage. The TopPIC database search for yielded roughly triple the raw identifications compared to either isolated separation methods yielding an average of 317 proteoforms identified and compares competitively with a recent paper published by other groups which combined CZE MS/MS with SDS-PAGE prefractionation, yielding the highest number of identifications in the paper being 225 (Fang, F. *et al.* PROTEOMICS 2024, 24 17). Differential expression analysis showed an increase in expression of acetylated H1 histone proteins in the SW620 sample, aligning with previous conclusions made about histone acetylation causing upregulated genetic expression or overexpression in cancer/disease conditions. The increased proteoform coverage from this workflow unlocks potential for increased understanding of mechanisms of disease, aging, and other relevant biological processes while retaining the macroscopic perspective of top-down proteomics. The modifications and alterations within the proteins give a unique perspective on the conditions of the biological system the proteins were pulled from, far greater than the raw peptide data and conclusions drawn from bottom-up proteomics.

**(G3)**

**Nanobubbles in Desorption Electrospray Ionization Mass Spectrometry**

*George Joseph, Bincy Binny, Andre Venter*

*Department of Chemistry, Western Michigan University, Kalamazoo, MI 49008*

Nanobubbles are buoyant, and unlike microbubbles, remain stable in solution for days or weeks. Nanobubbles (NBs) increase the solvent-air interface surface area and facilitate analyte transport to droplet surfaces. In addition, nanobubbles can act as surface cleaning agents through microstreaming and cavitation effects, removing bound contaminants and improving analyte accessibility. These characteristics make nanobubbles especially relevant for desorption electrospray ionization mass spectrometry (DESI-MS), where surface interactions play a central role. In this study, $N_2$ and $CO_2$ NBs were generated in gas-saturated aqueous solutions using flow-regime switching through a Tesla valve and characterized by nanoparticle tracking analysis. NB-enriched solutions were incorporated as the aqueous component of DESI spray solvents and evaluated using $N_2$ and $H_2$ nebulization gases across different spray voltages, source temperatures, and solvent compositions. Preliminary results demonstrated substantial enhancement of analyte signal intensity and signal-to-noise ratios in both positive- and negative-ion modes. In positive-ion mode, hydrocortisone showed up to 4-fold, while caffeine and glutathione showed up to 8-fold signal enhancement with NB incorporation. In negative-ion mode, ibuprofen and hippuric acid exhibited up to 6- and 4-fold enhancement, respectively, whereas benzoic acid showed up to 12-fold enhancement in additive free solvent systems. Analysis of a SPLASH LIPIDOMIX standard in negative mode further demonstrated compound-dependent effects, with $CO_2$ NBs producing 2- to 4-fold enhancement for multiple lipid species and $N_2$ NBs produced a dramatic enhancement of over 50-fold for selected phospholipids. These findings demonstrate the potential of NB enriched spray solvents as a simple strategy for improving DESI-MS sensitivity across diverse classes of small molecules and lipids.

**(G4)**

**Innovative Methods for Size-Resolved Organic Aerosol Composition Using Offline Aerosol Mass Spectrometry: NYC-METS 2023 Field Campaign**

*Xu He[1], Yao Xiao[2], Ruizhe Liu[3], Evan Dalton[2], Mitchell Rogers[4], Corin Tyler[1], Emily Costa[2], Nga Lee Ng[3,5], Drew Gentner,[4] Andrew P. Ault[2], Rachel E. O'Brien[1*]*

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Urban areas often suffer from high ozone and PM events, both of which can have negative effects on human health. New York City has periods of high particulate matter (PM) concentrations each summer, much of which is formed through secondary processes. To improve our understanding of the changes in the composition and size distribution of urban organic aerosols (OA), 12-hour aerosol particle samples were collected at a ground site in Manhattan during the summer of 2023 as part of the Atmospheric Emissions and Reactions Observed from Megacities to Marine Areas (AEROMMA) campaign using a Micro-Orifice Uniform Deposition Impactor (MOUDI). Samples were characterized with offline-AMS to evaluate the composition of OA as a function of size. A newly developed visualization tool based on delta analysis and delta functional group quantification methods were used to probe size-resolved structural and compositional features under varying air quality conditions. Functional groups vary with aerosol size with more carboxylic acids in the accumulation mode and more aliphatic groups in the largest and smallest size modes.

The impact of carbonate components from dust sources on aerosol composition measurements was examined, and a correction approach was developed for offline AMS analysis. Finally, isotopically labeled internal standards were applied to provide advanced insights into organonitrate characterization with offline AMS. Overall, these results are investigating size-resolved chemical composition and will improve our understanding of OA composition and possible sources within megacities as VOC emissions change.

**(G5)**

**Nanobubbles in Bulk Solution and Electrosprayed Microdroplets Accelerate Chemical Reactions**

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Bulk nanobubbles (NBs) are stable, long-lived gas-filled cavities in solution. They have large surface-to-volume ratios, strong affinity for hydrophobic surfaces, gas-dissolution capacity, and ability to generate reactive species. Chemical reactions are reported to be significantly accelerated within sprayed microdroplets during ESI-MS. Reported acceleration factors range from $10^3$ to $10^6$ relative to bulk. Proposed factors for acceleration include high electric field strength ($10^7$–$10^9$ V/cm), ordered reagent alignment, reagent confinement, partial solvation of reagents, and changes in droplet pH. Similar processes likely occur at gas-liquid interface of NBs, thereby increasing reaction rates. We show that deliberate NB addition accelerates bulk or microdroplet reactions. We demonstrate this for the Katritzky reaction and for the reactions between *N*,*N*-Dibutyl-1,3-propanediamine (DBPA) and $CO_2$. NB addition to bulk solution produced a 2X acceleration factor for the Katritzky reaction, whereas a 6X acceleration factor was observed in microdroplets. In the $CO_2$ sequestration reaction using DBPA, the reaction solvent is enriched with either $N_2$ or $CO_2$ NBs and paired with either $N_2$ or $CO_2$ nebulization gas. In all cases, addition of NBs (either $N_2$ or $CO_2$) produced between 2–50X acceleration factors, depending on generation methods and solvent fraction in which the NB is present. Our findings show that reagent utilization is more efficient when reagents are delivered as NB than by nebulization, as seen in the $CO_2$ sequestration reaction. Differences in magnitude of acceleration factors obtained with NB addition and microdroplets may be explained by differences in the surface area added by NB addition compared with droplet nebulization.

**(G6)**

**Evaluating Indoor Oxidation of Aerosol Particles Containing Quaternary Ammonium Compounds**

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Accurately measuring indoor chemical exposure risk requires a thorough understanding of chemical transport and transformation. For quaternary ammonium compounds (QACs), common in disinfectants and other personal care products, few studies examine QAC chemical lifetimes and oxidation products indoors, which likely affect high-risk populations (e.g., medical, educational, and custodial staff) exposed to elevated concentrations of these chemicals. Understanding chemical changes in aerosol particles is understudied in the indoor context, considering respiratory inhalation risk. To address this gap, we explore nontargeted QAC ozone oxidation in aerosol particles using a PTFE 0.25 $m^3$ chamber. We utilize high-resolution liquid chromatography tandem mass spectrometry (HR-LC-MS/MS) to identify QAC oxidation products

and resolve functionalized QAC isomers impacted onto a Teflon filter. We compare our offline HR-LC-MS/MS results to online aerosol mass spectrometer (AMS) spectra to validate online measurement capabilities. We work towards incorporating an AMS diagnostic peak at *m/z* 58 (C3H8N+) to elucidate oxidation kinetics. This future work will formalize the chemical fate of QACs indoors, expanding our kinetic and mechanistic understanding in the indoor environment. More importantly, our investigation provides crucial constraints to predict and model exposure risk indoors.

**(G7)**

**Systematic Evaluation of Gas Dynamics and Electrospray Emitter Position as Reagent-Free Supercharging Methods for Native Mass Spectrometry**

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Native Mass Spectrometry has become an important tool in structural biology. However, conventional optimization practices typically prioritize analyte desolvation and ion signal intensity, often evaluating the utility of specific in-source physical parameters, such as nanoelectrospray (nESI) emitter positioning and in-source gas flow dynamics, through only these limited figures of merit. Prior work has indicated that nESI ion source parameters can be tuned to produce conditions leading to protein and nucleic acid supercharging, although the broader impacts on gas-phase ion structure remain largely unexplored. Here, we systematically evaluate source parameters using ion mobility-mass spectrometry (IM-MS) and collision-induced unfolding (CIU) to improve the tunability, establish causal mechanisms, and evaluate the utility of the supercharged ions produced under such conditions. Our initial results indicate that in-source physical parameters can systematically alter the protein ion structures produced by nESI. Increasing purge gas flow (0–800 L/h) on the Waters Cyclic IMS yielded a ~5% increase in BSA arrival time centroid, while average charge state remained relatively stable. However, CIU of the 16+ state revealed significant shifts in CIU50-2 and CIU50-3 transition voltages, with a new CIU feature emerging at ~600 L/h. At 200 L/h, the CIU fingerprint resembled that of 0.25% sulfolane-based supercharging, though differences in the CIU50-3 region suggest distinct structural populations. Emitter position experiments on the Agilent 6560C showed that longitudinal displacement (up to ~15 mm) minimally affected BSA charge state distribution, yet CIU of 17+ ions revealed a ~7% decrease in CIU50-3 transition voltage. These findings suggest that structural integrity can be compromised despite the lack of a supercharging effect. All these data collectively underscore CIU as a sensitive probe for monitoring unintended structural alterations driven by in-source nESI conditions.

**(G8)**

**Stability Study of Different Types of Nanobubbles**

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Nanobubbles (NBs) are gas-filled spherical structures with diameters on the order of a few hundred nanometers. According to the Young–Laplace equation, the immense internal pressure generated by their high surface curvature should cause them to collapse or dissolve within milliseconds. Contrary to this classical prediction, however, nanobubbles have been experimentally observed to persist for days to weeks, and potentially up to months, making the mechanisms underlying their anomalous stability an open question. In this study, we investigate nanobubble longevity and characterize how zeta potential and bubble size evolve over time

across four solvent systems: 100% water, 3% ethanol–water, 50:50 methanol–water, and 100% methanol. Measurements are performed using a Nanoparticle Tracking Analyzer (NTA), which combines Brownian motion video analysis and laser-scattering microscopy with electrophoretic light scattering to determine particle size distribution and zeta potential. Preliminary data indicates that stability varies by solvent- and constituent-gas compositions but in all cases the NBs remain stable for at least a week. Our previous work has demonstrated that nanobubbles enhance the signal intensity of small molecules, proteins, and lipids in mass spectrometry techniques such as electrospray ionization (ESI) and desorption electrospray ionization (DESI). Given this analytical benefit, establishing nanobubble stability and shelf life is critical, determining how long they retain their properties after bulk preparation will directly inform their practical use in such applications.

**(G9)**

**Pushing the Limits: Investigation of Analytical Techniques for Halide Quantification in Ambient Particles Collected during Flights over the Arctic**

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Natural halogen cycles in the Arctic are sustained by multiphase reactions, yet the role of atmospheric particles in this chemistry is understudied, especially in the context of the rapidly changing Arctic. As the Arctic undergoes accelerated warming, more sea ice is fracturing to form leads, which are sources of sea spray aerosol that contain halides ($Cl^-$, $Br^-$, and $I^-$). Sea spray aerosol seed cloud droplets, participate in multiphase reactions, and propagate halogen chemistry. The CHemistry in the Arctic: Clouds, Halogens, and Aerosols (CHACHA) airborne field campaign was based in Utqiaġvik, AK, from February to April 2022. A particle-into-liquid sampler was deployed on a research aircraft to collect particles in water while flying over leads and through clouds. Due to the expected low halide concentrations and limited sample volumes, the analytical technique used for halide quantification must be extremely sensitive. Previously, neutron activation analysis was used to quantify halogens in airborne particles collected in the Arctic, but this technique typically requires large sample volumes and extensive sample preparation. More recently, ion chromatography coupled to inductively coupled plasma – mass spectrometry (IC-ICP-MS) has detected halides in smaller sample volumes. However, many IC-ICP-MS techniques exhibit a tradeoff between the limits of detection and sample volume, so the challenge of minimizing both for a sensitive analysis remains. This work explores the potential of several analytical techniques for these unique and valuable samples.

**(G10)**

**Analysis of Fluorescently Derivatized Anatoxin-a Using LC-FLD-MS**

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Anatoxins (ANAs) are neurotoxic alkaloids produced during cyanobacterial harmful algal blooms (cyanoHABs). Anatoxin-a (ANA-a), the most common ANA congener, is typically monitored in drinking water by ELISA. LC-MS/MS can separate and quantify ANA congeners, but derivatization with a fluorescent dye enables efficient analysis by reversed-phase LC with fluorescence detection (FLD). Herein, LC-FLD was coupled to a high-resolution mass spectrometer (HRMS) via post-column flow splitting for parallel detection of ANA-a derivatized with 4-fluoro-7-nitrobenzofurazan (NBD-F) (James *et al.*, 1996), with the goal of improving identification and quantification of ANA congeners. UHPLC-FLD-MS analysis of underivatized and derivatized ANA-a standards, as well as water samples from Grand Lake St. Marys, Ohio, was performed. The underivatized ANA-a standard eluted at 2.68 min (*m/z* 166.1224), and LC-HRMS confirmed its identity in a cyanoHAB sample (retention time 2.69 min, *m/z* 166.1224). FLD detected NBD-F-derivatized ANA-a (*m/z* 329.1244) at 530 nm and MS detected it at 4.69 and 4.72 min, respectively, and MS/MS spectra confirmed its identity. FLD gave $1.5\times10^{6}$ emission counts, and MS gave $1.79\times10^{6}$ signal intensity per 20 µL injection, reflecting each detector's sensitivity. The present LC-FLD-MS approach enables parallel analysis of ANA-a in cyanoHAB samples using accurate mass measurements, MS/MS, and fluorescence detection.

**(G11)**

**Canadian Wildfire Smoke over Michigan in Summer 2026: A Size-Resolved View of Aerosol Chemistry**

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During the summer of 2026, smoke from Canadian wildfires was transported into Michigan, resulting in elevated particulate matter ($PM_{2.5}$) concentrations and degraded air quality. Statewide air quality alerts were issued, and Air Quality Index (AQI) readings reached hazardous levels at several monitoring sites. These smoke events highlight the impact of transported smoke on downwind communities and the need to characterize wildfire aerosols in detail. The organic fraction is a major component of submicron wildfire particles, and its composition can be changed during atmospheric transport. These processes can alter the organic composition and distribution across particle sizes as well, highlighting the importance of size-resolved chemical characterization of the transported smoke particles. Such measurements can provide insights into $PM_{2.5}$ mass concentrations and chemical information relevant to examining smoke exposure in affected communities. Here, we examine the size-resolved smoke particles collected on polytetrafluoroethylene (PTFE) filters using a micro-orifice uniform deposit impactor (MOUDI) at the University of Michigan on July 16-17, 2026. Samples were analyzed by offline aerosol mass spectrometry (AMS) to determine elemental ratios and average carbon oxidation state for each size fraction. We further apply our laboratory's delta analysis, which analyzes mass spectra with homologous $CH_2$ series, alongside functional group distribution analysis to estimate the relative contributions of alkyl, aromatic, carboxylic acid, ketone, and alcohol groups. By combining functional group distributions with elemental ratios and carbon oxidation state, we can better characterize how the organic composition of Canadian wildfire smoke transported to Michigan varies across particle size.

**(G12)**

**Measurements of Wildfire Smoke Transported to Southeast Michigan Using a Suite of Gas- and Particle-phase Instrumentation**

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The frequency and severity of fires across the globe is rising, in part due to rising temperatures. Wildfires are becoming a norm in parts of the United States and Canada. In recent years, Michigan has experienced long-range transport of smoke plumes from both western United States and Canadian wildfires. Wildfire smoke is harmful to human health; poor air quality puts vulnerable individuals with respiratory issues at higher risk. Wildfire smoke can also negatively affect many businesses as Michigan's tourism industry will be affected due to poor visibility, it can also cause dangerous conditions for aviation, including flight delays and cancellations, causing even more economic losses. Smoke from wildfires can contribute to high levels of nitrogen oxides ($NO_x$ = NO and $NO_2$), ground level ozone ($O_3$), and volatile organic compounds (VOCs). $NO_x$ and VOC emissions affect local and continental air quality and atmosphere, especially as they react with atmospheric oxidants to create secondary organic compounds during long-range transportation. To improve our understanding of the chemical composition and health and climate impacts of wildfire smoke plumes, the Pratt lab at the University of Michigan deployed a large suite of both particle-phase and gas-phase instruments to make online, *in-situ* measurements of the smoke plumes reaching Michigan from the Canadian wildfires this summer (2026). Here the particle sizing data collected via Scanning Mobility Particle Sizer (SMPS) and Aerodynamic Particle Sizer (APS); $O_3$ and $NO_x$ data collected via monitors in the lab and other monitoring stations across Michigan will be presented.

**(G13)**

**Evaluating Data-Dependent Acquisition and Intelligent Acquisition with AcquireX for High-Resolution Mass Spectrometry-Based Non-Targeted Per- and Polyfluoroalkyl Substances (PFAS) Analysis**

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Per- and polyfluoroalkyl substances (PFAS) are persistent anthropogenic contaminants widely detected in the environment and humans and associated with adverse health outcomes. Although EPA's CompTox Chemicals Dashboard lists more than 21,000 PFAS structures, targeted analysis typically monitors fewer than 100 analytes, leaving most PFAS unidentified and uncharacterized. Non-targeted analysis (NTA) using high-resolution mass spectrometry (HRMS) is a key tool for discovering emerging PFAS. However, acquisition strategy strongly influences feature detection, MS/MS coverage, and reproducibility. This study evaluates conventional data-dependent acquisition (DDA) and the intelligent AcquireX Deep Scan workflow for PFAS NTA across matrices of increasing complexity. Materials from the 2024 NIST PFAS NTA Interlaboratory Study were analyzed using a Thermo Vanquish UHPLC coupled to an Orbitrap Exploris 240 over three measurement weeks. System performance was monitored with an interleaved PFAS quality-control standard mixture, with retention-time CVs below 1% and peak-area variation below 20%, supporting stable instrument performance. Data were processed with FluoroMatch and compared by feature detection, confident annotation, and inter-week reproducibility. In the simple PFAS standard mixture (NIST A), AcquireX yielded 386 unique likely PFAS features and 47 confirmed

identifications, compared with 180 features and 31 identifications by DDA. In the AFFF-impacted soil extract (NIST C), AcquireX yielded 1,464 features and 132 confirmed identifications, compared with 472 features and 82 identifications by DDA. AcquireX also recovered more reproducible features overall, although DDA showed a higher reproducibility rate. These findings demonstrate that iterative intelligent acquisition substantially expands PFAS coverage, with increasing benefit as matrix complexity increases.

**(G14)**

**Single-Particle Chemical Characterization and Source Identification of Wintertime Atmospheric Particles in Polluted Salt Lake City, Utah**

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Salt Lake City (SLC), Utah, experiences severe wintertime air pollution as temperature inversions trap urban emissions near the surface, leading to elevated concentrations of fine particulate matter ($PM_{2.5}$, aerodynamic diameter < 2.5 μm) that pose significant health risks. Bulk measurements, which measure average $PM_{2.5}$, show mainly secondary ammonium nitrate; however, particle-resolved information on the heterogeneity of aerosol composition and sources remains limited. Single-particle measurements enable assessment of the contribution of different emission sources and the distribution of chemical species across individual particles. In this study, atmospheric particles with diameters between 0.18 and 3.2 μm were collected in SLC during January–February 2024 using a miniature micro-orifice uniform deposit impactor (mini-MOUDI). A total of 12,590 individual particles were analyzed using computer-controlled scanning electron microscopy with energy-dispersive X-ray spectroscopy (CCSEM-EDX). These measurements reveal the composition and morphology of individual particles, which helps identify their sources and how they have changed in the atmosphere since emission. Particle size and elemental composition were used to classify particles into distinct groups, enabling source attribution across different pollution events. Focus is placed on nitrogen-containing aerosols, including nitrogen-rich C/O/S (carbon/oxygen/sulfur) particles, road salt, and dust particles, due to their potential roles in heterogeneous chemistry and secondary nitrate formation. The single-particle measurements enable the detection of metal-containing aerosols that are poorly characterized by many conventional aerosol techniques and reveal their mixing with other elements. These particle-level mixing relationships provide insight into the sources and chemical transformation of wintertime aerosols in the Salt Lake City urban basin.

**(G15)**

**Proteomic Evaluations of Transmembrane Protein Enrichment in Nanodiscs**

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Membrane proteins are critically important pharmaceutical targets and thus their analytical characterization is vital to drug development efforts. However, compared to cytosolic proteins, membrane proteins are generally more difficult to purify and/or analytically characterize in part due to their amphipathic nature. Nanodiscs (NDs) have become a popular membrane mimetic

system offering a well-defined lipid bilayer environment to stabilize membrane proteins for in vitro analyses. NDs based on membrane scaffold proteins (MSPs) offer advantages in terms of their amenability to purification and control over lipid composition. Here we investigated the utility of MSP NDs that have different diameters and lipid compositions to enrich membrane proteins isolated from cells with liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis. Of the top 100 proteins with the highest intensities, we found that transmembrane proteins were highly prevalent, suggesting that NDs provide a mechanism to enrich these proteins in a bottom-up proteomic workflow. Additionally, when compared to the detergent micelle conditions, most proteins that were enriched in the ND samples were transmembrane proteins. These findings lay the foundation for developing ND synthesis conditions that can enrich transmembrane proteins while maintaining their original functions and activities.

**(G16)**

**Tabular Foundation Models Enable Multiplexed Sensors with Enhanced Predictive Ability and Dynamic Self-Adjustment**

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Deep learning artificial intelligence models are increasingly integrated with multi-analyte biosensors, but high-quality implementation requires signal preprocessing, large datasets, application-specific model development, and sensor modalities with fingerprinted spectra or imageable readouts. Herein, we illustrate how deep learning may be readily applied to any multiplexed sensor without requiring users to train domain-specific models. Briefly, multiplexed outputs from silicon photonic microring resonator immunoarrays were added to the context window of an open-source tabular transformer model (TabPFN), enabling signal processing and probabilistic clinical predictions via in-context learning. TabPFN successfully derived analyte concentrations from unprocessed assay sensograms and displayed superior immunoarray-based clinical predictions relative to random forest and XGBoost models across 519 patient samples. Single forward-pass TabPFN predictions were improved by averaging results from multiple context windows, with 20 or more windows per sample yielding high-quality estimates. Finally, TabPFN context windows engineered with periodized calibration sensograms demonstrated prospective signal prediction abilities, potentially facilitating automated self-modulating assay designs. These findings may be readily applied to other multiplexed platforms.

**(G17)**

**Ultra-Long Capillary Zone Electrophoresis-Electrospray Ionization-Tandem Mass Spectrometry for Enhanced Native Proteomics**

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Native mass spectrometry provides a powerful approach for characterizing intact proteins, preserving biologically relevant non-covalent interactions during analysis. Capillary zone electrophoresis coupled to electrospray ionization-tandem mass spectrometry (CZE-MS/MS) has proved useful for native proteomics due to its strong separation and sensitive detection capabilities. Challenges of CZE include a low sample loading capacity and narrow separation window. Our previous work has utilized a 1-meter fused silica capillary containing a neutral coating on its inner wall and a highly efficient dynamic pH junction-based protein stacking method to combat these issues. To further increase the separation window and sample loading capacity of our CZE-MS/MS system, this study employs an ultra-long 3-meter separation capillary for

native analysis of a standard protein mixture consisting of carbonic anhydrase (CA), bovine serum albumin (BSA), and myoglobin. This extension leads to a lower electric field across the capillary, resulting in a much wider separation window as the electrophoretic velocity of proteoforms decreases. This allows for a greater acquisition of MS/MS spectra for proteoform identification. Additionally, the extended capillary allows for a larger sample loading volume while maintaining separation efficiency. With a 180-min separation window, the use of an ultra-long capillary provides greater resolution of intact protein species for native analysis. Separation of individual protein aggregates and oligomers has been observed with differing charge-state distributions. These results demonstrate the potential of an extended separation capillary to further increase proteoform coverage of native samples. The use of more complex biological samples, such as human plasma, will further validate this strategy.

**(G18)**

**Investigation of Transported Boreal Wildfire Smoke using Single-Particle Mass Spectrometry on a Research Aircraft**

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Wildfires are a significant source of aerosols and gases and are increasing in frequency and intensity globally. Transported Canadian boreal wildfire smoke impacts both the Arctic and mid-latitude regions (including Michigan). As it is transported in the atmosphere away from the fire source, smoke undergoes chemical reactions that alter the smoke properties. Due to the wide range of chemical processes that occur, identification of aged biomass burning aerosols is a challenge for analytical techniques. Atmospheric models also struggle to reproduce value ranges for the physical and chemical properties of aged smoke, producing outputs with large ranges and. During the Summer 2024 NASA Arctic Radiation-Cloud-Surface Interaction Experiment (ARCSIX), individual aged biomass burning aerosols from boreal fires were detected in real-time using the aircraft aerosol time-of-flight mass spectrometer (A-ATOFMS) aboard the NASA P-3 aircraft. Here, we report results of the analysis and interpretation of single-particle mass spectra collected during a transit flight from Pituffik, Greenland to Wallops Island, Virginia, USA that included a wide spatial extent of transported smoke. Periods of aged smoke influence are identified based on mass spectral markers of individual aerosols. The presence of specific chemical markers can also be used to identify specific chemical reactions which are known to be a part of smoke aging. This work seeks to improve the understanding of aged smoke chemical composition and its physical properties, as wildfires become more prevalent.

**(G19)**

**Abstract Withdrawn**

**(G20)**

**Release Profiles of Organics, PFAS and Inorganic Elements During Irrigation Events in Commercial Containerized Horticulture Crop Production**

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Ornamental plants have exploded in popularity as modern decor, while also offering a rewarding hobby for consumers. Commercial horticulture generated $18 billion in sales in 2024 in the United States and consumed over one billion plastic nursery planters and containers. Water consumption for irrigation in container-based productions can be up to 18 $Lm^{-2}day^{-1}$ heavily relying on irrigation runoff capture and reuse. While the industry is contributing to the national economy, production sites create a unique chemical environment worth closer attention to the monitoring of irrigation runoff beyond traditional parameters and constituents, e.g., pH, salinity, suspended solids, and nutrients. Therefore, we investigated the impact of organic compounds, with particular interest on agrochemical- and plastic industry related compounds, per- and polyfluoro alkyl substances (PFAS) and trace level elements, in particular rare-earth elements (REEs) along with "heavy metals" on the quality of irrigation water and runoff. This study focused on investigating release profiles as a function of time of the abovementioned analytes during irrigation events using automated sample collection systems. Due to high dilution factors, analytes of interest were preconcentrated and removed from the matrix by specialized extraction methods before being analyzed by gas chromatography–mass spectrometry (GC–MS) for untargeted screening of volatile and semi-volatile organics, liquid chromatography–tandem mass spectrometry (LC–MS/MS) for fourteen targeted PFAS species and inductively coupled plasma–tandem mass spectrometry (ICP–MS/MS) for targeted analysis of forty elements. The identification of accumulated organic compounds and inorganic elements, and their time-dependent profiles in irrigation runoff will be discussed.

**(G21)**

## Proteoform Barcode: An Intuitive Visualization Framework for Top-Down Proteomics Results

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Over the past several years, top-down proteomics has demonstrated strong capability in identifying large numbers of proteoforms. However, results are most often presented simply by reporting the total number of identified proteoforms, which provides limited biological insight, particularly in clinical studies. Effective visualization is essential for clearly interpreting proteomic differences between patients and healthy individuals. Here, we introduce a proteoform barcode to intuitively visualize top-down proteomics results. Proteoforms are grouped by gene along the x-axis, and bar color represents relative proteoform intensity, with darker colors indicating higher abundance. This approach enables rapid, intuitive interpretation of complex proteoform data. Histone extracts from two human colorectal cancer (CRC) cell lines, SW480 andSW620, were analyzed using a CZE–Orbitrap 480 system, with 20 runs performed for each cell line following previously reported procedures. Proteoform identification was carried out using TopPIC. Identified proteoforms were then grouped by gene and annotated by biological function and pathway using the R packages clusterProfiler, ReactomePA, and org.Hs.eg.db. Proteoform barcodes were generated using ggplot2 for visualization. In addition, previously published serum proteoform datasets were used to demonstrate barcode-based differentiation between healthy individuals and Alzheimer's disease (AD) patients. Our preliminary results demonstrate that the proteoform barcode enables clear and intuitive discrimination between the colorectal cancer cell lines SW480 and SW620 across three independent runs. Within each cell line, barcodes exhibit high similarity

across runs, indicating strong run-to-run reproducibility. In contrast, when reproducibility between runs is compromised, the corresponding barcodes become visually disordered and inconsistent, highlighting the ability of this approach to directly reflect data quality and experimental stability. Beyond cell line data, we applied the proteoform barcode to previously published serum proteomics datasets from AD patients and healthy individuals. The barcode representation revealed that the primary differences between the two groups are associated with proteoforms derived from the HBA_HUMAN and HBB_HUMAN genes. Although these proteins are not currently considered core AD biomarkers, their proteoform-level differences are clearly captured by the barcode and enable effective visual separation between healthy and AD samples. This observation underscores the value of proteoform-resolved visualization, as subtle yet systematic changes that may be overlooked in conventional numerical summaries can be readily identified. Together, these results demonstrate that the proteoform barcode not only facilitates biological comparison across conditions but also serves as a practical tool for assessing reproducibility and uncovering meaningful proteoform-level patterns in complex clinical proteomics datasets.

**(G22)**

## Spectroscopic Characterization and Mass Spectrometric Identification of Phycobiliproteins from a Cyanobacterial Extract

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Phycobiliproteins (PBPs) play a significant role in light harvesting and photosynthesis in cyanobacteria. C-phycocyanin (C-PC), allophycocyanin (APC) and C-phycoerythrin (C-PE) have been reported as major cyanobacterial PBPs. Analysis of PBPs and other proteins in cyanobacteria provides information on their identities, quantities and molecular structures. Herein, proteins in a cyanobacterial extract were identified and quantified using different analytical methods. Cyanobacterial proteins were extracted from cyanobacteria collected at the shore of Lake Erie. Total protein concentration in the extract was determined using bicinchoninic acid (BCA) assay. C-PC amount in the extract was measured by fluorescence spectroscopy (FS). Initial characterization of the PBPs in the extract was done using UV-visible (UV-vis) spectroscopy. The proteins in the extract were separated by native poly acrylamide gel electrophoresis (Native PAGE) and sodium dodecyl sulfate-poly acrylamide gel electrophoresis (SDS-PAGE). Protein bands were detected using fluorescence imaging and Coomassie blue staining. Stained protein bands were excised from the gel and subjected to trypsin digestion. The resulting in-gel digest peptides were extracted and analyzed by liquid chromatography-electrospray ionization mass spectrometry (LC-ESI-MS). Acquired MS and tandem mass spectrometry (MS/MS) data were processed using “Proteome Discoverer” (Thermo) software for protein identification. UV–vis spectra showed absorption maxima at 570 nm and 620 nm, indicating the presence of C-PE and C-PC in the extract, respectively. FS analysis yielded a C-PC concentration of ~0.31 mg/mL, while total protein concentration was 0.58 ± 0.01 mg/mL. LC-ESI-MS analysis of in-gel protein digests and peptide-spectrum matching resulted in identification of several proteins, including C-PC and APC.

**(G23)**

**Developing a Method for Quantification of Saxitoxins in Water by Coupling Hydrophilic Interaction Liquid Chromatography with Mass Spectrometry**

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Saxitoxins (STXs), also known as paralytic shellfish toxins (PSTs), are highly polar neurotoxic alkaloids associated with harmful algal blooms (HABs). Their analysis by liquid chromatography–mass spectrometry (LC–MS) is complicated by their high polarity, matrix-induced ion suppression, in-source fragmentation, and the presence of structurally similar congeners. A multidimensional analytical approach combining hydrophilic interaction liquid chromatography (HILIC) with mass spectrometry was investigated to improve the separation and selective detection of STXs. Ultra high-pressure liquid chromatography (UHPLC) conditions were optimized using an ethylene-bridged hybrid (BEH) HILIC stationary phase to improve retention and peak shape of highly polar STXs. A STX congener eluting from the HILIC column was ionized by electrospray ionization (ESI)-MS and quantified by using a triple quadrupole mass spectrometer in selected reaction monitoring mode. The present approach demonstrated the utility of integrating a new sample preparation and injection protocol with BEH HILIC column for quantification of a STX by UHPLC-MS/MS. This strategy is currently applied toward enhancing trace-level determination of STX congeners in lake water collected during HABs.

**(G24)**

**Detecting Underground VOC Contamination via Phytoscreening: A Pilot Study in Elkhart, Indiana**

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In Elkhart, Indiana, the U.S. EPA has established six Superfund sites and identified three vapor intrusion risk areas from underground volatile organic compound (VOC) contamination. Phytoscreening, an emerging technique that detects underground contaminants by analyzing plant tissue, has proven effective for identifying chlorinated VOCs such as trichloroethylene (TCE) at sites with known spills in Detroit, Michigan. This pilot study asked two questions: can Detroit-style phytoscreening be used in Elkhart, and does phytoscreening data spatially correlate with EPA groundwater contamination data? We collected 10 plant root samples in and around EPA Superfund sites in Elkhart, targeting one vapor intrusion risk area identified by the EPA at Lusher Street. Root samples were analyzed for TCE using headspace SPME-GC-MS/MS. We matched each plant sample to the nearest groundwater monitoring well and assessed the relationship using Kendall's tau. TCE was detected in 5 of 10 plant root samples (0.3-22.7 ng/g). TCE concentrations in plant roots and nearest neighbor groundwater wells showed a moderate positive correlation (Kendall's tau = 0.43, p = 0.12, 95% CI: -0.11 to 0.97). Phytoscreening of weedy plants detected underground VOC contamination at a known Elkhart contamination site, consistent with prior Detroit applications. TCE detection patterns in plants generally match groundwater detection patterns. Although the correlation was moderate and did not reach statistical significance, these findings support the need for a larger, more comprehensive study to evaluate whether opportunistic phytoscreening can serve as a reliable, low-cost surrogate for groundwater and soil sampling to support vapor intrusion risk assessments.

**(G25)**

## Cyanotoxin Distribution in Freshwater Systems and Fish: Spatial and Temporal Trends and Matrix-Matched UPLC–MS/MS Method Development

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Cyanobacterial harmful algal blooms (cHABs) are widespread events that threaten aquatic ecosystems and human and wildlife health through the production of bioactive metabolites, including microcystins (MCs) and anabaenopeptins (Aps), which inhibit protein phosphatases and carboxypeptidases, respectively. Green Bay (GB), Wisconsin, and Grand Lake St. Marys (GLSM), Ohio, have extensive histories of harmful algal blooms. We used targeted liquid chromatography–tandem mass spectrometry (LC-MS/MS) to investigate spatial patterns in GB and temporal trends in GLSM, while developing a method to quantify 14 MC and six AP congeners in fish tissue. In GLSM, cyanotoxins were detected from 2022-2026 with concentrations generally peaking near October, except for a pronounced MC increase in May 2025. Several individual toxins reached approximately 10 µg/L or greater. Comparisons of filtered and unfiltered samples indicated that toxins were predominantly associated with the particulate/intracellular fraction. Aps were more abundant than MCs in both systems, with AP-F prominent in water samples. In GB, both toxin groups were detected throughout the bay in 2024, with concentrations generally increasing toward the southern bay near the Fox River. Fish tissue analysis detected AP-F in carp from both systems at concentrations up to 1.660 µg/kg. Shad exhibited the highest reported total AP concentrations, ranging from 0.500 to 2.297 µg/kg. These findings demonstrate substantial cyanotoxin diversity, spatial and temporal variability, and toxin occurrence in fish, underscoring the value of monitoring multiple toxin classes in freshwater ecosystems.

# Research Associate & Industrial Posters

**Untargeted Analysis of Blended Fruit and Vegetable Beverages (Smoothies) Using Head-Space Solid Phase Microextraction, Thermal Desorption, Enhanced Chromatography, and High-Performance Time-of-Flight Mass Spectrometry**

*Noah Houseworth, David E. Alonso, and Joe Binkley*
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Blended beverages are complex food matrices made up of fruits, vegetables, and supplemental ingredients that contribute to a wide range of compounds. These compounds influence flavor and aroma, and can serve as indicators of freshness, processing, or contamination. Advanced analytical techniques are necessary to effectively analyze these mixtures. The goal of this study was to evaluate headspace solid-phase microextraction (HS-SPME) gas chromatography (GC), and thermal desorption (TD) GC–mass spectrometry (GC–MS) for profiling the compounds in these nutrient-rich beverage samples. A range of commercially available and laboratory-supplied beverages were analyzed. Samples were subjected to HS-SPME for the extraction of volatile compounds, while complementary analysis using thermal desorption enabled capture of semi-volatile constituents. GC and GC–MS systems were used for compound separation and detection. Data were processed using automated non-targeted peak detection workflows. Compound identification was achieved through spectral library matching (NIST/Wiley), retention index alignment. Data were normalized and subjected to principal component analysis (PCA) to visualize clustering patterns and identify major sources of variance. The combined HS-SPME-GC-MS and TD-GC–MS workflow enabled comprehensive profiling of beverage components. Detected compounds included esters, alcohols, aldehydes, ketones, terpenes, and organic acids associated with characteristic fruit and vegetable aromas and flavors. Semi-volatile compounds such as phenolics, additives, and trace contaminants related to processing or packaging were also observed. HS-SPME demonstrated strong sensitivity for highly volatile compounds, while thermal desorption expanded analytical coverage to less volatile species. Statistical analysis revealed clear differentiation between smoothie types, with distinct compositional profiles driven by ingredient composition and processing conditions. Key discriminant compounds included specific esters, terpenes, and phenolic compounds. The integration of HS-SPME and TD-GC–MS provides a complementary approach for the comprehensive characterization of beverage matrices. This methodology is well-suited for applications in food quality assessment and authenticity verification.

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| Graduate Poster Judges | Marwa Abdel Latif<br>Will Colin<br>Matt Fhaner<br>Jon Kirchoff<br>Ashley Lalonde<br>Irfana Muqbil<br>Donna Seibert<br>Andre Venter |

Special Thanks to Volunteers Who Assisted at the Symposium ! ! !

## Notes

MARK YOUR CALENDAR and SAVE THE DATE

# Anachem

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# 2027

VisTaTech Center
Schoolcraft College, Livonia, Michigan
November 4, 2027