EASTERN ANALYTICAL SYMPOSIUM & EXPOSITION 2023

Better life with Analytical Chemistry

Crowne Plaza Princeton Conference Center Plainsboro, NJ **November 13–15, 2023**

Final Program



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The Eastern Analytical Symposium & Exposition is sponsored by the Analytical Division, the North Jersey and the New York Sections of the American Chemical Society; the American Microchemical Society; the Chromatography Forum of Delaware Valley; the Coblentz Society; the New York Microscopical Society; the Delaware Valley, New England, & New York Sections of the Society for Applied Spectroscopy; the Association of Laboratory Managers; the New Jersey Association of Forensic Scientists; and the Chinese American Chromatography Association

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For updates and discussions follow us on:



Parking & Shuttle Services

Parking is available at the nearby Princeton Alliance Church at 20 Schalks Crossing Road, Plainsboro which is just 0.7 miles away. EAS Trolley shuttle service will be available every 10 min. from 7:00 AM to 6:30 PM on Monday & Tuesday to transport you from the overflow Church parking lot to & from the Conf. Center.

Better Life with Analytical Chemistry Frank Romano, EAS 2023 President



Welcome to the Eastern Analytical Symposium and Exposition! Thank you to our EAS Board, Exhibitors, Sponsors, Crowne Plaza staff and all those who have helped contribute to the success of this year's symposium. The EAS 2023 theme is *Better Life with Analytical Chemistry*, depicted by a beautiful and relaxing sunny beachscape. Society relies on science and technology to improve the quality of our lives through the development of better products and services in many industries including Pharmaceuticals, Forensics, Environmental, Cosmetics, Food and Flavors, Cannabinoids, Clinical Diagnostics, Energy, Science Education, and others. The technology available to today's scientists continues to become increasingly more powerful and critical to our success. While you're attending EAS 2023, please take the time to enjoy that *Better Life* and stop by our beach mural for photo ops in the lobby of the Convention Center for a reminder.

Our Keynote Lecture speaker, Dr. Vasilis Vasiliou, Yale University, is giving a talk on "Exposome and Human Disease; From Neurological Disorders to Diabetes and Cancer" on Monday afternoon at 4:15 PM. Dr. Vasiliou is the Susan Dwight Bliss Professor of Epidemiology and the Chair of the Department of Environmental Health Sciences at Yale School of Public Health.

Early risers will be rewarded with our Tuesday morning Breakfast Lecture at 8:00 AM, featuring Dr. Frank Nichols, who will be speaking on "Fractionation and Characterization of Bacterial Complex Lipids using Analytic Chemical and Mass Spectral Approaches". Dr. Nichols is a Professor in the Division of Periodontology at the University of Connecticut School of Dental Medicine. He has served as curriculum director for undergraduate Periodontics didactic/clinical program as well as the Periodontics residency program director.

On Wednesday, Professor Sibrina Collins, Lawrence Technical University, will give a Plenary Lecture on "Inclusive Stories in Chemistry: Celebrating Dr. Marie Maynard Daly". Dr. Collins served as the Founding Executive Director of the Marburger STEM Center on the campus of Lawrence Technological University (2016-2023). Beginning January 2023, she was appointed as Executive Director of STEM Education for the College of Arts and Sciences (CoAS) at Lawrence Tech.

The EAS Board is proud to sponsor several awards recognizing distinguished career achievements across analytical sub disciplines. Congratulations to the following EAS 2023 Awardees: Professor Robert Kennedy, University of Michigan, Outstanding Achievements in the Fields of Analytical Chemistry; Professor Mary Wirth, Purdue University, Outstanding Achievements in Separation Sciences; Professor James Prestegard, University of Georgia, Outstanding Achievements in Magnetic Resonance; Professor John McLean, Vanderbilt University, Outstanding Achievements in Chemometrics; and Professor Emanuela Gionfriddo, University of Toledo, Young Investigator Award. We also congratulate our eight undergraduate and graduate student awardees!

We hope you find the time to visit our Expo where many of the vendors will be presenting their state-of-the-art technology products and services Monday through Wednesday. This year our Technology Tour has been renamed Passport to Prizes. As you explore the Expo, stop by the booths of the participating vendors listed in the Passport and get your passport "stamped". Completed Passports can be submitted to the Souvenir Booth in Stockton B for a special gift. Your name will be entered for a chance to win a free EAS 2024 Registration or Short Course.

The centerfold of this program lists our exhibitors and special events taking place during the symposium. Join in and participate in some fun activities on Monday and Tuesday nights, Crowne Plaza Hotel, 2nd floor, across from the Flight Lounge. Don't forget to stop by our Souvenir Booth, located in Stockton B, to pick up your EAS 2023 memento.

Please download our EAS 2023 app for the most current program updates. Follow us on Instagram, LinkedIn and/ or Facebook. On behalf of the entire EAS Board, we thank you for attending EAS 2023. Special thanks to our Key Committee Chairs, our Executive Secretary, Bernadette Taylor and our Exposition Director, Janine Kishbaugh for their tireless efforts in preparing for EAS 2023. Enjoy the Symposium!

Frank Romano EAS 2023 President

Conferences-in-Miniature

2023 EAS Conferences-in-Miniature

BIOANALYSIS, PROTEOMICS & METABOLOMICS

Technical Sessions

- Revolutionizing Bioanalysis: Cutting Edge Analytical Advancements (11/14 PM)
- EAS Young Investigator Award, Honoring Emanuela Gionfriddo, University of Toledo (11/15 AM)
- Applications of Analytical Chemistry in Proteomic Research (11/15 PM)

Short Courses

• Practical Bioanalytical Method Validation by LC-MS/MS (11/14)

CHEMOMETRICS

Technical Sessions

- Applied Chemometrics and Machine Learning (11/13 AM)
- EAS Award for Outstanding Achievements in Chemometrics, Honoring John Kalivas, Idaho State University (11/13 PM)
- Accelerating Pharma R&D: Automation, Machine Learning, Predictive Sciences, and Image Analytics (11/14 AM)
- Unleashing the Power of Data with Quality-by-Design and Chemometrics (11/14 PM)
- Chemometrics: Using Data to Solve Tomorrow's Problems (11/15 PM)

Short Course

Non-Linear Machine Learning for Calibration and Classification (11/12)

CHROMATOGRAPHY

Technical Sessions

- EAS Award for Outstanding Achievements in Separation Science Honoring Mary Wirth, Purdue University (11/13 AM)
- EAS Award for Outstanding Achievements in the Field of Analytical Chemistry, Honoring Robert Kennedy, University of Michigan (11/13 PM)
- Chromatographic Solutions for Modern-Day Challenges (11/13 PM)
- Multidimensional Separations: Theory & Practice (11/13 AM)
- Separations in Pharmaceutical Applications (11/13 PM)
- Fifty Years of Innovations in HPLC Columns (11/14 AM)
- What You Actually Need to do to Make Your Separations Sustainable? (11/14 PM)
- Recent Developments in High Performance Thin Layer Chromatography (11/14 PM)
 Evaluating and Understanding Extremely Large Molecules Through Various Separation
- Techniques (11/15 AM)
- Beyond Boundaries: Expanding Horizons of Liquid Chromatography (11/15 AM)
- Advances in Chromatography with Applications in the Biomedical / Clinical Diagnostics Field (11/15 PM)

Short Courses

- HPLC and UHPLC for Practicing Scientists 1 and 2: Fundamentals, Method Development, and Troubleshooting (11/12-11/13)
- Practical LC-MS Method Development and Sample Preparation (11/12-11/13)
- Chromatographic Methods of Analysis of Oligonucleotides, siRNA, and mRNA (11/12)
- High-Performance Thin-Layer Chromatography an Alternative Approach to Quality: Standardization, Quantification and Automation (11/12)
- Supercritical Fluid Chromatography (SFC): A Powerful and Greener Tool for Analytical and Preparative Separations (11/15)
- 2D Liquid Chromatography for Pharmaceutical Analysis (11/14)
- Getting the most from GC and GC/MS (11/14)

CONSERVATION SCIENCE

Technical Sessions

- From Brushstrokes to Chemical Signatures: Uncovering the Mysteries of Artworks through Forensic Analytical Techniques (11/13 PM)
- Conservation Science: Beyond Art & Forensics (11/15 AM)
- Analytical Studies in Heritage Discovery, Authentication and Attribution (11/15 PM)

ENVIRONMENTAL & CONSUMER ANALYSIS

Technical Sessions

- Food Safety Analysis (11/13 AM)
- Advancing Approaches for Analyzing Fine Microplastics and Nanoplastics (11/13 AM)
- Forever Bounded: PFAS and Other Xenobiotics in the Environment and Analytical Challenges (11/13 AM)
- · Human Exposures to PFASs from Everyday Sources (11/13 PM)
- · Protecting the Food Chain: Developments in Food and Beverage Analysis (11/13 PM)
- Beyond Traditional Methods: Exploring Next Generation Innovations in Environmental Science (11/14 AM)
- Analytical Approaches to Cosmetic Chemistry (11/15 AM)
- Measurement Challenges in Cannabis-Derived Products (11/15 PM)

FORENSIC ANALYSIS

Technical Sessions

- Research from our Emerging Forensic Scientists (11/13 AM)
- State-of-the-Art Innovation in Forensic Science (11/13 AM)
- From Brushstrokes to Chemical Signatures: Uncovering the Mysteries of Artworks through Forensic Analytical Techniques (11/13 PM)
- Explosives & GSR: Present & Future Directions (11/14 AM)
- Forensic Microscopy "What is it? Who does it? (11/14 PM)

LABORATORY MANAGEMENT

Technical Session

• Lab Managers Basics: Essentials Every Lab Manager Should Know (11/13 PM)

Short Courses

- The Fundamentals of Laboratory Management Managing People (11/12)
- Prepare Your Analytical Laboratory for Quality Audit and Inspection (11/13)
- Design of Experiments (DoE): Key to Effectiveness and Continuous Improvement in the Laboratory (11/13)

MASS SPECTROMETRY

Technical Sessions

- Shaping the Future of Cancer Research: Exploring Mass Spectrometry Innovations (11/13 AM)
- Mass Spectrometry: Unlocking a World of Applications (11/13 PM)
- EAS Award for Outstanding Achievements in Mass Spectrometry, Honoring John McLean, Vanderbilt University (11/14 AM)
- Quantitative Mass Spectrometry through Drug Development Life Cycle (11/14 PM)
- Applications of Ion Mobility Mass Spectrometry (11/15 AM)

Short Courses

- Practical LC-MS Method Development and Sample Preparation (11/12-11/13)
- Getting the most from GC and GC/MS (11/14)
- Practical Bioanalytical Method Validation by LC-MS/MS (11/14)

NMR SPECTROSCOPY

Technical Sessions

- NMR: The Swiss Army Knife of Analytic Methods (11/14 AM)
- EAS Award for Outstanding Achievements in Magnetic Resonance, Honoring James Prestegard, University of Georgia (11/14 PM)

PHARMACEUTICAL ANALYSIS

Technical Sessions

- Accelerating Pharma R&D: Automation, Machine Learning, Predictive Sciences, and Image Analytics (11/14 AM)
- Infectious Diseases Diagnostics, Treatment and Prevention (11/14 AM)
- Applying Analytical Technologies to Drug Development (11/14 PM)
- Risk Mitigation in the Pharma QC Laboratory (11/14 PM)
- Overcoming the Complexity of Biological Drug Products through Experimental and Computational Characterizations (11/15 AM)
- Analytical Advancements Driving Pharmaceutical Excellence (11/15 PM)

Short Courses

- Sample Preparation: The Chemistry Behind the Techniques (11/12)
- Analytical Method Validation and Lifecyle Management FDA, ICH and USP Expectations (11/12)
- Prepare Your Analytical Laboratory for Quality Audit and Inspection (11/13)
- Analytical Method Validation: A Quality by Design Approach (11/14)
- 2D Liquid Chromatography for Pharmaceutical Analysis (11/14)
- An Overview of Drug Development, Drug Quality, Regulatory, and Quality Control Processes (11/15)

POSTER SESSIONS

- Monday Poster Session AM (11/13)
- Monday Poster Session PM (11/13)
- Tuesday Student Award Poster Session (11/14)
- Tuesday Poster Session AM (11/14)
- Tuesday Poster Session PM (11/14)
- Wednesday Poster Session PM (11/15)

POWERHOUSE SESSIONS

Technical Sessions

- Advancing Approaches for Analyzing Fine Microplastics and Nano-plastics (11/13 AM)
- Separations in Pharmaceutical Applications (11/13 PM)

SPECIAL LECTURES

Technical Sessions

- Keynote Lecture by Dr. Vasilis Vasiliou, Yale University (11/13 PM)
- Breakfast Lecture by Dr. Frank Nichols, University of Connecticut (11/14 AM)
- Plenary Lecture by Dr. Sibrina Collins, Lawrence Technical University (11/15 AM)

SPECTROSCOPY

Technical Sessions

- Coherent Nonlinear Optical Spectroscopy and Imaging (11/13 AM)
- PAT: Eyes in the Process (11/13 PM)
- Highlighting Early Career Scientists in Spectroscopy and Analytical Chemistry (11/14 AM)
- New York/New Jersey Section of the Society for Applied Spectroscopy Gold Medal Award, Honoring Curtis Marcott, Light Light Solutions (11/14 PM)
- Portable Instrumentation in the Field (11/15 AM)
- Sub-mMicron IR and Raman Spectroscopies (11/15 AM)
- Exploring Diverse Applications of Spectroscopic Techniques (11/15 PM)

Short Courses

- Introduction to Quantitative Spectroscopy for Near Infrared and Raman Instrumentation (11/13)
- Practical Raman Microscopy (11/14)

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Conferences-in-Miniature

2023 Technical Program

Monday Morning, November 13, 2023

EAS Award for Outstanding Achievements in Separation Science Honoring Mary Wirth, Purdue University

Sponsored by Restek Corporation

Chair: Shelley Claridge, Purdue University

9:00	1	Plenty of Room at the Top: From Molecular to Macroscopic Chemical Patterning and Characterization of Soft Materials, <u>Shelley Claridge</u> , Purdue University
9:30	2	Drug Discovery Using Mass Spectrometry for Synthesis and Analysis, Graham Cooks, Purdue University
10:00		Break
10:30	3	Interfacial Chemistry within Porous Chromatographic Silica – The Inside Story Revealed by Confocal Raman Microscopy, <u>Joel Harris</u> , Jay P. Kitt, Grant J. Myres, David A. Bryce, University of Utah
11:00		Presentation of the EAS Award for Outstanding Achievements in Separation Science
11:05	4	Surface Science Underlying Protein Chromatography, Mary Wirth, Purdue University
Nanoplas Chairs: A Universit	sho	s ok Deshpande, NOAA, Beizhan Yan, Columbia
9:00	5	Distribution and Transport of Microplastics and Associated Pollutants in New York Harbor Waters, <u>Hui Ping Deng</u> , Beizhan Yan, Columbia University
9:30	6	Rapid Single-Particle Chemical Imaging of Nanoplastics by SRS Microscopy, <u>Naixin Qian</u> , Wei Min, Beizhan Yan, Columbia University
10:00		Break
10:30	7	Characterization of Microplastics by Using a Novel Method of Pyrolysis GC-MS, <u>Ashok Deshpande</u> , NOAA
11:00		Panel Discussion
		ional Separations: Theory & Practice by ACS Division of Analytical Chemistry

Sponsored by ACS Division of Analytical Chemistr Chair: James Grinias, Rowan University

9:00	8	Comprehensive Two-Dimensional Gas Chromatography: The Future of Nontargeted VOC Analysis, <u>Katelynn</u> <u>Perrault Uptmor</u> , College of William and Mary
9:30	9	Adventures in Two-Dimensional Liquid Chromatography Separations of Therapeutic Oligonucleotides, <u>Dwight Stoll</u> , Gustavus Adolphus College
10:00		Break
10:30	10	Trapping Mode Two-Dimensional Liquid Chromatography for Quantitative Low-Level Impurity Enrichment in Pharmaceutical Development, <u>Ziqing Lin</u> , Qinggang Wang, Yiyang Zhou, Jonathan Shackman, Bristol Myers Squibb
11:00	11	LCxMSy: Exploring Different Combinations of Multi- Dimensional Liquid Chromatography with Multiple Parallel Mass Spectrometry, <u>William Byrdwell</u> , United States Department of Agriculture
	-	

Applied Chemometrics and Machine Learning Chair: Brandye Smith-Goettler, Merck & Co., Inc.

- 9:30 13 Detecting and Quantifying Solid-Phase Impurities by Leveraging Morphological Differences Using Image-Based PAT, Hossein Salami, Merck & Co., Inc 10:00 Break 10:30 14 Scalable Continuous Photochemical and Electrochemical Reactions: Reactors and PAT Challenges and AI: From Picoseconds to Tonnes, Michael George, University of Nottingham 11:00 15 Brandye Smith-Goettler, Merck & Co., Inc. The Research from our Emerging Forensic Scientists Sponsoredby New Jersey Association of Forensic Scientists Chair: Monica Joshi, West Chester University of PA 9:00 16 Detection of Yellow Fever Virus in Human Remains Using Mass Spectrometry-Based Protein Identification, Kyra
- <u>Miller</u>, Kimberlee Moran, Carla Cugini, Rutgers University
 9:30 17 Determining the Variability in Color in Human Head Hair, <u>Emma Redman</u>, Lawrence Quarino, Cedar Crest College
 10:00 Break
- 10:30 18 A Novel FTIR Method for the Detection and Quantitation of Ruhemann's Purple in Latent Fingerprint Analysis, <u>Kira</u> <u>Bochard</u>, Heather Harris, Arcadia University, Kimberlee Moran, Rutgers University-Camden, Cynthia Tidwell, University of Montevallo
- 11:00 19 Evaluation of Gas Chromatography-Triple Quadrupole Mass Spectrometry for the Identification of Organic Gunshot Residues from Known Shooters and Non-Shooters, <u>Thomas Ledergerber</u>, Monica Joshi, Luis Arroyo, Tatiana Trejos, West Virginia University

Shaping the Future of Cancer Research: Exploring Mass Spectrometry Innovations

- Chair: Costel Darie, Clarkson University
 - 9:00 20 Proteomics Analysis of Breast Milk for Early Detection of Breast Cancer: A Mass Spectrometry Approach, <u>Aneeta</u> <u>Arshad</u>, Danielle Whitham, Costel Darie, Clarkson University, Brian T. Pentecost, Kathleen F. Arcaro, University of Massachusetts-Amherst
 - 9:20 21 Proteomic Analysis and Comparison of Stage IIA T1N1 ER/PR Negative Breast Cancer Serum to Controls for Identification of Potential Biomarkers for Breast Cancer, <u>Pathea S. Bruno</u>, Costel Darie, Clarkson University, Brian T. Pentecost, University of Massachusetts Amherst
 - 9:40 22 A Proteomic Investigation of Human Serum from Donors with Stage IIB Breast Cancer and Matched Controls to Identify Protein Biomarkers for Earlier Breast Cancer Detection, <u>Danielle Whitham</u>, Panashe Mutsengi, Brian T. Pentecost, Costel Darie, Clarkson University
 10:00 Break
- 10:30 23 A Proteomic Investigation of Human Serum from Donors with Triple Negative Breast Cancer and Matched Controls to Identify Potential Protein Biomarkers for Breast Cancer Detection, <u>Norman Haaker</u>, Isabelle Sullivan, Danielle Whitham, Brian T. Pentecost, Costel Darie, Clarkson University
- 10:50 24 A Proteomics Investigation of Human Sera from African American Donors with Invasive Ductal Carcinoma Breast Cancer and Matched Controls, <u>Logan Seymour</u>, Panashe Mutsengi, Danielle Whitham, Brian Pentecost, Costel Darie, Clarkson University
- 11:10 25 A Case Study Investigation for Biomarker Discovery: Proteomics Analysis of Sera from an Asian American Woman with Triple Negative Breast Cancer and a Matched Controls, <u>Hailey Morrissiey</u>, Panashe Mutsengi, Danielle Whitham, Costel Darie, Clarkson University, Brian Pentecost, University of Massachusetts-Amherst

Technical Program

Coherent Nonlinear Optical Spectroscopy and Imaging Sponsored by Coblentz Society Chair: Kenneth L. Knappenberger, Pennsylvania State University

	Analysis
29	The Interactions of Electrolyte Solutions with Charged Monolayer Films at the Air/Water Interface, <u>Paul Cremer</u> , Penn State University
28	Investigating the Influence of Chaperones on Desmin Fragment-Related Cardiomyopathy via Two-Dimensional Infrared Spectroscopy, <u>Ariel Alperstein</u> , University of Delaware
	Break
-1	Second Harmonic Investigations of Bacterial Membrane Complexity, <u>Tessa Calhoun</u> , University of Tennessee
27	

9:00	30	Dairy Ingredients Safety for the Global Market, Erin
		Aungier-Markoff, Cayuga Milk Ingredients
9:30	31	Analysis of PFAS, Pesticides, and Mycotoxins in Food ar Agriculture, <u>Volker Bornemann</u> , Avazyme, Inc.
10:00		Break
10:30	32	Flexible Natural Toxin Methods for Food to Meet Current and Future Regulatory Requirements, <u>Emily Britton</u> , Narendra Meruva, Waters Corporation
11:00	33	Multi-Residue GC/MS/MS of Pestcides Analysis in Infant Food, <u>Douglas Stevens</u> , David Gould. Stuart Adams, Simon Hird, Frank Dorman, Waters Corporation

State-of-the-Art Innovation in Forensic Science Chair: Dave Trimble, Northrop Grumman Corp

- 9:00 34 Determining the Time Since Deposition of Variable Heated Bloodstains Utilizing Raman Spectroscopy and Chemometrics, <u>Alexis Weber</u>, Igor K. Lednev, University at Albany, SUNY
- 9:20 35 Investigating the Dynamics of Soil Chemistry and its Related Microbiome through Liquid Chromatography and Mass Spectrometry, <u>Jessica Grace Prudence Hay</u>, Deakin University
- 9:40 36 The Application of Particle-Correlated Raman Spectroscopic Analysis of Soils to Mock-Casework Scenarios, <u>Samantha Gong</u>, Marisia Fikiet, Brooke Kammrath, University of New Haven, Peter De Forest, Forensic Consultant
- 10:00 37 Capabilities and Limitations of Particle Correlated Raman Spectroscopy (PCRS) for the Analysis Forensic Soil Minerals, <u>Jasmine Kaur</u>, Joshua Christensen, Ella Galvan, Marisia Fikiet, Virginia Maxwell, Brooke W. Kammrath, University of New Haven, Ethan Groves, Skip Palenik, Chis Palenik, Microtrace LLC, Peter De Forest, Forensic Consultants
- 10:20 Break

Forever Bounded: PFAS and Other Xenobiotics in the Environment and Analytical Challenges Chairs: Kaitlyn Campbell, Christopher Perkins, University of Connecticut

9:00 38 Transport and Deposition of Emerging PFAS Through Rainfall, <u>Jennifer Faust</u>, Yubin Kim, Jameson Sprankle, Donald Conley, Rebekah Gray, Paul Edmiston, The College of Wooster, Kyndal Pike, University of Wisconsin-Madison

			Technical Program
	9:3	0 39	Developing and Testing of Passive Samplers for Dissolved PFAS, <u>Rainer Lohmann</u> , Jitka Becanova, Matthew Dunn, Jarod Snook, University of Rhode Island
	10:0	0	Break
llar	10:3	0 40	Investigating the Role of Coastal Wetland on Per- and Polyfluoroalkyl Substances (PFAS) Transport, <u>Mi-Ling Li</u> , University of Delaware
<u>Hai-</u> ane	11:0	0 41	PFAS Method Development and Bioaccumulation in Long Island Sound, <u>Kaitlyn Campbell</u> , Jessica Brandt, Christopher Perkins, Anthony Provatas, University of Connecticut
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	44	Method	relopment of a Fit-For-Purpose Assay Degradation HPLC I Using Open Lab Software, <u>Deliana Arias</u> , Zack Zhiqiang erck & Co., Inc.
d and	45	Novel V Navalka) Analysis of an Industrial Perfluorinated Alkylamine in /ehicles to Support <i>In-Vivo</i> Studies, <u>Fabricio Beltran</u> , Nikita ar, Bo Tokarski, Geoff Clay, Charles River Laboratories
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fant	47	HAART	ements in the Analysis of Synthetic Peptide Enfuvirtide and Drugs Utilizing MaxPeakTM High Performance Surfaces Brianna Clements, Waters Corporation
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nd sity at	49	Chroma	Im Ion Assay for Coral Tank Monitoring via Ion atography with Suppressed Conductivity Detection, <u>Kayry</u> a, William LaCourse, University of Maryland Baltimore
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- 53 Monitoring the Estrogen-Inducible Proteins in Lake Trout (Salvelinus namaycush) from Great Lakes upon Exposure to Environmental Contaminants, <u>Taniya Jayaweera</u>, Bernard Crimmins, Sujan Fernando, Thomas Holsen, Costel C. Darie, Clarkson University
- 54 Targeted Lipidomic Analysis of Fatty Acids in Marine Dietary n3-PUFA Supplements, <u>Yifan Li</u>, Fereshteh Zandkarimi, Columbia University
- 55 Determination of Illegal Dyes in Chili Powder Using UPLC-MS/ MS, <u>Stephanie Nauth</u>, Andres Campiglia, Christian Febres Collazo, University of Central Florida
- 56 Assessments and Comparisons of Chiral Chromatography with Fully Porous Particles and 2.7-um Superficially Porous Particles in HPLC and SFC, <u>Melissa Wilcox</u>, Edward Franklin, Gay Lowden, Regis Technologies, Inc.

Technical Program

- 57 Fractionation of Complex RNA Mixtures for Enhanced Modification Mapping via LC-MS/MS, <u>Cassandra Herbert</u>, Jennifer Kist, Patrick Limbach, University of Cincinnati
- 58 Withdrawn by the author.
- 59 Synthesis, Characterization, and Electrochemical Properties of Derivatized Naphthoquinone Electron Acceptors, <u>Brinda</u> <u>K. Narayana</u>, Megan Schlogl, Patrick Landry, K.V. Lakshmi, Rensselaer Polytechnic Institute, Vasily Kurashov, John H. Golbeck, Pennsylvania State University
- 60 Analytical Impacts on the Belzutifan Next-Gen End-game Chemistry Development, <u>Hong Li</u>, Rekha Gangam, Wenjun Liu, Diane Lee, Clara Hartmanshenn, Timothy Wright, Jiaxuan Yan, Daniel Dirocco, Jonathan Mcmullen, Merck & Co., Inc.
- 61 Analysis of WCU Andean Headwear Collection, <u>Sadie Patterson</u>, Zachary Voras, West Chester University of Pennsylvania

Monday, November 13: E-Poster Session; 12:30pm – 1:25pm

- 62 AQbD and Green Chemistry Principles Driven Method to Determine Mycophenolate Mofetil Impurities-Identification of Degradation Products by QToF LCMS, <u>Siva Krishna Muchakayala</u>, Naresh Kumar Katari, Vishnu Murthy Marisetti, Catalent Pharma Solutions
- 63 Cipher Software as a Tool for an Improved Data Integrity for Dissolution Testing in GMP Space, <u>Monika Baraniak</u>, Bristol Myers Squibb
- 64 Replacing Electropolished Stainless Steel Tubing with a Silicon-Based CVD Coating for Higher Inertness, Lower Wet-Up and Dry Down Performance, and Greater Corrosion Resistance for Gas and Fluid Transfer, <u>Jesse Bischof</u>, SilcoTek Corporation
- 65 To Mix or Not to Mix: Effect of Using Solvent Blends as Modifier in Chiral SFC, <u>Daipayan Roy</u>, Larry Miller, Amgen Research
- 66 Polysaccharide-Based Chiral Stationary Phases for the Separation of Atropisomers, <u>John Ferraro</u>, Weston Umstead, Daicel Chiral Technologies
- 67 Gefapixant Citrate (MK-7264) Sulfonamide Step Speciation Study: Investigation into Precipitation-Dissolution Events During Addition of Chlorosulfonic Acid, <u>Nelo Rivera</u>, Ryan Cohen, Si-Wei Zhang, Zachary Dance, Holst Halsey, Siqing Song, Xiaodong Bu, Mikhail Reibarkh, Hong Ren, Alfred Lee, Darryl Chang, Sachin Lohani, Merck & Co., Inc.
- 68 Novel End-Capping Method with Silyl-Reagent Including Ethylene Chain, <u>Norikazu Nagae</u>, ChromaNik Technologies Inc.
- 69 The Determination of Nutritional and Toxic Elements in Plant-Based Foods Using ICP-MS, <u>Andrea Palpini</u>, PerkinElmer
- 70 LC and LC MS Methods for Analysis of mRNA Poly(A) Tail, <u>Martin</u> <u>Gilar</u>, Catalin Doneanu, Waters Corporation
- 71 Lego® Blocks as 'Standard' Samples for Evaluation of Fluorescence, Richard Crocombe, Crocombe Spectroscopic Consulting, <u>Brooke Kammrath</u>, University of New Haven, Pauline Leary, Noble
- 72 Withdrawn by the author.
- 73 A Qualitative Comparison of the Fast Fourier Transform and the Morlet Wavelet Transform for Potential Depression Diagnosis Using Resting-State Electroencephalographic Data, <u>Eliana Du</u>, West Windsor Plainsboro High School South
- 74 Investigation of the Effects of Overexpression of Human Jumping Translocation Breakpoint (JTB) Protein Using In-Solution Digestion-Based Proteomics, <u>Krishan Weraduwage</u>, Madhuri Jayathirtha, Danielle Whitham, Costel C. Darie, Clarkson University
- 75 Assessing the Memory Effect of Trifluoroacetic Acid (TFA) on Various Reversed-Phase HPLC Stationary Phases, <u>Matthew</u> <u>Swoyer</u>, Colleen Dugan, GSK
- 76 Structural Characterizations of Multiple Strawberry Fiber Fractions by NMR, <u>Gary D. Strahan</u>, Hoa K. Chau, Arland T. Hotchkiss Jr., USDA/ARS

- 77 Rapid Timeframe Biophysical Characterization of Vaccine Intermediates Under Accelerated Stability Conditions, <u>Donald</u> <u>Kotowski</u>, Andrea Gomez, Walter Wasylaschuk, Michael McNevin, Merck & Co., Inc.
- 78 Universal Ion Chromatography Method for Anions in Active Pharmaceutical Ingredients Enabled by Computer-Assisted Separation Modelling, <u>Dolee Merai</u>, Tianyu (Kelvin) Yuan, Matthew J. Gunsch, Ryan Peters, Sachin Lohani, Frank Bernardoni, Michael A. Zompa, Imad Haidar Ahmad, Erik L. Regalado, Merck & Co., Inc., Christopher A. Pohl, CAP Chromatography Consulting
- 79 Using Novel Stationary Phase Selectivity to Address Potential NDMA Over-Quantification due to Isobaric Interference in the LC-MS/MS Analysis of Nitrosamines, <u>Geoff Faden</u>, MAC-MOD Analytical, Matt James, Anthony Edge, Avantor Sciences
- 80 Building a Project Centric Database for Immediate Use or in a Low Resource Environment, <u>Michael Barrett</u>, Anna Shternin, Hannah Dvorak, Shari Sellers, Graciela Terife, Merck & Co., Inc.
- 81 Modifying the Method for Industry-Wide Content Analysis of Polysorbate 80 (PS80) on HPLC-ELSD, <u>Daniel Steyer</u>, Kennedy Guillot, Katie Carnes, Sina Mortazavi, Suraj Hettiarachchi, Michelle Ward, Lee Oliver, GSK

Monday Afternoon, November 13, 2023

EAS Award for Outstanding Achievements in the Field of Analytical Chemistry

Honoring Robert Kennedy, University of Michigan Sponsored by Bristol Myers Squibb Chair: James Grinias, Rowan University

1:30		Presentation of the EAS Award for Outstanding Achievements in the Fields of Analytical Chemistry
1:35	82	Using Microfluidic Droplet Technology to Improve Throughput for Chemical Analysis, <u>Robert Kennedy</u> , University of Michigan
2:00	83	Small Separations and Big Data: Using Analytical Chemistry to Address the Challenges of Cancer Detection, <u>Rebecca Whelan</u> , University of Kansas
2:30		Break
3:00	84	Two-Dimensional Liquid Chromatography for Advanced Characterization of Industrial Polymers and Sustainable Materials, <u>Peilin Yang</u> , Dow Chemical Company
3:30	85	Low-Cost, Open-Source Tools for Chemical Analysis, James Grinias, Samuel Foster, Deklin Parker, Christopher Piccolo, Joeachin Obasi, Catherine Seltzer, Matthew Will, Rowan University

EAS Award for Outstanding Achievements in Chemometrics Honoring John Kalivas, Idaho State University Sponsored by Eigenvector Research Chair: Peter Harrington, Ohio University

- 1:30 86 AI, Machine Learning, Chemoinformatics, and Chemometrics: What's the Deal, <u>Peter Harrington</u>, Ohio University
 2:00 87 Temporal Surface Mode Decomposition for Transient Kinetics Analysis, <u>Matthew Kunz</u>, Debtanu Maiti, Rebecca Fushimi, Idaho National Laboratory
 2:30 Break
- 3:00 88 Photonic Data Science: Model Transfer for Raman Spectra and FAIR Data Storage for Vibrational Spectroscopic Data, <u>Thomas Bocklitz</u>, Leibniz-Institute of Photonic Technology
 3:30 Presentation of the EAS Award for Outstanding
- Achievements in Chemometrics
- 3:35 89 Rashomon Effect on Model Interpretability and Improving Model Generalizability, <u>John Kalivas</u>, Idaho State University

POWERHOUSE SESSION: Separations in Pharmaceutical Applications Chairs: Erik Regaldo & Imad Haidar, Merck & Co., Inc.

1:0	30	90	Strategies and Tools to Simplify and Support Method Development in Two-Dimensional Liquid Chromatography - A Progress Report, <u>Dwight Stoll</u> , Gustavus Adolphus College
2:0	00	91	Pharmaceutical Portfolio Delivery by Benefit of Strategic Method Development and Automation for Large and Small Molecule Separations, <u>Kaitlin Grinias</u> , Colleen Dugan, Mark Sleeper, Daniel Steyer, Katie Carnes, Sina Mortazavi, Stephanie Lehman, Justin Shearer, GSK
2:3	30		Break
3:0	00	92	Coupling Separation and Sample Preparation Methods for Pharmaceutical Analysis, <u>Jared Anderson</u> , Danial Shamsaei, Shu-An Hsieh, Iowa State University
3:3	30		Panel Discussion

Chromatographic Solutions for Modern-Day Challenges Chair: Enju Wang, St. John's University

1:30	93	Development of Limit Test for Residual Spermine and Putrescine in Monoclonal Antibody In-Process Samples, <u>Sina Mortazavi</u> , GSK
1:50	94	Small Molecule HPLC Method Optimization Using an Acidic, Basic, and Neutral Panel and Superficially Porous Particles, <u>Conner McHale</u> , Advanced Materials Technology
2:10	95	Nonstoichiometric Pseudoprotic Ionic Liquids as Media for Metal Separations, <u>Mark Kobrak</u> , Brooklyn College
2:30		Break
3:00	96	The Benefits of Reducing Metal Ion Introduction into HPLC Flow Paths via Silicon-Based CVD Coatings, Jesse Bischof, SilcoTek Corporation
3:20	97	Modeling and Visualizing Mass Transfer of Monoclonal Antibodies (mAb) in Size Exclusion Chromatography (SEC) Columns, <u>Sornanathan Meyyappan</u> , Fabrice Gritti, Waters Corporation,
3:40	98	The Systematic Screening Protocol: A Streamlined Way to Develop Fast and Robust Reversed-Phase Liquid Chromatography Methods, <u>Kenneth Berthelette</u> , Kim Haynes, Waters Corporation

From Brushstrokes to Chemical Signatures: Uncovering the Mysteries of Artworks through Forensic Analytical Techniques, organized by the New Jersey Association of **Forensic Scientists**

Chair: David Fisher, New Jersey Institute of Technology

Mass S	pectr	ometry: Unlocking a World of Applications
		Jackson Pollock, Nicholas Petraco, John Jay College
3:30	102	The Authentication of Untitled: Red, Black, and Silver by
3:00	101	Thiago Piwowarczyk, NY Art Forensics
2:30		Break
2:00	100	Science in the Museum: How Analytical Techniques Inform Art History, Conservation, and Museum Practice, <u>Marco</u> <u>Leona</u> , Metropolitan Museum of Art
1:30	99	Materials Analysis and Art Historical Research on a 16th Century Painting of St. Catherine of Alexandria, <u>Jeffrey</u> <u>Taylor</u> , NY Art Forensics

Chair: Michelle Case, Bristol Myers Squibb

103 Investigation of the Effects of Human Jumping 1:30 Translocation Breakpoint (hJTB) Protein Using Mass Spectrometry Based Proteomics, Taniya Jayaweera, Madhuri Jayathirtha, Danielle Whitham, Costel C. Darie, Clarkson University

- Technical Program
- 1:50 104 Development of an Automated Matrix Assisted Laser Desorption Ionization Mass Spectrometry Workflow for Formulation Risk Assessment of Novel, Engineered Cytokine Proteins, Gregory Pirrone, Erik Munsell, Alexey Makarov, Heidi Ferguson, Suman Luthra, Mohammad Al-Sayah, Merck & Co., Inc. 2:10 105 Optimization of the In-Gel Sample Preparation for Mass
- Spectrometry-Based Proteomics, Danielle Whitham, Costel C. Darie, Brindusa Alina Petre, Clarkson University
- 2:30 Break
- 106 Evaluation of LC-MS Instruments for Multi-Attribute 3:00 Method (MAM) Implementation, Catherine O. Brown, Kelsey T. Morgan, Matthew D. Maust, Justin W. Shearer, Nicole A. Schneck, Emily L. Gill, GSK
- 107 Moving into PROTACs Drug Discovery: Considerations for 3:20 LC-MS Analysis, Sharon Tentarelli, AstraZeneca

PAT: Eyes in the Process

Chair: James Rydzak, Specere Consulting

- 108 Do You Really Understand Your Crystallization The Value 1:30 of PAT, Norman Wright, Mettler Toledo
- 2:00 Development of Adaptable and Scalable Quantitative Mid-109 Infrared Spectroscopy Models for In-line Monitoring of the Continuous Synthesis of Furosemide Using Dynamic Calibration Methodology, Roudabeh Sadat Moazeni Pourasil, Yuma Miyai, Matthew Glace, Rachel Vallejo, James Rydzak, Thomas D. Roper, University of Virginia Commonwealth

2:30 Break

- 3:00 110 Expanding the Role of In-line Spectroscopy in the Pharmaceutical Environment, John Wasylyk, Robert Wethman, Ming Huang, Bristol Myers Squibb
- 3:30 111 Near-Infrared Spectroscopy: From a Simple Lab-Based Tool for Raw Material Qualification to a Key Component in PAT/QbD and Continuous Manufacturing, Emil Ciurczak, Doramaxx Consulting

Protecting the Food Chain: Developments in Food and **Beverage Analysis**

Chair: Shelby Zangari

1:30	112	Multivariate Regression of Chili Capsaicinoids for
		Absorbance-Transmittance Excitation Emission Matrix
		(A-TEEM) Spectroscopy and UPLC-DAD Data, Adam
		Gilmore, HORIBA Instruments, Uwe Nienaber, Kalsec Inc.

- 1:50 113 Accurate and Reliable Analysis of Food Samples Using ICP-MS with Argon Gas Dilution, Andy Fornadel, Sukanya Sengupta, Bhagyesh Surekar, Richard Fussell, Daniel Kutscher, Thermo Fisher Scientific
- 2:10 114 Analytical Testing Solutions for Method Validation Studies on PFAS Testing of Drinking Water and other Samples Matrices by UHPLC/MS/MS, Cole Strattman, PerkinElmer 2:30 Break
- 3:00 115 Determination of Cannabinoids in Animal Feeds by Liquid Chromatography-Tandem Mass Spectrometry, Xin Xu, Lisa Murphy, University of Pennsylvania
- 3:20 116 Wet Chemistry Automation for Increasing Laboratory Productivity in Environmental, Food & Beverage Testing, Gary He, Thermo Fisher Scientific

Lab Managers Basics: Essentials Every Lab Manger Should Know

Chair: Denis Swijter, ALMA

- 1:30 117 Transitioning from the Bench to Lab Leadership, Scott Hanton, Lab Manager Magazine
- How to Recruit, Hire and Onboard New Staff, Dwayne F. 2:00 118 Henry, Montgomery College 2:30 Break

3:00	119	Improving Productivity Through the Use of SharePoint,
		Veronica Godley, San Antonio Water System
3:30	120	How to Manage the Budget, <u>Tarshae Drummond</u> , Fayetteville State University

Human Exposures to PFASs from Everyday Sources Chair: James D. Stuart, University of Connecticut

- 1:30 121 Dietary Pathways and Routes of Human Exposure to PFAS, Dana McCue, EHS Support
- 2:00 122 Using Non-Targarted Analyses to Probe PFAS Exposure from Sources Ranging from Nonstick Pans to Fish, <u>Erin</u> <u>Baker</u>, James Dodds, Anna Boatman, Greg Kudzin, Ashlee Falls, University of North Carolina, Kaylie Donelson, North Carolina State University

2:30 Break

- 3:00 123 Bioaccumulation of Per/Polyfluoroalkyl Substances (PFASs): What we can Learn Through High-Resolution Mass Spectrometry Analysis of Complex Mixtures, <u>Carrie</u> <u>McDonough</u>, Carnegie Mellon University
- 3:30 124 PFAS in Foods: Modified Expansion and Results, <u>Susan</u> <u>Genualdi</u>, Wendy Young, Elsie Peprah, Cynthia Srigley, Stacey Wiggins, William Limm, Christine Fisher, Brian Ng, Lowri deJager, United States Food & Drug Administration

KEYNOTE LECTURE

Monday, November 13, 4:15 PM

Room:

Paper Number: 125

Exposome and Human Disease: From Neurological Disorders to Diabetes and Cancer Dr. Vasilis Vasiliou, Yale University

All registered Conferees, Attendees and Exhibitors are invited to attend. A reception will be held immediately following the lecture.

Tuesday Morning, November 14, 2023

BREAKFAST LECTURE

Tuesday, November 14, 8:00am

Room:

Paper Number: 126

Fractionation and Characterization of Bacterial Complex Lipids Using Analytic Chemical and Mass Spectral Approaches

Dr. Frank Nichols, University of Connecticut

All registered Full Conferees and Full-Time Student Conferees are invited to attend the Breakfast Lecture. A light breakfast will be provided.

EAS Award for Outstanding Achievements in Mass Spectrometry

Honoring John McLean, Vanderbilt University Sponsored by the American Microchemical Society Chair: Erin Baker, University of North Carolina

9:00	Presentation of the EAS Award for Outstanding
	Achievements in Mass Spectrometry

- 9:05 127 Advanced Molecular Phenomics in Systems, Synthetic, and Chemical Biology, John McLean, Vanderbilt University
 9:30 128 Identifying and Quantifying Cellular and Media Metabolites
- Predictive of Mesenchymal Stromal Cell Potency by Metabolomics Coupled to Machine Learning, <u>Facundo</u> <u>Fernández</u>, Georgia Institute of Technology 10:00 Break

- 10:30 129 Ion Mobility-Mass Spectrometry for High-Throughput Multi-Omics, <u>Kelly Hines</u>, University of Georgia
- 11:00 130 Advancing Lipidomic Measurements and Informatics Tools to Enable Better Health Assessments, <u>Erin Baker</u>, James Dodds, Jack Ryan, Amie Solosky, University of North Carolina, Jessie Chappel, North Carolina State University

Accelerating Pharma R&D: Automation, Machine Learning, Predictive Sciences, and Image Analytics Chairs: Daniel Skomski, Merck & Co., Inc & Kim Huynh-Ba, Pharmalytik

- 9:00 131 SubVision: Deep Learning to Accelerate Biopharmaceutical Formulation Development, <u>Yue-Ming</u> <u>Chen</u>, Shubing Wang, Andy Liaw, Yongchao Su, Daniel Skomski, Merck & Co., Inc.
- 9:30 132 Development of a Viscosity Optimization Algorithm through Automated Experimentation, <u>Peter Soler</u>, Stephen Thomas, Bristol Myers Squibb
- 10:00 Break
- 10:30 133 Automated Data Pipeline for Organic Solubility High-Throughput Screening Workflows in Pharmaceutical Drug Development, <u>Michael Rerick</u>, GSK
- 11:00 134 Investigating Oral Solid Dosage Excipient Compatibility Via Automation and High-Throughput Experimentation, <u>Alexander Chin</u>, Merck & Co., Inc.

Highlighting Early Career Scientists in Spectroscopy and Analytical Chemistry

Chair: Fay Nicolson, Dana-Farber Cancer Institute

9:00	135	Getting the Most Out of Portable Instrumentation: Handheld LIBS Method Development for Timber Analysis, <u>Caelin Celani</u> , Helder Carneiro, Maria Delgado, Karl Booksh, University of Delaware, Erin McClure-Price, United States Fish & Wildlife Service, James Jordan, Tyler Coplen, United States Geological Survey
9:30	136	Academics to Industry: Becoming a Pharmaceutical Forensics Chemist, <u>Britany Handzo</u> , Bristol Myers Squibb
10:00		Break
10:30	137	PCR-Less, Enzyme-Free Methods for Sensitive Detection of Disease Biomarkers, <u>Samuel Mabbott</u> , Texas A&M University
11:00	138	From Crime Scenes to Clinics: Raman Hyperspectroscopy of Body Fluid Stains and Chemometrics for Forensic Purposes and Diseases Diagnostics, <u>Bhavik Vyas</u> , Igor Lednev, University of Albany-SUNY, Lenka Halamkova, Texas Tech University
NMR: T	ne Sv	viss Army Knife of Analytic Methods

NMR: The Swiss Army Knife of Analytic Methods Chair: Jeffrey C. Hoch, University of Connecticut

- 9:00 139 Applications of NMR and Statistical Methods in Establishing Analytical Comparability and Process Consistency for mAbs, <u>Igor Dikiy</u>, William Matousek, Simona Horsa, Polat Abdubek, Dylan Howie, Cody Secor, Michael Rosconi, Erica Pyles, Regeneron Pharmaceuticals
- 9:30 140 Leveraging Quadrupolar Nuclei in Solid-State NMR, <u>Alexander Paterson</u>, University of Wisconsin-Madison
 10:00 Break
- 10:30 141 Highly Standardized NMR-Metabolite Biomarker Discovery Using Clinical Samples, <u>Alessia Trimigno</u>, Kari Boardman, Chen Dong, Jifang Zhao, Keri Sheehan, Elizabeth O'Day, Olaris, Inc.
- 11:00 142 Painting a Portrait of a Protein that Won't Sit Still, <u>Alexandra Pozhidaeva</u>, Yulia Pustovalova, Irina Bezsonova, Oksana Gorbatyuk, Jeffrey Hoch, UConn Health

Explosives & GSR: Present & Future Directions Chairs: Gina Guerrerra, US Federal Bureau of Investigation, Brooke Kammrath, University of New Haven

9:00	143	Nanoparticle Enhanced Laser Induced Breakdown Spectroscopy (NELIBS) for the Analysis of Gunshot Residue, <u>Alyssa Marsico</u> , University of New Haven		
9:30	144	Isotopic Profiling of Explosives Using Gas Chromatography Triple Stage Quadrupole Isotope Ratio Mass Spectrometry, <u>Stephan Hlohowskyj</u> , United States Federal Bureau of Investigation		
10:00		Break		
10:30	145	Capabilities and Limitations of Canine Training Across an Explosive Odor Spectrum, <u>Melissa Singletary</u> , Auburn University		
11:00	146	Development of Strategic Analytical Methods to Support the Modernization of Gunshot Residue Practice in Forensic Science, <u>Tatiana Trejos</u> , Luis Arroyo, Kourtney Dalzell, Thomas Ledergerber, Leah Thomas, Madison Lindung, West Virginia University		

Beyond Traditional Methods: Exploring Next Generation Innovations in Environmental Science Chair: Shirley Fischer-Drowos, Widener University

9:00	147	Sorption and Desorption of 17alpha-ethinylestradiol (EE2)
		and Beta-Estradiol (E2) on Montmorillonite Clay, Christian
		Manuelli, Yuegang Zuo, University of Massachusetts
		Dartmouth
9:20	148	PFAS Dark Matter. Slippery Cannabis and Catechin

- 9:20 148 PFAS Dark Matter, Slippery Cannabis and Catechin Epimers: Disparate Problems with a Similar Path to a Solution, <u>Frederick Strathmann</u>, Thomas Lubinsky, Rachel Harris, Julie Wushensky, MOBILion Systems, Inc.
- 9:40 149 Your GC/MS Knows What You're Doing at Home...Sort of: Looking at VOC Makeup of New and Occupied Homes Using Pyrolysis Gas Chromatography, <u>Khadiza Mom</u>, Quantum Analytics
- 10:00 Break
- 10:30 150 Analytical Chemistry is Essential for Gaining Understanding of the Earth's Climate, Past Present and Future, <u>Roland Hirsch</u>
- 10:50 151 Photooxidation and Phenol Decomposition Processes on Hydrophobic Nanoparticles, <u>Alexander Greer</u>, Britney Singh, Serah Essang, Lloyd Lapoot, Brooklyn College, Graduate Center of the City University of New York
- 11:10 152 Rapid, Efficient and Safe Microwave-Assisted Digestion of Li Battery Components for Trace Metals Analysis, <u>Alicia</u> <u>Stell</u>, Samuel Heckle, Macy Harris, CEM Corporation

Infectious Diseases - Diagnostics, Treatment and Prevention Chair: David Banach, University of Connecticut School of Medicine

9:00	153	Applied Chemistry in Clinical Bacteriology, <u>Melissa</u> <u>Gitman</u> , Mount Sinai School of Medicine
9:30	154	CRISPR-Powered Microfluidics Biosensing Devices for Point of Care Detection of Infectious Diseases, <u>Changchun</u> <u>Liu</u> , University of Connecticut School of Medicine
10:00		Break
10:30	155	Advances in Sterilization and Disinfection in Healthcare Settings, <u>Scott Roberts</u> , Yale School of Medicine
11:00	156	The Treatment and Prevention of Clostridioides Difficile Infection, <u>David Banach</u> , University of Connecticut School of Medicine

Analytical Method Development and New Modalities in Biopharmaceutical Laboratories Chair: Brandon Presley, Janssen R&D

Fifty Years of Innovations in HPLC Columns Sponsored by Waters Corporation Chair: Thomas Walters, Waters Corporation			
		,	
11:00	160	Vaccine Analytical Development, <u>Kristen Feibelman</u> , Merck & Co., Inc.	
10:30	159	Large Molecule Bioassay Development: Strategies and Analytical Challenges, <u>Julie McIntosh</u> , Merck & Co., Inc.	
10:00		Break	
9:30	158	Controlling Process-Related Impurities in the Biopharma Setting, <u>Hope McMahon</u> , Chris Gerberich, Robert Luo, GSK	
9:00	157	Capillary Isoelectric Focusing (cIEF) Technology Bridging, <u>Christopher Cammarata</u> , Janssen R&D	

- 9:00 161 Fifty Years of Innovations in HPLC Column Reproducibility, Efficiency, Stability and Inertness, <u>Thomas Walters</u>, Waters Corp.
- 9:30 162 Fifty Years of Innovations in HPLC Column Selectivity, David Bell, Restek Corporation
- 10:00 Break
- 10:30 163 Innovations in HPLC Columns: Perspectives from a Pharmaceutical Analyst, <u>Michael Dong</u>, MWD Consulting
- 11:00 164 Innovations in HPLC Column Technology for Faster and More Efficient Separations of Large Biomolecules, <u>Szabolcs Fekete</u>, Matthew Lauber, Waters Corporation

Tuesday, November 14: E-Poster STUDENT AWARDEE Session 1; 11:30am – 12:25pm

- 165 Lipidomic Phenotype of Mitochondrial Acyltransferase Deficiency Revealed by Imaging Mass Spectrometry, <u>Yu Tin Lin</u>, Julia Bonney, Tingting Yan, Carolyn Dirain, Lexin Chen, Ramon Miranda Quintana, Peter Stacpoole, Boone Prentice, University of Florida, Manal Zabalawi, Charles McCall, Wake Forest School of Medicine, Lane Smith, University of Michigan Medical School
- 166 An Automated High Throughput Approach for Large Scale Retention Measurement in Liquid Chromatography, <u>Trevor Kempen</u>, Tina Dahlseid, Dwight Stoll, Gustavus Adolphus College, Bob Pirok, University of Amsterdam
- 167 Confocal-Raman Spectroscopy Investigation of the Interactions Between Porous-Silica immobilized DNA Aptamers and their Protein Targets, <u>Aric Potter</u>, Grant Myres, Jay Kitt, Joel Harris, University of Utah
- 168 Kinetic Profiling of Commercially Available Capillary Scale Columns, <u>Samuel Foster</u>, James Grinias, Rowan University, Elisabeth Gates, Paul Peaden, Serguei Calugaru, Raymond West, Milton Lee, Axcend
- 169 Advancing Planetary Probe Based Mass Spectrometry Through Machine Learning, <u>Nicole North</u>, Abigail Enders, Heather Allen, Ohio State University
- 170 Optoelectronic Impacts of Surface Ligands in Water Dispersible Copper Selenide Nanoparticles, <u>Riti Sen</u>, University of Pittsburgh
- 171 The Application of a Raman Spectroscopy Body Fluid Identification Model on Samples Exposed to Bluestar Forensic Spray, <u>Alexis</u> <u>Weber</u>, Igor K. Lednev, University at Albany-SUNY
- 172 Human Breastmilk as a Bio-Fluid for the Use of Protein Biomarkers for Breast Cancer, <u>Danielle Whitham</u>, Pathea Bruno, Norman Haaker, Brian T. Pentecost, Costel C. Darie, Clarkson University, Kathleen F. Arcaro, University of Massachusetts-Amherst

Technical Program

Tuesday, November 14: E-Poster Session 1; 11:30am – 12:25pm

- 173 Reduction of Perfluoroalkyl and Polyfluoroalkyl Substances in Drinking Water Using a Standard Filter Containing Activated Carbon Plus Ion Exchange Resin, Measured Using the QSight 420 UHPLC/MS/MS, <u>Cole Strattman</u>, PerkinElmer
- 174 Determination of PFAS in Drinking Water Using Automated FREESTYLE XANA-PFAS System, <u>Fred Foster</u>, GERSTEL, Inc.
- 175 Applications of HPTLC for Testing Essential Oils, <u>Gavin Brush</u>, doTerra
- 176 Automated Polysorbate 80 (PS80) Forced Degradation Screening Workflow to Accelerate Biopharmaceutical Upstream Processing, <u>Sharon Matamoros</u>, Ashley Reeder, GSK
- 177 Method Development for PFAS and Drugs of Abuse (DoA) Compounds Using a Virtual Method Development Tool, <u>Melinda</u> <u>Urich</u>, Chris Nelson, Justin Steimling, Tim Yosca, Samantha Herbick, Restek Corporation, John Garrett, Analytical Innovations
- 178 The Use of Short 10 mm Columns for Rapid LC-MS Analysis, Edward Faden, MAC-MOD Analytical, Matt James, Anthony Edge, Avantor Sciences
- 179 Method Development for Solid-Phase Extraction and Capillary LC-UV Analysis of Drugs of Abuse and Related Metabolites, <u>John</u> <u>Boughton</u>, Sangeeta Kurre, Ama Hackman, Samuel Foster, James Grinias, Rowan University
- 180 Deciphering the Function of RNA Modifications in the Central Nervous System and Single Cells: Strategies in Sample Preparation, Separations, and Mass Spectrometry, <u>Kevin Clark</u>, Tufts University
- 181 Analysis of the Electrochemical Oxidation of Lignin using Chemometrics, <u>Gobind Sah</u>, Staser John, Peter Harrington, Ohio University
- 182 Geospatial Origin Differentiation of Pinus Ponderosa Ash using Multivariate Classification and Inductively Coupled Plasma Mass Spectrometry, <u>Maria Delgado-Cornelio</u>, Helder Carneiro, Caelin Celani, Karl Booksh, University of Delaware, Collin White, Barry Lavine, Oklahoma State University, James Jordan, US Geological Survey, Michael Ketterer, Northern Arizona University

Tuesday, November 14: E-Poster Session 2; 12:30pm – 1:25pm

- 183 Innovations in Enhanced SFC: Complex Purifications Enabled by Recent Advances in Analytical and Preparative Enhanced Supercritical Fluid Chromatography (eSFC), <u>Jimmy DaSilva</u>, Imad Haidar Ahmad, Erik Regalado, Merck & Co., Inc.
- 184 False Positive Glycopeptide Identification via in-FAIMS Glycan Fragmentation, <u>Valentina Rangel Angarita</u>, Keira Mahoney, Catherine Kwon, Raibat Sarker, Taryn Lucas, Stacy Malaker, Yale University
- 185 Accurate Moisture and Accurate Potency, <u>Kerri-Ann Blake</u>, Metrohm USA
- 186 Determination of Trace Level Nitrite in Pharmaceutical Excipients Using Ion Chromatography with Conductivity Detection, <u>Weiqing</u> <u>Fu</u>, Qinggang Wang, Yongmei Wu, Britol Myers Squibb,
- 187 FIDIG, the Bolt that Allows Agilent FID's to Light Every Time, <u>Matthew Monagle</u>, AIC LLC
- 188 Application of Ultrafast Supercritical Fluid Chromatography in a High-Throughput Pharmaceutical Process Development Workflow, <u>Matthew Morgan</u>, Mark Hardink, Angel Diaz, Giselle Reyes, Pfizer
- 189 Direct Elemental Analysis in Cell Culture Media Using ICP-MS, Brady Frill, PerkinElmer
- 190 Investigation of Electrochemical Degradation of PFOA Using High Surface Area Electrodes, <u>XingZhi Chen</u>, Haverford College, Md Tanim-Al Hassan, Timothy Yaroshuk, Hao Chen, Omowunmi Sadik, New Jersey Institute of Technology
- 191 Extraction of CBD from Personal Care Products Followed by Liquid Chromatography Coupled with UV Detection, <u>Rachel Murphy</u>, Jacob Esposito, Isabella McGrath, University of Connecticut

- 192 Identifying Potentially Different Phytocannabinoids in Experimentally Grown Hemp Extracts Using High Performance Liquid Chromatography with UV PhotoDiode-Array Detection, <u>Austin Pelletier</u>, James Stuart, Angelica Velasquez, Cole Strattman, Anthony Provatas, CESE
- 193 Investigation of Extraction Protocols for the Analysis and Quantitation of Cannabinoids in Gummy Matrices using Liquid Chromatography and Ultraviolet Detection, <u>Aaron Urbas</u>, Walter Wilson, National Institute of Standards and Technology, Haley Jensen, Ira Lurie, George Washington University
- 194 The Challenges to Migrating Analytical Methods between Instruments, <u>Tony Reinhold</u>, Paula Hong, Waters Corporation
- 195 Evaluation, Performance and Comparison of a 1.5 mm Internal Diameter LC Column for Pharmaceutical Analysis, <u>Alan McKeown</u>, Marianna Gonzales, Vertex Pharmaceuticals Ltd.
- 196 The Effect of Solvent Choice on Limit of Detection Calculations in Gas Chromatography with Flame Ionization (GC-FID) Detection, James Mizvesky, Nicholas Snow, Seton Hall University
- 197 Analysis of Common Active Pharmaceutical Ingredients (APIs) Using Gas Chromatography-Flame Ionization (GC-FID) and Gas Chromatography-Vacuum Ultraviolet (GC-VUV) Detection as a Green Alternative to HPLC, <u>Alexander Bulsiewicz</u>, James Mizvesky, Nicholas Snow, Seton Hall University
- 198 All Carbon Stationary Phase Material for Biomolecule Separation: Design and Characterization, <u>Michael Parente</u>, Balaji Sitharaman, Millennial Scientific
- 199 Automated Solid Phase Extraction and Determination of Hallucinogenic Compounds in Serum and Urine Samples Using a Novel Robotic Autosampler and LC-MS/MS Platform, <u>Fred Foster</u>, GERSTEL, Inc.
- 200 Approaches for Reducing the Environmental Impact and Increasing the Throughput of LC Separations, <u>Jessica Hussey</u>, MAC-MOD Analytical, Matt James, Anthony Edge, Avantor Sciences

Tuesday Afternoon, November 14, 2023

EAS Award for Outstanding Achievements in Magnetic Resonance

Honoring James Prestegard, University of Georgia Sponsored by Bruker BioSpin and New Era Enterprises Chair: Darón I. Freedberg, United States Food & Drug Administration

- 1:30 201 NMR Illuminates the Conformational Ensembles of Nucleic Acids, <u>Hashim Al-Hashimi</u>, Columbia University
 2:00 202 An NMR Journey from Method Development to Practical Applications that all began in New Haven, <u>John Marino</u>, National Institute of Standards and Technology
 2:30 Break
 3:00 203 NMR: A Powerful Tool to Study Nature's Switches to Develop Biotech Tools and Therapeutics, <u>Kevin Gardner</u>, CUNY Advanced Science Research Center
- 3:30 Presentation of the EAS Award for Outstanding Achievements in Magnetic Resonance
- 3:35 204 Glycans on Glycoproteins; What NMR Can Tell Us, <u>James</u> <u>Prestegard</u>, University of Georgia

New York/New Jersey Sections of the Society for Applied Spectroscopy Gold Medal Award Honoring Curtis Marcott, Light Light Solutions

Chairs: Dana Garcia, Deborah Peru, DP Spectroscopy and Training

- 1:30 205 Industrial Spectroscopy Research Leading to the Development of Novel Bioplastics, <u>Isao Noda</u>, University of Delaware
- 2:00 206 Super-Resolution Photothermal Infrared Spectroscopy for Science and Industry, <u>Craig Prater</u>, Photothermal Spectroscopy Corp.

2:30 Break 3:00 207 Nano-Chemical Imaging and Spectroscopy to Unravel (bio)-Organic Matter towards the Single-molecule Level, Francesco Simone Ruggeri, Wageningen University 3:30 208 Characterizing the Microstructure of Novel Bioplastics

Using Photothermal Infrared Spectroscopy, <u>Curtis Marcott</u>, Light Light Solutions

What You Actually Need to do to Make Your Separations Sustainable

Sponsored by Chromatography Forum of DE Valley Chair: Mary Ellen McNally, FMC Corporation

- 1:30 209 Portable Capillary LC for In-Line UV Monitoring and MS Detection: Comparable Sensitivity and much Lower Solvent Consumption, <u>Michael Hicks</u>, Keith Mattern, Jonathan Fine, Shane Grosser, Daya Patel, Lauren Weisel, Pankaj Aggarwal, Merck & Co., Inc.
- 2:00 210 Development of the Analytical Control Strategy to Support a Continuous Drug Substance Process – New Thoughts on Green Chromatography, <u>Stephen Groskreutz</u>, Eli Lilly and Company
- 2:30 Break3:00 211 Evaluating your Method from a Sustainable Perspective,
- Mary Ellen McNally, FMC Corporation
- 3:30 212 Green Sample Preparation: It's All Green, <u>Douglas Raynie</u>, South Dakota State University

Quantitative Mass Spectrometry Through Drug Development Life Cycle

Chair: Carolina Cabral, Merck & Co., Inc.

1:30	213	Stereoisomer Separation of Drugs and Biomarkers Using Supercritical Fluid Chromatography to Support PK/PD
		Studies, <u>Fangbiao Li</u> , Bang-Lin Wan, Guanping Bi, Rena
		Zhang, Daniel Spellman, Merck & Co., Inc.

- 2:00 214 A Novel Hybridization LC-MS/MS Methodology for Quantification of siRNA in Plasma, CSF and Tissue Samples, Long Yuan, Biogen
 2:30 Break
- 3:00 215 Identification of Riboflavin as Novel BCRP Biomarker in Animal Models, <u>Linna Wang</u>, Yueping Zhang, Petia Shipkova, Bethanne Warrack, David Nelson, Runlan Huo, Jian Chen, Erika Panfen, Xue-Qing Chen, R.Marcus Fancher, Qian Ruan, Lisa Christopher, Yongjun Xue, Michael Sinz, Hong Shen, Bristol Myers Squibb
- 3:30 216 Hybrid LBA-LC-MS/MS Method for Glycan-Resolved PK Monitoring of a Therapeutic Fusion Protein, <u>Ines Santos</u>, Brian Melo, Linna Wang, Yury Chaly, Bonnie Wang, Y-J Xue, Jim Shen, Bristol Myers Squibb

Forensic Microscopy "What is it? Who does it? Sponsored by Agilent Technologies Chair: Thomas A. Kubic, John Jay College & The Graduate Center, CUNY

- 1:30 217 The Fatal Bullet Was it a Ricochet or Not, Peter Diaczuk, John Jay College CUNY
- 2:00 218 Microscopy and Microanalysis of Aluminum Powders Used in Improvised Explosive Devices (IED), <u>JoAnn Buscaglia</u>, JenaMarie Baldaino, Kayla Moquin, United States Federal Bureau of Investigation Laboratory, Jack Hietpas, John Jay College of Criminal Justice
- 2:30 Break
- 3:00 219 Investigative Leads from Microscopic Traces: A Lost Skill?, Skip Palenik, Microtrace
- 3:30 220 A Review of Dispersion Staining in Forensic Casework, Nick Petraco, Petraco Forensic Art Investigation

Unleashing the Power of Data with Quality-by-Design and Chemometrics

Chair: Pankaj Aggarwal, Merck & Co., Inc.

- 1:30 221 Mapping Key Elements in the USP <1220> and ICH Q14 Guidances to an Enhanced Quantitative Framework and Workflow for Analytical Procedure Development, <u>Richard</u> <u>Verseput</u>, S-Matrix Corporation
- 1:50 222 Faster, Cheaper, Greener! Joining HT Plate Readers and Chemometrics to Enable Enzyme Evolution, <u>Umme Ayesa</u>, Zachary Dance, Merck & Co., Inc.
- 2:10 223 Chemometrics Best Practices and the Impact on Quality Management, <u>Brian Rohrback</u>, Infometrix, Inc.
- 2:30 Break
- 3:00 224 Combining Analytical Data with Contextual Metadata through CDS Platform, Suite of Applications, and Spotfire Dashboards, <u>Henry Tat</u>, Jonathan Fine, Pankaj Aggarwal, Merck & Co., Inc.
- 3:20 225 Successful Replacement of Two Problematic HPLC Methods – One for API and One for Related Substances – with a Robust Single UHPLC Method Using the Enhanced QbD Approach, <u>Richard Verseput</u>, S-Matrix Corporation, Marina Mavrinac, J.G.L. Pharma, Gordan Dinter, Labtim Adria

Recent Developments in High Performance Thin Layer Chromatography

Chair: Leonel Santos

- 1:30 226 High-Performance Thin-Layer Chromatography PRO as a Quality Control Tool in Routine Analysis, <u>Wilmer Perera</u>, CAMAG Scientific, Inc., Shaune Liendo, Diana Catalan, Cape Fear Community College
- 1:50 227 Is Lipid Repair in Hair a Possibility or a Pipe Dream?, Ernesta Malinauskyte, TRI Princeton
- 2:10 228 High Performance Thin Layer Chromatography Accurate Mass Spectrometry for the Rapid Identification of Unknown Compounds, <u>James Kababick</u>, Stacy Wise, Chanze Jennings, Flora Research Laboratories, LLC
- 2:30 Break
- 3:00 229 USP Standards for European Elder Berry Dietary Ingredients: HPTLC Test Solutions to Address Quality and Adulteration Issues, <u>Maria Monagas</u>, United States Pharmacopeia Convention, Tiên Do, Eike Reich, CAMAG
- 3:20 230 Equivalency of DNA Sequencing vs. HPTLC Chromatographic Analysis vs. Botanical Microscopy Methodologies for Botanical Identity: A Statistical Evaluation, <u>Anthony Fontana</u>, Sidney Sudberg, Dinah Yu, Alkemist Labs, Robert LaBudde, Least Cost Formulations, Zhengfei Lu, Yanjun Zhang, Adam Faller, Herbalife

Revolutionizing Bioanalysis: Cutting Edge Analytical Advancements

Chair: Lydia Breckenridge, Bristol Myers Squibb

- 1:30 231 Exploration of Ultra High Pressure Liquid Chromatography for Bioanalysis, <u>Hayley Herderschee</u>, Robert Kennedy, University of Michigan, Noah Lancaster, Evgenia Shishkova, Austin Salome, Joshua Coon, University of Wisconsin-Madison
- 1:50 232 Rapid Label-Free Cell-Based Approach Membrane Permeability Assay Using MALDI-HDX-MS for Peptides in Drug Discovery, <u>Alexey Makarov</u>, Merck & Co., Inc.
- 2:10 233 Nanoparticle-Enhanced Laser Induced Breakdown Spectroscopy (NELIBS) on Lanthanide Micro Particles Tagged to Biomarker, <u>Ali Safi</u>, Helmar G. Adler, Joshua E. Landis, Kemal Efe Esseller, Noureddine Melikechi, University of Massachusetts Lowell, Yuri Markushin, Delaware State University

2:30 Break

- 3:00 234 Identifying Size-Dependent Toxin Sorting in Bacterial Outer Membrane Vesicles, <u>Aarshi Singh</u>, Justin Nice, Angela Brown, Nathan Wittenberg, Lehigh University
- 3:20 235 Mass-Activated Droplet Sorting for Selection of Lysine-Producing Escherichia Coli, <u>Emory Payne</u>, Bridget Murray, Laura Penabad, Robert Kennedy, University of Michigan, Eirc Abbate, Inscripta, Inc.

Applying Analytical Technologies to Drug Development Chair: Oscar Liu, Silver Springs Scientific LLC

1:3	30 236	Modernizing USP Methods According to <621> with Superficially Porous Particle Columns, <u>Stephanie Schuster</u> , Peter Pellegrinelli, Conner McHale, Advanced Materials Technology
1:5	50 237	Using Ion Chromatography to Assay for Citrate and Phosphate in Pharmaceutical Formulations, <u>Gary He</u> , Jingli Hu, Jeff Rohrer, Carl Fisher, Thermo Fisher Scientific
2:1	10 238	Direct Quantitation of Small-Molecule Impurities Using Molecular Rotational Resonance Spectroscopy, <u>Alexander</u> <u>Mikhonin</u> , Ann Adele Byars, Reilly Sonstrom, Voislav Blagojevic, Justin Neill, BrightSpec, Inc.
2:3	30	Break
3:0	0 239	Towards Globally Accepted Specifications of Pharmaceutical Products: A Summary of the Current State, Kaitlin Grinias, GSK
3:2	20 240	Analysis of Extractables and Leachables in Pharmaceutical and Medical Products using a Novel Simultaneous UHPLC-UV-CAD-HRMS Multi-Detector Platform, <u>Vedha Patel</u> , Rajesh Chennam Shetti, Dujuan Lu, Danny Hower, Chongming Lui, SGS Health Science
3:4	0 241	Isotopic Batch Process Understanding for Quality Control and Regulatory Compliance, <u>John Jasper</u> , Molecular Isotope Technologies, LLC, Anthony Sabatelli, Wiggin and Dana, LLP, Ann Pearson, Harvard University

Risk Mitigation in the Pharma QC Laboratory Sponsored by Waters Corporation Chair: Isabelle Vu Trieu, Waters Corporation

1:30	243	Analytical Quality by Design Based Method Development for the Analysis of Cold and Cough Formulations, <u>Fadi</u> <u>Alkhateeb</u> , Adam Bengtson, Isabelle VuTrieu, Paul Rainville, Waters Corporation
2:00	244	Continuous Monitoring of Method and Instrument Performance Across Various Instrument Vendors and Platforms Using a Variety of USP Monographs, Jennifer Simeone, Waters Corporation
2:30		Break

 3:00 245 Data Integrity and How it Will Impact Your Laboratory, Michael Barkan, Consultant
 3:30 Panel discussion

Wednesday Morning, November 15, 2023

EAS Young Investigator Award Honoring Emanuela Gionfriddo, University of Toledo Chair: Jared Anderson, Iowa State University

9:00	246	Employing Sustainable Solvents in Chemical Separations and Purification, <u>Jared Anderson</u> , Iowa State University
9:30		Presentation of the EAS Young Investigator Award
9:35	247	Addressing the Challenge of Small Molecule Separation in Complex Samples through Sustainable and High- Throughput Microextraction Techniques, <u>Emanuela</u> <u>Gionfriddo</u> , University of Toledo
10:00		Break

- 10:30 248 Diverse Applications of Compact Capillary LC, <u>James</u> <u>Grinias</u>, Samuel Foster, Benjamin Libert, Sangeeta Kurre, John Boughton, Ama Hackman, Rowan University
- 11:00 249 Gas Chromatographic Separations to Extract Chemical Data from Forensic Odors: Bugs, Bacteria and Bodies, <u>Katelynn Perrault Uptmor</u>, College of William and Mary

Evaluating and Understanding Extremely Large Molecules Through Various Separation Techniques Sponsored by Chromatography Forum of DE Valley Chair: Ray McClain, Merck & Co., Inc.

- 9:00 250 Redefining the Characterization Paradigm of RNA Lipid
- Nanoparticles, <u>Marshall Padilla</u>, Sarah Shepherd, Kushol Gupta, Michael Mitchell, University of Pennsylvania
 9:30 251 The Purification of Really Big (or Small?) Things: C-CP
- 9:30 251 The Purification of Really Big (or Small?) Things: C-CP Fiber Isolation of Exosomes from Diverse Matrices, Kenneth Marcus, Clemson University

10:00 Break

- 10:30 252 Analytical Characterization of a Pneumococcal Conjugate Vaccine, <u>James Deng</u>, Merck & Co., Inc.
- 11:00 253 Determining How Much, How Big and What "Stuff" is in a Complex Biotherapeutic Sample, <u>Wyatt Vreeland</u>, National Institute of Standards and Technology

Applications of Ion Mobility Mass Spectrometry Chairs: Gene Hall, Rutgers University, Anthony Pitts-McCoy, Merck & Co., Inc.

9:00 254 Advances in Polymer Characterization by Ion Mobility Mass Spectrometry, Chrys Wesdemiotis, University of Akron Leveraging High Resolution Ion Mobility Separations for 9:30 255 Pharmaceutical Applications, Komal Kedia, Merck & Co., Inc. 10:00 Break 10:30 256 Investigation of Tautomeric Forms of Gaseous lons by Ion Mobility, Athula Attygalle, Stevens Institute of Technology 257 Ion Mobility Spectrometry in Big Pharma, Gene Hall, 11:00 **Rutgers University**

New Applications of Quantitative Proteomics Chair: Jeremy Balsbaugh, University of Connecticut

- 9:00 258 A Proteomics Approach to Examine Brain Endothelial Cell Nuclear Protein Expression Level Changes in FTLD, <u>Olivia Durham</u>, Amy Kimble, Evan Jellison, Patrick Murphy, UConn Health, Jennifer Liddle, Jeremy Balsbaugh, University of Connecticut
- 9:30 259 Integrative Single-Organoid Proteomics in 3D Models of Ovarian Cancer Uncovers Remodeled Mitochondria Bioenergetics, <u>Krystal Lum</u>, John Muroski, Ileana Cristea, Princeton University, Oscar Pundel, Benjamin Neel, NYU Langone Health
- 10:00 Break
- 10:30 260 Proteogenomic Analysis of Pediatric Acute Myeloid Leukemia Diagnosis and Relapse Pairs, <u>Han Fisher</u>, Tina Glisovic-Aplenc, Lusha Cao, Kevin Nestler, Asif Chinwalla, Hossein Fazelinia, Yi Xing, Kathrin Bernt, Richard Aplenc, The Children's Hospital of Philadelphia, Saar Gill, Mingyao Li, Perelman School of Medicine, Jen Liddle, Jeremy Balsbaugh, University of Connecticut
- 11:00 261 Orbitrap Analysis of Cysteine PTMs in Signaling Proteins, <u>Hong Li</u>, Tong Liu, Rutgers University

Technical Program

Sub-Micron IR and Raman Spectroscopy Chair: Jing Qu, University of Delaware

Portable Instruments in the Field		
11:00	265	Tip-Enhanced Raman Spectroscopy and Nano-Imaging for 2D Materials, Peter Schuck, Columbia University
10:30	264	Visible to Mid-IR Spectromicroscopy with Top-Down Illumination and Nanoscale (≈10 nm) Resolution, <u>Devon</u> <u>Jakob</u> , Andrea Centrone, National Institute of Standards and Technology
10:00		Break
9:30	263	Recent Advances in Multimodal Optical-Photothermal Infrared Imaging and Spectroscopy, <u>Samuel Tenney</u> , Sabine Neal, Brookhaven National Lab
9:00	262	Correlated Micro- and Nano-Scale Analyses of Two Particles from the Near-Earth Asteroid Ryugu, <u>Timothy</u> <u>Glotch</u> , Stony Brook University

Sponsoredby the Rigaku Analytical Devices and New England SAS

Chair: Suzanne Schreyer, Rigaku Analytical Devices

- 9:00 266 Development of Alternate QC Techniques for More Rapid Screenings within LMIC Contexts, <u>David Jenkins</u>, Matthew Eady, Ed Bethea, Chris Harmon, FHI 360, Jonelle Caison, Melissa Growney, Campbell University
 9:30 267 Analysis of FDA-Regulated Products for the Presence of Active Pharmaceutical Ingredients Using Surface Enhanced Raman Spectroscopy Michael Thatcher Adam
 - Enhanced Raman Spectroscopy, <u>Michael Thatcher</u>, Adam Lanzarotta, Martin Kimani, Lisa Lorenz, Megan Sterling, Sara Kern, JaCinta Batson, United States Food & Drug Administration
- 10:00 Break
- 10:30 268 The Introduction of Raman Technology into Existing Law Enforcement Strategies to Degrade the Flow of Precursor Chemicals in Myanmar for the Production of Narcotics, <u>Michael Brown</u>, Rigaku
- 11:00 269 Street Chemistry: How Optical Spectrometries (FTIR and RAMAN) are Used to Solve Crimes, <u>Pakorn Patimetha</u>, NJ State Police

Beyond Boundaries: Expanding Horizons of Liquid Chromatography Chair: Peter Bratin, KLA

- 9:00 270 Method Migration of Amino Acid Analysis Across Multiple Instruments to Quantify Amino Acid Content in Commercially Available Supplements, <u>Kimberly Martin</u>, Paula Hong, Jennifer Simeone, Waters Corporation
- 9:20 271 Development of a Rapid LC Method for the Determination of 3-Chloropropionic Acid and 3-Chloropropionyl Chloride using EDC Derivatization, <u>Yuan Ren</u>, Qian Zhang, James Chadwick, Robert Menger, Yan Zha, Bristol Myers Squibb, John Orlet, Pfizer
- 9:40 272 The Development and Use of a Virtual Liquid Chromatography Method Development Tool, <u>Melinda</u> <u>Urich</u>, Justin Steimling, Jamie York, Chris Nelson, Tim Yosca, Restek Corporation, John Garrett, Analytical Innovations
- 10:00 Break
- 10:30 273 Quantification and Characterization of Intact Polysorbate 80, its Degradants, and its Subspecies in Biopharmaceuticals, <u>Katie Carnes</u>, Justin Shearer, Lee Oliver, Sina Mortazavi, Timothy Brown, Mike Morris, Michelle Ward, Josh Fuller, GSK, Roberto Delgadillo, Element Biosciences

- 10:50 274 Deeper Understanding of the Mechanism of Water Dewetting from Hydrophobic Mesoporous Silica Particles to Improve the Design of Stationary Phases in Reversed-Phase Liquid Chromatography, <u>Fabrice Gritti</u>, Waters Corporation
- 11:10 275 Separation of guide RNA for CRISPR: Methods, Mechanisms and Applications, <u>Bingchuan Wei</u>, Jenny Wang, Bifan Chen, Lulu Dai, Lance Cadang, Kelly Zhang, Genentech

Conservation Science: Beyond Art & Forensics Chairs: Jocelyn Alcantara-Garcia, University of Delaware, Rosie Grayburn, Winterthur Museum

- 9:00 276 Changing the Conversation for Biological Materials in Cultural Heritage: Integrating Multiple Disciplines with Multi-Faceted Scientific Approaches, <u>Julie Arslanoglu</u>, Metropolitan Museum of Art
- 9:30 277 The Current Understanding of the Organic Compositions of Chinese Export Lacquer Finishes, <u>Catherine Matsen</u>, Winterthur Museum
- 10:00 Break
 - 10:30 278 For the Culture: Collective Scientific Studies of Colonial-Era Art of the Spanish Americas, <u>Alicia McGeachy</u>, Elena Basso, Marco Leona, Metropolitan Museum of Art, Marc Vermeulen, National Archives, Annette Ortiz Miranda, The Walters Art Museum, Federica Pozzi, Institute of Science & Technology Chimiche, Diego Tamburini, British Museum, Marc Walton, M+ Museum
 - 11:00 279 Exploring Yale's Collection: XRF Scanning at Scale, <u>Marcie</u> <u>Wiggins</u>, Richard Hark, Aniko Bezur, Yale Institute for the Preservation of Cultural Heritage

Overcoming the Complexity of Biological Drug Products through Experimental and Computational Characterizations Chair: Yongchao Su, Merck & Co., Inc.

9:00 280 Fragmentation Pathways of Monoclonal Antibodies Induced by Visible Light, Christian Schoneich, University of Kansas 281 Nucleic Acid Lipid Nanoparticles: Development and 9:30 Process Optimization, Jeffery Smith, Merck & Co., Inc. 10:00 Break Understanding Protein Interactions Under Hydrodynamic 10:30 282 Stress with Multiphysics Simulation, Tonglei Li, Purdue University 11:00 283 Direct Assessment of Oligomerization of Chemically Modified Peptides and Proteins in Formulations Using DLS and DOSY-NMR, Kang Chen, United States Food & Drug Administration

Wednesday, November 15: E-Poster Session: 12:30pm – 1:25pm

- 285 Development and Validation of Stability Indicating RP-HPLC Method for Estimation of Aminocaproic Acid in Tablet Dosage Form, <u>Vrunda Patel</u>, Conestoga College
- 286 Efficient HPLC Column and Mobile Phase Screening Protocol for Developing Stability-Indicating Methods: Diphenhydramine Case Study, <u>Justin Mercado</u>, Josh Dalo, Chris Wood, Linnea Budge, FreeThink Technologies
- 287 Systematic Protocol Utilizing High Performance Surface Technology for the Improved Separation and Quantification of Synthetic Peptides and Associated Impurities, <u>Adam Bengtson</u>, Paul Rainville, Stephanie Harden, Waters Corporation
- 288 Understanding Excipient-Induced Solution Instability to Enhance Drug Product Development, <u>Margaret Brunell</u>, Merck and Co., Inc.
- 289 Plasticizers in Plants A Study on the Absorption of Plasticizers in Various Crops, <u>Victoria Sabatelli</u>, Elisa Uzeiri, Lakeland Regional High School

- 290 Comprehensive Profiles of Fragrance, Beverage, and Building Products - A Comparison of Techniques, <u>Megan Harper</u>, Nicole Kfoury, Jackie Whitecavage, Fred Foster, GERSTEL, Inc.
- 291 Rapid, Efficient and High-Throughput Extraction Method of PFAS from Soil, <u>Alicia Stell</u>, Benedict Liu, CEM Corporation
- 292 Use of a Derivatization Tag for Signal Enhancement of Organic Acids in Supercritical Fluid Chromatography-Mass Spectrometry, John Boughton, Yih Ling Saw, Faith Wroniuk, Peter Pellegrinelli, Samantha Calvez, Alexander Kaplitz, Lark Perez, James Grinias, Rowan University, Mahmoud Mostafa, James Edwards, Saint Louis University
- 293 Quantitatively Determining Isoniazid in Tablets with a Handheld NIR Spectrometer, <u>David Jenkins</u>, Matthew Eady, FHI360, Melissa Growney, Campbell University
- 294 Are You Analyzing "All" Your Extractables/Leachables? A Case Study Involving a Simple Switch from Acetonitrile to Isopropanol for Mobile Phase B in Liquid Chromatography/Mass Spectrometry, Yunyun Yuan, Ying Jiang, Yijun Lu, Ethicon, Johnson & Johnson
- 295 Method Validations of Trace Level Impurities in an Agrichemical Compound, <u>Nicholas Chubatyi</u>, Michael Harrington, FMC Corporation
- 296 Unified GC/MS Method for Detection of Alkyl and Benzyl Halides, Alex Dunleavy, Matt Bauerle, Exemplify BioPharma
- 297 Optical Characterization of 2D Ga2Se2 via Molecular Beam Epitaxy and Exfoliation for Quantum Computing Applications, Lottie Murray, Mingyu Yu, Eric Herrman, Xi Wang, Matthew Doty, University of Delaware, Stephanie Law, Penn State University
- 298 Biophysical Characterization of Proteins: Therapeutics, Vaccines and Plant Based, <u>Yelena Pyatski</u>, Rina Dukor, Kimberly Qinn, Juanita Sanchez, BioTools
- 299 Nanoscale Orientation-Sensitive IR Spectroscopy of Crystalline Samples, <u>Sung Park</u>, Padraic O'Reilly, Derej Nowak, Patrick O'Hara, Molecular Vista
- 300 Analytical Comparison of Genotoxic Impurities in Extracted Nicotine vs. Synthetic Nicotine, <u>Ayesha Nisathar</u>, Hui Chen, J-Star Research Inc.
- 301 Identification of Potential Degradation Impurities of Moxidectin, Mechanistic Explanation on Degradation Pathway and Establishment of a Stability-indicating Analytical Method, <u>Yao An</u>, Tyler Chen Huang, Frank Rinald, J-STAR Research

Wednesday Afternoon, November 15, 2023

PLENARY LECTURE

Wednesday, November 15, 11:45am – 12:45pm Paper Number: 284

Inclusive Stories in Chemistry: Celebrating Dr. Marie Maynard Daly Dr. Sibrina Collins Lawrence Technical University All registered Attendees are invited to attend

The Critical Role of Chromatography in Advancing Discovery and Development of Novel Medicines Sponsored by the Chinese American Chromatography Association

Chair: Yi He, John Jay College of Criminal Justice

- 1:30 302 Accelerating Drug Discovery by High-Throughput Purification and Physico-Chemical Characterization by HPLC/MS, Laszlo Varady, Rilas Technologies
- 2:00 303 Separation Workflows Coupled with Mass Spectrometry for Biotherapeutic Development, <u>Nicole Schneck</u>, Matthew D. Maust, Robert J. Schuster, Paul MacGregor, Catherine O. Brown, Mark Jennings II, Sonya Kennedy-Gabb, GSK
 2:30 Break

- 3:00 304 Advanced Chromatographic Tools for Accelerated Development of Nucleic Acid Based Medicines, <u>Balasubrahmanyam Addepalli</u>, Makda Araya, Maissa Gaye, Martin Gilar, Matthew Lauber, Waters Corporation
- 3:30 305 Challenges and Solutions in Analyzing Variants in Antibodies and Related Substances: Some Real-Life Case Studies, <u>Xiaodong Liu</u>, NanoChrom Technologies

Measurement Challenges in Cannabis-Derived Products Chair: Aaron Urbas, National Institute of Standards and Technology

- 1:30 306 Things WE'ED Like to Avoid Circumventing Measurement Challenges When Analyzing Cannabinoidinfused Complex Matrices, <u>Rabi Musah</u>, Benedetta Garosi, Megan Chambers, University at Albany - SUNY
 2:00 307 The Importance of Digestion Temperature on Trace Metals Analysis, <u>Samuel Heckle</u>, CEM Corporation
- 2:30 Break
- 3:00 308 The Characterization of Delta-9-Tetrahydrocannabinol Stereoisomers in Various Cannabis Products, <u>Brandy</u> <u>Young</u>, Andrea Andreeva, Certainty Analytical Labs
- 3:30 309 Accurate Identification and Quantitation of Contaminants - Understanding the Impact of the Cannabis Matrix, Jini Glaros, ModernCanna Labs

Advances in Chromatography with Applications in the Biomedical/Clinical Diagnostics Field Chair: David Bell, Restek Corporation

- 1:30 310 Leveraging Multi-Mode Microextraction and Liquid Chromatography for Quantitative Analysis of Neurotoxic Non-Proteinogenic Amino Acids, Emanuela Gionfriddo, Ronald Emmons, Endri Karaj, L. M. Viranga Tillekeratne, University of Toledo, Erasmus Cudjoe, PerkinElmer, David Bell, Restek Corporation Separation and Analysis of Oligonucleotides for Clinical 2:00 311 Diagnostics, Jared Anderson, Derek Eitzmann, Shashini De Silva, Iowa State University 2:30 Break 312 Simplifying Clinical LC-MS Development by Leveraging 3:00 Unique Stationary Phase Selectivity, Samantha Herbrick, **Restek Corporation** 313 Utilization of Hydrophilic Interaction Liquid 3:30 Chromatography (HILIC) in Clinical Analyses, David Bell, **Restek Corporation** Analytical Advancements Driving Pharmaceutical Excellence Chair: Sharla Wood, Bristol Myers Squibb
 - 1:30 314 Improved Drug Product Development and Control through Detailed Characterization of API Epimerization, <u>Nathan</u> <u>Contrella</u>, Steven Tignor, Colin Lam, Margaret Brunell, Alexandra Andrews, Josey Topolski, Devin Swiner, Tamara Cabalu, Zhoupeng Zhang, Ryan Cohen, Brittany Kassim, Merck & Co., Inc.
 - 1:50 315 Efficiency of Ultrafiltration / Diafiltration in Removing Organic and Elemental Process Equipment Related Leachables, <u>Bin Sun</u>, Cytiva
 - 2:10 316 Application of XRF in the Pharmaceutical Industry, <u>Sergey</u> <u>Mamedov</u>, HORIBA Scientific
 - 2:30 Break
 - 3:00 317 Pharmaceutical Applications Utilizing LUMA Vacuum Ultraviolet Detection: Advancements in Moisture Content, Impurity Analysis, and FAMEs Analysis, <u>Rafael Acosta</u>, Ryan Schonert, VUV Analytics

3:20 318 First-Principle-Based Investigation of Column Selectivities - Using Multidimensional Analytical Design Space Models as Tools to Find Equivalent Working Ranges Across Various Stationary Phases, <u>Arnold Zoeldhegyi</u>, Molnar-Institute, Róbert Kormány, Egis Pharmaceuticals Plc.

Chemometrics: Using Data to Solve Tomorrow's Problems Chairs: Caelin Celani & Helder Carneiro, University of Delaware

1:30	319	Application of Self-Optimizing Support Vector Classifier- Radial Basis Function for Multivariate Classification of Maca Metabolomic Mass Spectral Profiles from China and Peru, <u>Qudus Thanni</u> , Peter Harrington, Ohio University
2:00	320	Self-Modeling Curve Resolution of Raman Spectra from Mixed Deuterated and Protiated Phospholipid Membranes Reveals Isotopically-Segregated Lipid Domains, <u>Jay Kitt</u> , University of Utah
2:30		Break
3:00	321	Error Propagation-based Optimal Threshold Determination for Classification Models: Advancing Boundary Calculation in Chemical Information Analysis, <u>Helder Carneiro</u> , Caelin Celani, Karl Booksh University of Delaware
3:30	322	Transcending the Black Box: A Semi-AutoML Approach to Collaborative Model Building, <u>Manuel Palacios</u> , Sean Roginski, Barry Wise, Robert Roginski, Eigenvector

Applications of Analytical Chemistry in Proteomic Research Chair: Kate Jackson, Colgate Palmolive

Research

- 1:30 323 New Technologies and Techniques for the Separation of Oligonucleotides and Polypeptides, <u>Weston Umstead</u>, Daicel Chiral Technologies
- 1:50 324 Assessing Chromatographic Systems for Use in Phosphopeptide Mapping Studies, <u>Corey Reed</u>, Paula Hong, Robert Birdsall, Jennifer Simeone, Waters Corporation
- 2:10 325 Don't Go to Pieces on Me: Importance of Particle Architecture and Backpressure on Oligonucleotide Characterization, <u>Hillel Brandes</u>, Cory Muraco, Clinton Corman, MilliporeSigma
- 2:30 326 Increased Efficiency of Protein and Peptide Separations by Varying Particle Size, Column Dimension, and Pore Size of Superficially Porous Particle Columns, <u>Peter Pellegrinelli</u>, Ben Libert, Stephanie Schuster, AMT

2:50 Break

Exploring Diverse Applications of Spectroscopic Techniques Chair: Dana Garcia

- 1:30 327 Thermodynamic Stabilization of Conformations in Lewis Antigens, <u>Darón Freedberg</u>, Jeahoo Kwon, Hugo Azurmendi, Jasmin Zarb, Marcos Battistel, CBER/FDA, Alessandro Ruda, Göran Widmalm, Stockholm University, Liang Liao, France-Isabelle Auzanneau, University of Guelph
- 1:50 328 i-HMBC: Unequivocal Identification of Two-Bond Heteronuclear Correlations in Natural Products at Nanomole Scale, <u>Xiao Wang</u>, Merck & Co. Inc
- 2:10 329 Developing Benchtop NMR Spectrometer into QC and PAT, <u>Hector Robert</u>, Anh Le McClain, Magritek
- 2:30 Break
- 3:00 330 Nanoscale Chemical Analysis of Surfaces and Monolayers of Intentional and Unintentional Molecules, <u>Graceson</u> <u>Aufderheide</u>, Sung Park, Padraic O'Reilly, Derej Nowak, Patrick O'Hara, Molecular Vista
- 3:20 331 Optical Imaging and Spectroscopic Analysis of Polysulfide Speciation in Li–S Battery Electrolyte, <u>Gbenga Taiwo</u>, Ali Rashti, Mritunjay Mishra, Koffi Yao, University of Delaware

3:40 332 Can Magnetic Resonance Force Microscopy Detect and Image Individual Nitroxide Spins?, <u>John Marohn</u>, Michael Boucher, Peter Sun, Russell Burgett, Pamela Nasr, Corinne Isaac, Roger Loring, Cornell University, Lee Harrell, U.S Military Academy, Robert McMichael, National Institute of Standards and Technology

Analytical Studies in Heritage Discovery, Authentication and Attribution

Sponsored by Kenescott Fdn; NY Microscopical Society Chair: John Scott, Kenescott Fdn; NY Microscopical Society

- 1:30 333 Dangers in the Library: Poison Book Covers, Altered Illuminations, and Toxin-Dusted Fore Edges, <u>Jennifer L.</u> <u>Mass</u>, Bard Graduate Center, Aaron Shugar, Queens University, Adam Finnefrock, Teresa Duncan, Scientific Analysis of Fine Art, Heidi Nance, Philadelphia College of Osteopathic Medicine
- 2:00 334 Considerations and Misinterpretations: Practical Notes on Authenticity, from a Paintings Conservator, <u>Kristin</u> <u>deGhetaldi</u>, deGhetaldi Fine Art Restoration
- 2:30 Break
- 3:00 335 Correlating Visual Changes with the Chemistry of Latex Browning in Works of Art, <u>Teresa Duncan</u>, Satoko Tanimoto, Hannah Duggan, Scientific Analysis of Fine Art, LLC, Esther Chao, Lena Stringari, Solomon R. Guggenheim Museum
- 3:30 336 Development, Application, and Relevance of Artificial Intelligence for Art Discovery, Authentication and Attribution, <u>Lauryn Smith</u>, The Frick Pittsburgh

Analytical Approaches to Cosmetic Chemistry Chair: Andrew Koutrakos, KX Technologies

- 1:30 337 Chromatography and Mass Spectrometry Based Approaches for Raw Materials Characterization and Finished Goods Analysis in Consumer Goods Samples, <u>Chad Herman</u>, Unilever R&D
- 2:00 338 Using Biology as Inspiration for Dynamic Optical Materials, Lelia Deravi, Northeastern University
- 2:30 Break
- 3:00 339 Multivariate Data Analysis for Cosmetic Formulations Powered by Umetrics, <u>Gregory Casee</u>, Sartorius
- 3:30 340 Balancing Moisture: Karl Fischer Analysis in Cosmetic Formulations, <u>Kerri-Ann Blake</u>, Metrohm USA

Technical Program

2023 EAS Awards

EAS Award for Outstanding Achievements in the Fields of Analytical Chemistry, sponsored by Bristol Myers Squibb

On Monday, November 13, 2023, Professor Robert Kennedy, University of Michigan, will receive the EAS Award for Outstanding Achievements in the Fields of Analytical Chemistry.



Robert Kennedy is the Hobart H. Willard Distinguished University Professor of Chemistry and Professor of Pharmacology at the University of Michigan. He earned a PhD at University of North Carolina in 1988 where his work focused on using open tubular LC to analyze single cells. After a post-doc in neuroscience he started his own research program at University of Florida in 1991 before moving to University of Michigan as the Hobart H. Willard Professor of Chemistry in 2002. His research has combined his interest in biology with chemical analysis, separations and microfluidics. A theme of his group has been development of new chemical analysis tools that can be used at the nanoscale for several applications including screening of drugs, engineering enzymes, monitoring neurotransmitters in the brain, and studying the secretion of insulin and other hormones. Key technical areas including ultra high pressure LC, droplet microfluidics, and mass spectrometry. His work has been recognized by several awards including the American Chemical Society Award in Chromatography, the Ralph Adams Award in Bioanalytical Chemistry, and two NIH MERIT awards. He has held several service posts including Department Chair and is presently Associate Editor of Analytical Chemistry and ACS Measurement Science Au.

EAS Award for Outstanding Achievements in Separation Science, sponsored by Restek

On Monday, November 13, 2023, Professor Mary J. Wirth, Purdue University, will receive the EAS Award for Outstanding Achievements in Separation Science.



Mary J. Wirth is the W. Brooks Fortune Distinguished Professor Emerita at Purdue University. She received her B.S. in chemistry from Northern Illinois University, where she became fascinated by separation science while taking a graduate course from Professor Joseph Pesek. She received her Ph.D. from Purdue University, working under the direction of Professor Fred Lytle, where she learned to invent new instrumentation to investigate chemical phenomena. Dr. Wirth's research interests have focused on understanding silica interfaces to advance chromatography, electrophoresis, and optical spectroscopy, for which she employed tools such as optical microscopy, AFM, SEM, solid-stateNMR, FTIR, and single-molecule spectroscopy. Her research has been recognized with awards that include the Spectrochemical Analysis Award from the ACS Analytical Division, the Gold Medal Award from the Society for Applied Spectroscopy, the Dal Nogare Award from the Chromatography Forum of the Delaware Valley, the Jubilee Award from the Chromatography Society (Europe), and the EAS Award for Outstanding Achievements in the Fields of Analytical Chemistry.

EAS Award for Outstanding Achievements in Chemometrics, sponsored by Eigenvector Research

On Monday, November 13, 2023, Professor John H. Kalivas, University of Idaho, will receive the EAS Award for Outstanding Achievements in Chemometrics.



John H. Kalivas is a Professor in the Department of Chemistry at the primary undergraduate institution Idaho State University (ISU). He obtained his PhD at the University of Washington in 1982 under the direction of Bruce Kowalski. After two temporary lectureship positions at University of Minnesota-Morris and Texas A&M University, he started his tenure track position at ISU in 1985. He has been named the Most Influential Professor eight times by graduating undergraduates receiving the ISU Outstanding Academic Achievement Award. In 1994 he was named ISU Distinguished Researcher and also awarded a Camille and Henry Dreyfus Scholar Award. In 2003 he was named a Fellow of the International Union of Pure and Applied Chemistry (IUPAC). Recently he received the Idaho Jean'ne M. Shreeve NSF EPSCoR Research Excellence Award in 2021 and the Society of Applied Spectroscopy Fellows Award in 2022. Since 1990, 1993, 1998 and 2007 he has been respectively serving on the editorial boards for the Journal of Chemometrics, Analytical Letters, Applied Spectroscopy, and Talanta. He became an Associate Editor for Applied Spectroscopy in 2010 and an Editor for the Journal of Chemometrics in 2013. In 2012 he spearheaded the formation of the Bruce R. Kowalski Award in Chemometrics administered by the Society of Applied Spectroscopy. He is the author or

co-author of over 130 professional papers, book chapters, and books dealing with chemometrics. Much of his research has spanned methodology developments for autonomous optimization of multivariate calibration and classification processes. He has also completed extensive work developing multivariate figures of merit. His recent work established model updating methods concentrating on transfer learning approaches using unlabeled data (transductive semi-supervised learning). These new processes include an autonomous model selection algorithm for up to three metaparameters (tuning parameters) specifically directed towards predicting analyte amounts in a collection of new target samples. Recent work also involved developing a new local modeling strategy that mines a spectral library leveraging hidden sample physicochemical and physiochemical properties to identify matrix matched calibration sample sets relative to predicting each new target sample. With his research team, he advanced a unique in-house fusion process that removes the optimization step for many classification methods. His current focus is pushing the chemometric frontier using immersive analytics for virtual reality (VR) data visualization to produce new hybrid data analysis structures by combining the computer with human cognitive skills to make more efficient and accurate decisions. Immersive VR allows the user to see inside data configurations as well as feel the inherent data structure with haptic gloves. Presently, the focus is resolving complex classification situations where autonomous algorithms fail.

EAS Award for Outstanding Achievements in Magnetic Resonance, sponsored by Bruker BioSpin and New Era Enterprises

On Tuesday, November 14, 2023, Professor James H. Prestegard, University of Georgia, will receive the EAS Award for Outstanding Achievements in Magnetic Resonance.



James H. Prestegard, currently GRA Eminent Scholar, Professor Emeritus of Chemistry, and Professor Emeritus of Biochemistry and Molecular Biology at the University of Georgia, was born in Minneapolis, Minnesota in January of 1944. He remained in the state until he received his BS in Chemistry from the University of Minnesota in 1966. He then moved to California to attend graduate school at Caltech. While he intended to pursue research in physical organic chemistry, he quickly became fascinated with the biophysical chemistry going on in Professor Sunney Chan's group and produced a thesis exploring applications of Nuclear Magnetic Resonance (NMR) to both nucleic acids and ion-transport antibiotics. While he intended to pursue postdoctoral studies involving the biophysics of membrane systems, a looming economic downturn dictated looking for a more permanent position. He joined the Chemistry Department of Yale University as an Assistant Professor in 1970. Ever since his appointment in the Chemistry Department at Yale University, the Prestegard laboratory has specialized in the development and application of NMR methods for the study of systems of biological interest. Focus has evolved from lipid membranes to proteins to carbohydrates, and now to combinations of these systems. The laboratory produced its first NMR structure of a protein in 1988

(acyl carrier protein), a structure which stood as the only structure of a fatty acyl carrier protein until a crystal structure appeared in 2001. It has produced many protein structures since that time, including one of the first integral membrane protein systems, the glycophorin dimer, in 1997. In the course of this activity new methodology was developed, including the use of lipid bicelles as an orientable medium for characterizing glycolipids and residual dipolar couplings (RDCs) as a new source of information on protein structure. In 2002 Dr. Prestegard, along with Aksel Bothner-By and Ad Bax, was recognized for the introduction of RDCs by the Award of the Laukien Prize for an outstanding contribution to experimental NMR. Since joining the Complex Carbohydrate Research Center at the University of Georgia, interest has turned to glycan-protein interactions and glycoprotein structure. Accomplishments here include the NMR structure determination of a glycosylated proteins. During the course of his career Professor Prestegard has mentored nearly 100 doctoral and postdoctoral students. He has published more than 400 papers and he is one of the editors of the leading textbook in the field of glycobiology, "Essentials of Glycobiology", now in its fourth edition.

EAS Award for Outstanding Achievements in Mass Spectrometry, Sponsored by the American Microchemical Society

On Tuesday, November 14, 2023, Professor John A. McLean, Vanderbilt University, will receive the EAS Award for Outstanding Achievements in Mass Spectrometry.



John A. McLean is Stevenson Professor of Chemistry, Chair of the Department of Chemistry, Associate Provost for Graduate Education, and Director of the Center for Innovative Technologies at Vanderbilt University. He is an elected Fellow of the National Academy of Inventors and the American Association for the Advancement of Science. He earned his PhD at George Washington University in 2001 in the development of inductively coupled plasma mass spectrometry instrumentation for ultratrace elemental analysis. He subsequently performed postdoctoral research at Forschungszentrum Jülich in Germany and then at Texas A&M University before beginning at Vanderbilt University in 2006. McLean and colleagues have focused on the conceptualization, design, and construction of ion mobility-mass spectrometers and structural mass spectrometers, specifically targeting complex samples in systems, synthetic, and chemical biology. His group applies these strategies to forefront translational research areas in drug discovery, personalized medicine, and 'human-on-chip' synthetic biology platforms. McLean has received a number of awards, including his laboratory serving as an Agilent Thought Leader Laboratory, a Waters Center of Innovation, the Chancellor's Award for Research, the Thomas Jefferson Award, Excellence in Teaching Award from the student members of the

American Chemical Society, a Defense Threat Reduction Agency Research Award, an American Society for Mass Spectrometry Research Award, and the Bunsen–Kirchhoff Prize from the GDCh (German Chemical Society), among others. He has served in many service roles to the profession including serving terms on the boards of professional societies, scientific companies, and major journals. He has published over 200 manuscripts and received over 30 patents in these and allied areas..

EAS Young Investigator Award

On Wednesday, November 15, 2023, Professor Emanuela Gionfriddo, University of Toledo, will receive the EAS Young Investigator Award.



Emanuela Gionfriddo is an Assistant Professor of Chemistry at the Department of Chemistry and Biochemistry of The University of Toledo (OH, USA). Research work in the Gionfriddo's lab focuses on developing advanced analytical separation tools for the analysis of complex biological and environmental samples using green extraction methodologies. She received her Ph.D. in Analytical Chemistry (2013) at the University of Calabria (Italy). She joined Prof. Pawliszyn's group at the University of Waterloo (Ontario, Canada) in 2014 as a Post-Doctoral Fellow and manager of the Gas-Chromatography section of the Industrially Focused Analytical Research Laboratory (InFAReL), and within three years, became a Research Associate. Dr. Gionfriddo has authored over 50 peer-reviewed contributions, including a patent on PTFE-based SPME coatings. Dr. Gionfriddo is one of the founding members of the Dr. Nina McClelland Laboratory for Water Chemistry and Environmental Analysis at The University of Toledo and she is appointed to the Ohio Attorney General Yost's Environmental Council of Advisors. Dr. Gionfriddo is the 2022 recipient of the ACS Analytical Division Satinder Ahuja Award for Young Investigators in Separation Science and the 2023 LCGC Emerging Leader in Chromatography Award. She also serves as the Secretary of the ACS Analytical Chemistry Subdivision on Chroma-

tography and Separation Chemistry. Her research program is currently funded by the National Science Foundation through the 2022 CAREER Award, the National Oceanic and Atmospheric Administration, and several industrial partnerships..

New York/New Jersey Society for Applied Spectroscopy Gold Medal Award

On Tuesday, November 14, 2023, Dr. Curtis Marcott, Light Solutions LLC, will receive the New York Society for Applied Spectroscopy Gold Medal Award.

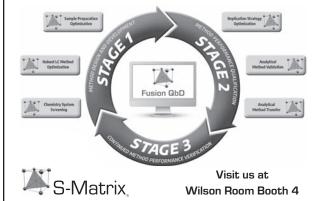


Curtis Marcott is a Senior Partner at Light Light Solutions LLC, a spectroscopic consulting firm. He received a B.S. in math and chemistry at Concordia College and his PhD from University of Minnesota. Following his PhD, he joined The Procter & Gamble Company where he worked for over 28 years in the Optical Spectroscopy Laboratory and was named Research Fellow in 1997. Dr. Curtis Marcott joined Light Light Solutions LLC in 2008. Dr. Marcott contributed to a number of innovative developments in vibrational spectroscopy: vibrational circular dichroism (VCD), near-IR measurements of interfacial phase boundaries, 2D correlation spectroscopy, publication of the first polarization modulation grazing angle FT-IR measurements of monolayers on metals and the first FT-IR spectroscopy using photothermal infrared (PTIR), including AFM-PTIR, optical PTIR (0-PTIR), and the simultaneous measurement of 0-PTIR and Raman spectra. Dr. Marcott has authored and co-authored more than 150 publications, given more than 650 presentations at national and international meetings. He is a past president of the Society for Applied Spectroscopy and has served on numerous conference organizing committees and

journal editorial advisory boards. For his work Dr. Marcott received the 1993 Williams-Wright Award from the Coblentz Society for achievement in industrial vibrational spectroscopy and was named the 2001 Cincinnati Chemist of the Year. Dr Marcott was previously Visiting Assistant Professor of Chemistry, University of Utah, Adjunct Professor of Chemistry, Miami University, and is currently Affiliated Professor of Materials Science and Engineering, University of Delaware.

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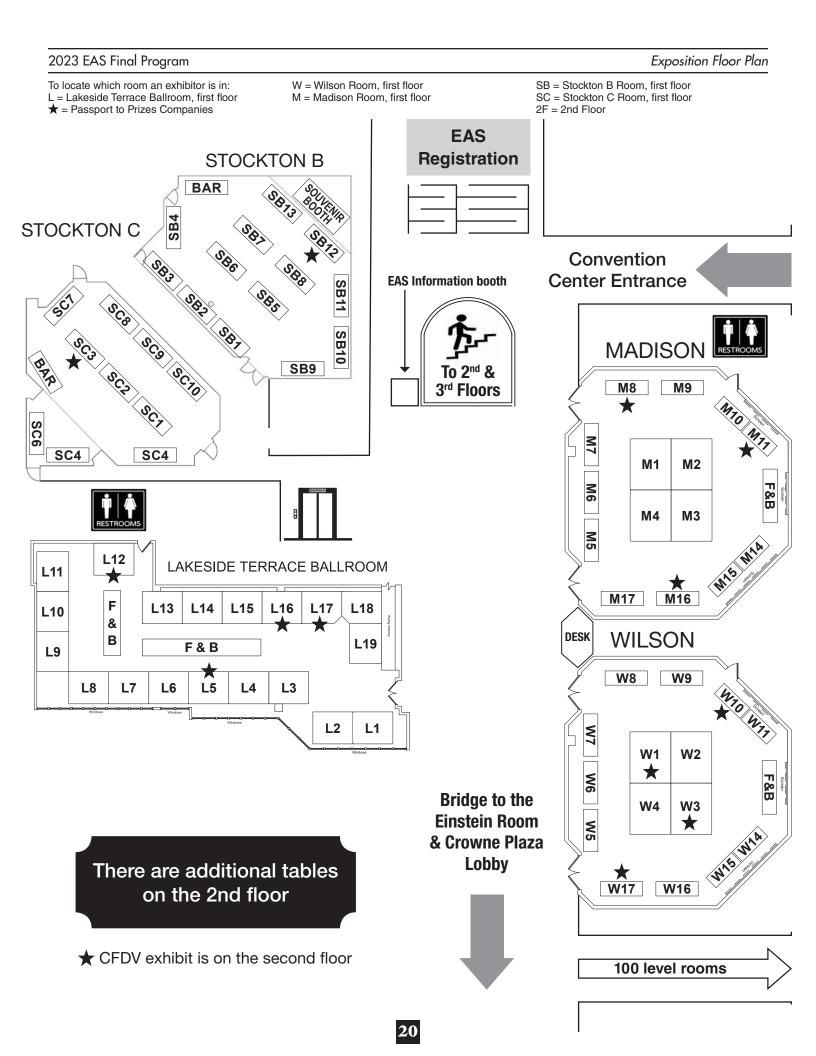
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Visit These Exhibitors at the 2023 EAS

Last updated November 07, 2023

ALMA – 2F	Molecular Vista, Inc. – SC3 Passport to Prizes
Advanced Materials Technology - W10 Passport to Prizes	Molnár-Institute for Applied Chromatography – L3
Advion Interchim Scientific – SB11	NJACS Topical Discussions Group – 2F
Agilent Technologies – L4	NY/NJ SAS – 2F
Alliance Calibrations Group – M3	Neta Scientific – W2
American Chemical Society, NY Local Section – 2F	New York Microscopical Society – 2F
Anton Paar – SB10	Nexomics Inc - SB12 Passport to Prizes
Argento Scientific – SC7	Omicron Scientific, Inc. – SB7
Axcend – M6	Parker – SB4
Bettersize Inc. – L14	PDR-Separations - L12 Passport to Prizes
Bruker Corporation – L15	PEAK Scientific, Inc. – L7
Buchi Corp – SB5	Photothermal Spectroscopy Corp. – SC8
CAMAG Scientific, Inc – SB13	Plasmion – W15
CDS Analytical, LLC – W6	Porton USA – SC2
CFDV - 2F Passport to Prizes	Pyvot - W17 Passport to Prizes
Catalent Pharma Solutions – SB8	Quantum Analytics – M7
Coblentz Society, Inc., The – 2F	Regis Technologies - M11 Passport to Prizes
Daicel Chiral Technologies – W7	Renishaw, Inc. – M9
Dissolution Technologies - M8 Passport to Prizes	Restek Corporation – L16 Passport to Prizes
ELGA LabWater – W9	Rudolph Research Analytical – L17 Passport to Prizes
Elementar Americas, Inc. – L11	S-Matrix Corporation – W4
Entech Instruments – L18	SCAT Americas Inc – M2
Frontage Laboratories, Inc. – SC4	SCIEX – M1
GERSTEL, Inc. – L5 Passport to Prizes	Schmidt + Haensch / Lazar Scientific, Inc. – M4
GFS Chemicals – W8	Shimadzu Scientific Instruments, Inc. – L2
HORIBA Scientific - M16 Passport to Prizes	SOTAX – L8
INTEGRA Biosciences – SB9	Spectrum Chemical Mfg. Corp. – SC6
Inorganic Ventures – L6	Stevens Institute of Technology – SC5
IonBench Corporation – W16	TA Instruments, a division of Waters - W3 Passport to Prizes
JEOL USA, Inc – L19	Tecan – W5
LCGC & Spectroscopy – M5	Thermo Fisher Scientific – L13
LECO Corporation – SC9	Thomson Instrument Company – W14
Logan Instruments Corp. – SC10	Trajan LEAP PAL Parts – SB2
MAC-MOD Analytical – L10	VELP Scientific – SB1
Mandel – M15	VICI DBS USA – SB3
Martel Instruments LLC – M10	Waters Corporation - W1 Passport to Prizes
Mestrelab Research – M17	Welch Materials, Inc. – SB6
Metrohm USA – L9	Wessex press – W11
MicroSolv Technology Corporation – L1	Wilmington PharmaTech – M14
Millennial Scientific – SC1	111

For more information, please contact Janine Kishbaugh at exposition@eas.org or 610-509-2354

Exposition & Special Events

Monday, November 13th Tuesday, November 14th Wednesday, November 15th 10:00am to 6:30pm 10:00am to 5:30pm 10:00am to 3:00pm

Demonstration Rooms



Visit the Agilent booth (L-4) and Demo Room 110A to learn about two newly launched LCMS systems. We will also be featuring products from molecular spectroscopy and consumables. In our demo room we will be showing a variety of chromatography and mass spec instruments. Stop by and discuss your research challenges with our experts. We will also have two lunch presentations (lunch will be provided but seating is quite limited). Please register: https://bit.ly/48ZAItE

<u>Monday Nov 13 , 12:00 PM – 1:00 PM:</u> The Power of 2DLC – Live demo Speaker: Bob Giuffre, Agilent Pre-sales Application Engineer

<u>Tuesday Nov 14 th 12:00 PM – 1:00 PM:</u> Changing Isocratic and Gradient Compendial Methods per USP 621 Speaker: Dr. William Long, Agilent Pre-sales Application Engineer



Waters Demo Room: Meet Your New Lab Ally

Waters Corporation is proud to showcase Andrew+ the pipetting robot and the Alliance iS HPLC system on Monday, Tuesday and Wednesday, 9:00 AM - 4:00 PM in Room 109. Visit the Waters demo room to discover our intuitively simple solutions for the laboratory and engage with our scientists.

For more information about the Waters Demo Room, please contact lsabelle_VuTrieu@waters.com

Receptions



Join us at booth L15 - Monday as we focus on a new enticing application, come raise a glass of wine with us! We are happy to support the Monday Evening Reception.

KEYNOTE, PLENARY & BREAKFAST LECTURES

We are excited to announce our special lectures! Join us to hear these experts:



Keynote Speaker

Monday, November 13, 4:15 PM Amphitheatre, 1st Floor

Exposome and Human Disease: From Neurological Disorders to Diabetes and Cancer

Dr. Vasilis Vasiliou Yale University

All registered attendees and exhibitors are invited to join us for the Keynote reception in the Expo Rooms immediately following the lecture.



Breakfast Lecture

Tuesday, November 14, 8:00 AM Einstein Room; 1st Floor

Fractionation and Characterization of Bacterial Complex Lipids Using Analytic Chemical and Mass Spectral Approaches

Dr. Frank Nichols University of Connecticut *A light breakfast will be offered during the lecture*



Plenary Lecture Wednesday, November 15, 11:45 AM Einstein Room; 1st Floor

Inclusive Stories in Chemistry: Celebrating Dr. Marie Maynard Daly Professor Sibrina Collins Lawrence Technical University

2023 EAS Student Awards

EAS continues to actively support a Student Awards program to recognize students involved in research in the broad field of analytical chemistry. We have expanded the Student Awards to include both graduate and undergraduate students. In the spring of each year, we encourage professors to identify undergraduate Juniors in college and graduate students who demonstrate special talent in research. Nomination criteria include excellent grades, appraisals of how the students handle their investigations, their approach and how they resolve problems and publicly disseminate their work.

In 2023, three undergraduates and five graduate students have been selected based on these criteria to receive EAS Student Awards. The following outstanding students have been chosen from a very worthy field of candidates:





Samuel Foster Rowan University Nominated by Prof. James Grinias



Nicole North Ohio State University Nominated by Prof. Heather Allen



Riti Sen University of Pittsburgh Nominated by Prof. Jill Millstone



Alexis Weber State University of New York - Albany Nominated by Prof. Igor Lednev

Danielle Whitham Clarkson University Nominated by Prof. Costel Darie

The Governing Board of the 2023 EAS congratulates these awardees for their outstanding achievements.

The Student Awardees' posters will be presented on Tuesday, November 14, 2023 in the Poster Area on the Bridge to the hotel from 11:30 PM – 12:25 PM

Workshops/Employment Bureau/Seminars

WORKSHOPS

Take advantage of this FREE workshops to improve your job seeking skills!

Monday, November 13, 12:00 PM - 1:00 PM

Career Change – Unlocking Your Potential

Reno DeBono, Ph.D., QC Manager – Analytical & Metals

EMD Electronics (Electronic Business of Merck KGaA, Darmstadt Germany)

Location: Room 110 B

This workshop will provide attendees with the opportunity to discover and communicate core skill sets during breakout sessions. The objective of the workshop is to help the experienced technical person to identify and win opportunities outside their current area of specialty.

- Understanding and communicating your core skills
- Understanding and identifying the core skills required in new careers
- · Identifying the gaps and problems of a position/company in the new area you can bring value to
- Identifying your success stories
- How to generalize highly specialized knowledge

Tuesday, November 14, 12:00 PM – 1:00 PM

A Guide to the Job Search for Young Professionals

Shelby Zangari, Ph.D.

Location: Room 110 B

The modern employment search is very different in 2023 than in previous years, and it can be difficult to navigate if you have never experienced the process before! In this session, we will discuss tips for how to search for job opportunities and how to tailor your resume to improve your chances of receiving a call back. We will also discuss how to prepare for the interview and make a positive impression on your future employer. You'll receive tips and tricks from someone who has recently gone through the job hunt. Bring your resume if you are interested in receiving some feedback as well!

EMPLOYMENT BUREAU

EAS continues to be invested in connecting employers with skilled scientific minds. All registered and onsite hiring manager's will have an opportunity to submit positions for posting on the employment bureau bulletin board. For consideration, submit your single page job posting including clearly identifiable on-site contact information to job_postings@eas.org. EAS will print and post the job postings on the employment bureau bulletin board for easy access to attendees. Using the provided posting contact information, EAS attendees will be able to contact the hiring managers directly to express their interest or to provide your application materials. There is no fee to post job openings.

Employer:

- Someone from your company must register and attend EAS. Job postings may be submitted on your Company stationery (please include job title, description, location, and contact information).
- Job postings will be accepted any time after your company has registered for EAS. These may be submitted in a hard copy form with the Employment Bureau on site.

Employee:

- Postings of current job openings will be available for your review in the Job Posting Area located in Room 201 on the 2nd Floor. Access to
 these postings is offered to all registered attendees of EAS.
- If you wish to contact an employer regarding a job posting, you may contact them directly using the information provided on the job posting.
- EAS will not be collecting resumes; you can submit it directly to the contact person per the instructions listed for that job opening.

ALVIN BOBER SEMINAR SERIES

EAS offers seminars essentially for high school students and teachers and college students. Seminars are included with the college student registration.

> Tuesday, November 14, 2023; 10:00 AM – 12:00 PM Spectroscopy and the World Around Us

Dr. Sharla Wood, Bristol Myers Squibb

Location: 3rd Floor

Join Dr. Sharla Wood, Bristol Myers Squibb, as we discover how light can be used to understand the world around us. Through a series of fun experiments, we will learn how spectroscopy, or the study of light and how it interacts with matter, can help us identify and learn more about materials just by how they absorb and emit light.

ALVIN BOBER SEMINAR SERIES (Continued)

Wednesday, November 15, 2023; 10:00 AM – 12:00 PM Careers in Science "Looking Back Through the Journey & Science of Color" Debbie Peru, DP Spectroscopy and Training Location: 3rd Floor

This seminar introduces the student to the various types of degrees and industrial positions available for scientists with two-year, four-year degrees or advanced degrees in chemistry, biology, engineering, etc. Part I of this seminar provides a look back through the journey of working in the energy, specialty chemical, pharmaceutical, and consumer product sectors. The seminar describes how analytical thinking and instrumental methods are used to solve problems and develop products that are used every day such as; gasoline, catalysts, plastic, soap, toothpaste, dietary supplements, roofing, etc. Part II of the seminar reviews the science of color and includes fun hands-on experiments to learn more about light including separation, reflectance, refraction, and how Beer's law describes the relationship between absorption and concentration. These hands-on experiments are intended to demonstrate how scientists use these basic principles every day during their career.

Looking for Career Advice? Join us for Speed Mentoring!

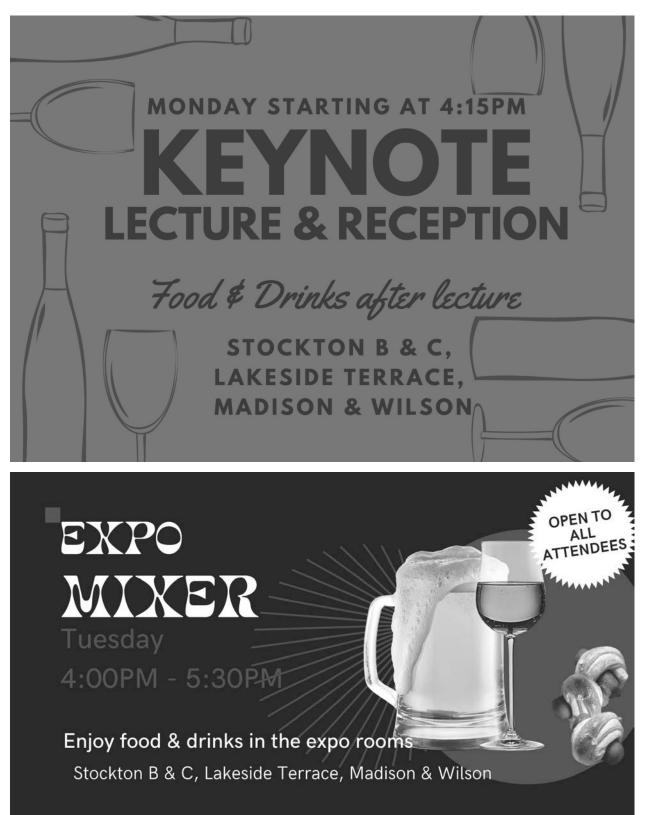
The Coblentz Society will offer an in-person Speed mentoring event on Monday, November 13 from 11:45 AM – 1:15 PM on the 3rd Floor. Speed Mentoring is a fun and fast paced session that enables a structured interaction with two dozen or more scientists from various industries, academia, and government labs that enable the mentees to get an understanding of what it's like to work in those areas. These interactions can be the basis of an ongoing mentoring relationship session if that is of interest and is a wonderful networking opportunity for job hunting or just getting a better understanding of life as a scientist. This is a great way to connect students with a variety of mentors and spark conversations in many possible career paths.



Lunch is provided; space is limited, and we encourage you to register in advance.



Exposition & Special Events



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