2024 Technical Program

Monday Morning, November 18, 2024

Sustainability: Driving the Next Major Developments in the Analytical Laboratory
Sponsored by Chromatography Forum of DE Valley
Chair: Mary Ellen McNally, FMC Corporation

9:00 1 Sustainability in Present-Day Forensic Science, Tom Brettell, Cedar Crest College

9:30 2 Driving Sustainability Goals Through GSK's Global Chromatography Technique Network, Daniel Fabry, GSK

10:00 Break

10:30 3 Continuous Manufacturing of Tirzepatide Using Online UHPLC-Based PAT: An Enabling Technology for Commercialization of a Synthetic Peptide, Bradley Campbell, Eli Lilly & Company

1 1:00 4 Incorporating Sustainable Practices in the Analytical Laboratory, Mary Ellen McNally, Austin Whittington, Mary Grace Guardian, Xiaoyan Wang, Anna Grifo, FMC Corporation

Pushing the Boundaries of Structure Elucidation
Chair: Sloan Ayers, Bristol Myers Squibb

9:00 5 Charge Detection Mass Spectrometry for Viruses, Vaccines, and Particles: Mass Spectrometry in the Megadalton Regime, Martin Jarrold, Indiana University

9:30 6 i-HMBC and Isotope-Shift-Based NMR Structure Elucidation Strategy, Mikhail Reibarkh, Merck & Co., Inc.

10:00 Break

10:30 7 Structural Characterization of Macrocyclic Peptido-Mimetic Compounds by NMR Spectroscopy, Christine Jorge, Luciano Mueller, Purnima Khandelwal, Alexander Brueckner, Janet Caceres-Cortesm Bristol Myers Squibb, Ajay Jain, Ann Cleves, Optibrium Limited

11:00 8 Small Molecule Crystallography to Solve Big Problems, Amy Sarjeant, Bristol Myers Squibb

From Pixels to Insights: Hyperspectral Techniques in Analytical Chemistry and Biological Imaging Analysis
Chair: Vanessa Castro, Rutgers University

9:00 9 Vibrational Spectroscopy & Hyperspectral Imaging Analyses for Biomedical Related Applications, Frank Weston, Tobias Gokus, Artem Danilov, Attocube Systems

9:30 10 Biomedical Applications of MALDI MS Imaging: Spatial Metabolomics and Beyond, Ye He, CUNY Graduate Center

10:00 Break

10:30 11 FTIR/Raman and TOF-SIMS Imaging, Samuel Gourion-Arsiquaud, TRI Princeton

11:00 12 High-Dimensional Mass Spectrometry Imaging Enables Prediction of Cancer Recurrence, Drew Jones, NYU Langone Health

Analytical Advancements in Bioanalysis
Chair: Neil Jespersen

9:00 13 Improving PS80 Content Analysis of Biopharmaceutical Therapeutics by Incorporation of Protein Precipitation, Daniel Steyer, Kennedy Guillot, Katie Carnes, Sina Mortazavi, Suraj Hettiarachchi, Michelle Ward, Lee Oliver, GSK

9:20 14 Multi-Dimensional Separation for Vaccine Component Analysis and Characterization, Arthur Arcinas, Rodell Barrientos, Mohamed Hamdi Said Hemida, Gunjan Dixit, Heather Wang, Andrew Singh, Emmanuel Appiah-Amponsah, Erik Regalado, Merck & Co., Inc.

9:40 15 Directly Detecting the Degradation of mRNA in mRNA Vaccine Model System Using Deep UV Resonance Raman Spectroscopy, Lamyaa Almehmadi, Massachusetts Institute of Technology, Sergei Reverdatto, Igor Lednev, Alexander Shekhtman, State University of New York-Albany, Vladimir Ermolenkov, The RNA Institute

10:00 Break

10:30 16 Two-Dimensional SEC-SEC-UV-MALS-dRI Workflow for Streamlined Analysis and Characterization of Biopharmaceuticals, Ophelia Ukaegbu, ARD, Rodell Barrientos, Andrew Singh, Mohamed Hemida, Heather Wang, Imad Haidar Ahmad, Hang Hu, Zachary Dunn, Emmanuel Appiah-Amponsah, Erik Regalado, AR&D

10:50 17 Enhancing Quantitative Analysis of Xenobiotics in Blood Plasma through Cross-Matrix Calibration and, Bayesian Hierarchical Modeling, Emanuela Gionfriddo, University at Buffalo, Nipunika H Godage, Song S. Qian, University of Toledo, Erasmus Cudjoe, Perkin Elmer Inc.

Analytical Chemistry: Studies in Environmental Science
Chair: Alexander Greer, Brooklyn College - CUNY

9:00 18 Effects of Radiolysis on the Stability and Chemical Fate of Pertechnetate under Solvent Extraction Conditions for Nuclear Waste Reprocessing and Long-Term Storage, Donna McGregor, Rachel Greenberg, Hossam Elshendidi, Benjamin Burton-Pye, Lehman College of the City University of New York, Lynn Francesconi, Hunter College of the City University of New York

9:30a 19 A Novel Method to Quantify and Prevent Fouling Using Superhydrophobic Surfaces, Louis Pimpinella, Graduate Center-CUNY

10:00 Break

10:30 20 NMR Detection of Primary and Secondary Products from the Photooxidation of a Phenolic Compound on Silica Particles and in Solution, Serah Essang, Brooklyn College

11:00 21 Biomimetic Photooxidation of a Geranylated Phenol to Reach Natural Product-Like Dihydrobenzofuran and Allylic Hydroperoxides: Synthesis, Homogeneous, and Singlet Oxygen Quenching Studies, Kamrun Nahar, Brooklyn College

Diverse Applications of Spectroscopy and NMR
Chair: Dana Garcia

9:00 22 Preliminary Characterization of Cultural Heritage Objects in the West Chester University Museum Collections, Zachary Voras, West Chester University

9:20 23 Imaging of Fluorescent and Autofluorescent Biomaterials and Photosynthetic Microorganisms via Fluorescence Detected Widefield Photothermal Infrared Spectroscopy, Eoghan Dillon, Jay Anderson, Craig Prater, Ting Yan, Photothermal Spectroscopy Corp., Kathleen Gough, University of Manitoba

9:40 24 A Collaborative Study on Platform 1H Quantitative NMR Method: Towards Capacity Building for Novices, Yang Liu, United States Pharmacopeia

10:00 Break

10:30 25 Automatic qNMR Data Analysis Approach: Prototype of qQMSA-Based Digital Product, Sunil Paudel, Yang Liu, Ben Shapiro, United States Pharmacopeia, Joo-Won Nam, Yeungnam University, Reino Laatikainen, University of Eastern Finland, Pekka Laatikainen, Spin Discoveries

10:50 26 Measuring Therapeutic Proteins (TPs) Particulates Using Submicron IR (O-PTIR), Microscopy from >100µm to <500nm, Jay Anderson, Mustafa Kansiz, Eoghan Dillon, Photothermal Spectroscopy Corp.

Problem Solving with Mass Spectrometry
Chair: James Stuart, University of Connecticut

9:00 27 Absolute Quantitation of Peptides and Proteins by Coulometric Mass Spectrometry, Hao Chen, New Jersey Institute of Technology

9:20 28 A Comprehensive Analysis of Serum from Women with Breast Cancer and Age-Matched Controls to Determine Candidate Protein Biomarkers, Logan Seymour, Danielle Whitham, Pathea Bruno, Costel Darie, Clarkson University, Brian Pentecost, University of Massachusetts-Amherst

9:40 29 Protein Biomarkers in Human Whole and Lactoferrin-Depleted Breast Milk: Mass Spectrometry-Based In-Solution Proteomics Analysis for Facilitating Early Detection and Treatment of Breast Cancer, Tochukwu (Victor) Njoku, Lilian Corrice, Costel Darie, Clarkson University, Brian Pentecost, Kathleen Arcaro, University of Massachusetts-Amherst

10:00 Break

10:30 30 GC/MS Approach for Analysis of Extractables and Leachables (E&L) in Complex Matrices Using Spectral Deconvolution and Retention Indices, Anastasia Andrianova, Bruce Quimby, Eric Fausett, Sofia Nieto, David Weil, Agilent Technologies

10:50 31 Rapid Screening of Enzymatic Reactions via Droplet-APCI-MS and FIA-MS, Bridget Murray, Robert Kennedy, University of Michigan, Moritz Pott, BASF SE, Jules Beekwilder, Isobionics BV

11:10 32 Strategic Analytical Method Development for Trace Levels of EDC and EDU in API Material by LC-MS, Sondrica Goines, Cong Bi, Jonathan Shackman, Robert Menger, Bristol Myers Squibb

Analytical Innovations Driving Pharmaceutical Excellence
Chair: Oscar Liu, Silver Springs Scientific LLC

9:00 33 New Insights into and Applications of Tandem-Column Liquid Chromatography, Joe Foley, Megan Marrazzo, Zhiyang Liu, Drexel University

9:20 34 Development and Application of a Selectively Tunable, Universal 1H and 19F Quantitative NMR Standard, Ryan Cohen, Jared Wood, Xiao Wang, Mikhail Reibarkh, Merck & Co., Inc., Thomas Williamson, University of North Carolina

9:40 35 Fast and Simple Quantitation of GC-Unfriendly Impurities Using Headspace-MRR, Alexander Mikhonin, Voislav Blagojevic, Reilly Sonstrom, Steven Shipman, Justin Neill, BrightSpec, Inc.

10:00 Break

10:30 36 Pharmaceutical Formulation Stability Studies with BeScan, Beverly Barnum, Annika Jurgilewicz, Bettersize, Inc.

10:50 37 What Is a Scientifically Sound Method? Examples of Form FDA 483s and Warning Letters Under CFR211.160(b), Xiaohui (Sherry) Shen, United States Food and Drug Administration

Monday, November 18: E-Poster Morning Session; 11:30am – 12:25pm

38 Deducing Melanin Biosynthesis and Supramolecular Organization, Dhairavi Shah, Dhaara Shah, Subhasish Chatterjee, Kean University

39 Determination of Glucose in Blood by Applying Imbedded Enzyme Technology, Ben Sutter, Kevin Schlueter, Xylem

40 Probing Binding Affinities, RNA Compaction, and Complex Stoichiometry for SARS CoV-2 Nucleocapsid Protein and RNA Using Single-Molecule FRET, Alec Garasimowicz, Madison Stringer, Jasmine Cubuk, Kathleen Hall, Melissa Stuchell-Brereton, Andrea Soranno, Washington University School of Medicine

41 Automation of a Capsid ELISA Method for Support of Manufacturing Process Development of AAV Therapeutics, Monica Bond, Jeanna Hill, Daniel Konovalov, Zhichao Fang, Thomas Slaney, Gloria Li, Anthony Leone, Bristol Myers Squibb

42 Lipid Profiling of Human Hair Fibers Using MALDI-TOF Imaging: Insights from Root to Tip in Scalp Sections, Ernesta Malinauskyte, Vanessa Castro, TRI Princeton

43 Interaction Between Fluorescent Gold Nanoclusters with Proteins and Cells, Maima Bogar, Jingqiu Hu, West Chester University, Jah'dir Cartegena-Rivers, Lankenau Hs

44 Ion Chromatography-Based Quantification of Tris(2-Carboxyethyl) phosphine in Antibody-Drug Conjugates, Suji Lee, Michael Zompa, Frank Bernardoni, Tao Liang, David Schenk, Casey Dougherty-Gunsch, Teng Peng, Neil Williams, Xinxin Han, Mirlinda Biba, Patrick Fier, Paul Bulger, Merck & Co., Inc.

45 Suppress or Not to Suppress?!... – CRAFT it! Extracting Essential Biomarker Signals Directly from the Full 1H NMR Spectrum of Serum Samples, István Pelczer, James Chen, Ayelet Yablon, Christina Metaxas, Mateus Guedin, Joseph Hu, Kenith Conover, Princeton University, Krish Krishnamurthy, Chempacker LLC

46 Optimizing Oligonucleotide Extraction by SPE, Geoff Faden, MAC-MOD Analytical, Colin Pipe, David Dunthorne, Tony Edge, Matt James, Avantor

47 A Proteomics Analysis of Serum from African American Donors with Invasive Ductal Carcinoma Breast Cancer Compared to Matched Controls, Celeste A. Darie, Logan Seymour, Panashe Mutsengi, Danielle Whitham, Brian T. Pentecost, Costel Darie, Clarkson University

48 Proteomic Study and Comparison of Sera from Controls and Stage IIA T1N1 ER/PR Cases for the Discovery of Possible Breast Cancer Biomarkers, Angiolina Hukovic, Niyogushima Nuru, Norman Haaker, Isabella Pelkey, Pathea Bruno, Brian T. Pentecost, Costel Darie, Clarkson University

49 Monitoring the Estrogen-Inducible Proteins in Lake Trout (Salvelinus namaycush) from Great Lakes upon Exposure to Environmental Contaminants, Taniya Jayaweera, Krishan Weraduwage, Sujan Fernando, Thomas Holsen, Costel Darie, Clarkson University, Bernard Crimmins, AEACS

50 Rapid Machine Learning Identification of Rhodamine-B in Ballpoint Pen Ink, Alisha Khodabocus, Eden Fitsum, Walker Knapp, Sinead McWeeney, Benjamin Steinman, Kristin Wustholz, College of William & Mary

51 Japanese Woodblock Prints Analysis, An Art History and Chemistry Collaboration, Kayla Geulen, Kennedy Short, Rutgers University

52 Detecting the Presence of PFAS "Forever Chemicals" in Commonly Used Infant Care Products, Anthony Provatas, Kevon Rattigan, Angelica Velasquez, Abigail Manka, Christopher Perkins, University of Connecticut

53 Testing and Validation of Elemental Impurities in Pharmaceutical Products According to ICH Q3D and USP <232>/<233> Using ICP-MS, Brady Frill, PerkinElmer

54 Navigating Challenges in Extractables & Leachables Characterization of Polyethylene Glycol-Based Medical Devices, Yunyun Yuan, Ying Jiang, Yijun Lu, Johnson & Johnson MedTech

55 Novel Optimal Tryptic Digestion Methods Using Bovine Serum Albumin in-gel Sample Preparation for Mass Spectrometry-Based Proteomics, Niyogushima Nuru, Pathea Bruno, Danielle Whitham, Norman Haaker, Hailey Morrissiey, Costel C. Darie, Brindusa Alina Petre, Clarkson University

56 Proteomic Analysis of Varying Protein Contents in Different Plant Milk Types Using Gel-Based Mass Spectrometry Analysis, Alivia Sochia, Celeste A. Darie, Angiolina Hukovic, Niyogushima Nuru, Taniya Jayaweera, Pathea Bruno, Costel C. Darie, Clarkson University

57 Utilizing Monodisperse Fully Porous Particles (MFPP) for improvements in LC-MS based Metabolomics for Disease Detection, Edward Faden, MAC-MOD Analytical, Tim Garrett, University of Florida, Mark Woodruff, Fortis Technologies

Monday, November 18: E-Poster Afternoon Session; 12:30pm – 1:25pm

58 Removal and Recovery of Lead and Cadmium Ions with Biowaste Adsorbent from Aqueous Solutions, Liang Feng, Enju Wang, St. John's University

59 Detection of "Forever Chemicals" per and poly-fluoroalkyl Substances (PFAS) in Water Using Surface Enhanced Raman Spectroscopy (SERS), Syed Islam, Eastern Connecticut State University

60 Liquid Chromatography-Tandem Mass Spectrometry for Determination of 40 PFAS Compounds, Elizabeth Smiley, Dongmei Alvi, Joan Wirt, Occoquan Lab

61 New Capillary C18, Carbon, and HILIC HPLC Columns for Bio-Analysis, Breanne Smith, William Maule, Michael Ye, Olga Shimelis, Cory Muraco, MilliporeSigma

62 Method Development Made Easy for GC×GC Users, Kira Fisher, Katelynn Perrault Uptmor, William & Mary

63 Comparison Between Plasma and Serum Matrices for Perfluoroalkyl and Polyfluoroalkyl Substance Detection, Diana Mathes, New Jersey Department of Health

64 Identification of the Estrogen-Inducible Proteins in Fishes from the Great Lakes Upon Exposure to Environmental Contaminants, Krishan Weraduwage, Taniya Jayaweera, Sujan Fernando, Thomas Holsen, Costel Darie, Clarkson University, Bernard Crimmins, AEACS

65 Green Chromatographic Method for assay, Impurities, and Preservatives from Ketoconazole Cream Formulation: Identification of Degradants by Q-ToF LCMS and Robustness by Design of Experiments, Siva Krishna Muchakayala, Naresh Kumar Katari, GITAM University, Vishnu Murthy Marisetti, ScieGen Pharmaceuticals Inc.

66 Scalability of Solid-Core Particles for Chromatographic Analyses, Maureen DeLoffi, Gabrielle Zabala, Gary Izzo, Weiqiang Gu, Thomas Walter, Cheryl Boissel, Daniel Walsh, Waters Corporation

67 Mitigation of the Non-Specific Binding during HILIC Analysis of Metal Sensitive Compounds, Tony Reinhold, Paula Hong, Martin Gilar, Andrew Steere, Waters Corporation

68 Evaluation of Hybrid Silica C18 End-capped with Bidentate Silylating Reagent for HPLC, Norikazu Nagae, ChromaNik Technologies Inc., Scott Sliver, Pyvot

69 Application of RP-HPLC with Fluorescence Detector for Analysis of Bisphenol Analogues in Infant and Toddler Products, Viral Shah, Louis Fleck, Axel Martinez, Intertek, Tyler Horvath, Academic

70 Preparation of Capillary LC Columns in Tube-in-Manifold Microfluidic Devices, Christopher Piccolo, James Grinias, Rowan University, M. Keller, T. Austin, G. Shelver, D. J. Czarnecki, IDEX Health & Science

71 Porous Graphitic Carbon Chromatography Columns: Retention Mechanisms and Applications, Egidijus Machtejevas, Merck Life Science, Clinton Corman, Sigma-Aldrich Corp.

72 Structure Elucidation of Trace Impurities in Commercial Compounds by Nuclear Magnetic Resonance, Yao An, Sloan Ayers, Ziyu Wang, Bristol Myers Squibb

73 Arrayed Spin Lock Durations in One Dimensional Total Correlation NMR Spectra for Structural Characterization, Alexander Marchione, Sara Maute, Michael Davis, Chemours

74 Sustainable Synthesis and Surface Functionalization of Cellulose Derived Carbon Quantum Dots (CQDs) for Applications in Drug Delivery, Sarah Watson, Simret Asefa, Abbie Ganas, West Chester University

75 Dynamic Partitioning of Surfactants into Non-Equilibrium Emulsion Droplets Analyzed by Quantitative Mass Spectrometry, Wangyang Xue, Parvin Bayati, Stewart Mallory, Lauren Zarzar, The Pennsylvania State University, Rebecca Balaj, Dow Chemical

Monday Afternoon, November 18, 2024

The Emerging Role of Oligonucleotides in Pharmaceutical Sciences

Sponsored by the Chinese American Chromatography Association

Chair: Yi He, John Jay College of Criminal Justice

1:30pm 76 The Challenges and Solutions to Develop the Ultra-Sensitive Hybridization LCMS Assay for Oligonucleotides, David Zuluaga, Resolian

2:00pm 77 Oligonucleotide and Metabolites Bioanalysis Using LC-MS/MS Technique: Case Studies, Xiangji Liu, Frontage Laboratories

2:30pm Break

3:00pm 78 Probing the Structure of sgRNA Through Advanced Analytical Tools, Wei Bingchuan, Genetech

3:30pm 79 Recent Advances in LC-MS of Oligonucleotides, Vidya Annavarapu, University of Georgia

The Evolving Role of Analytical Chemistry in PFAS Environmental Issues

Chair: Charles R. Powley, Center for PFAS Solutions

1:30 80 The Evolving Role of Analytical Chemistry in PFAS Environmental Issues, Charles R. Powley, Center for PFAS Solutions

2:00 81 Current LC Approaches for Analysis of PFAS Referencing Short and Long Chain Mixtures, Barry Boyes, Conner McHale, Advanced Materials Technology, Inc.

2:30 Break

3:00 82 Hunting the Missing Fluorine in Aqueous Film-forming Foams Containing Per- and Polyfluoroalkyl Substances, Min Liu, Gabriel Munoz, Sung Vo Duy, Sébastien Sauvé, University of Montreal, Caitlin M. Glover, Jinxia Liu, McGill University

3:30 83 A Non-Targeted Approach for PFAS Analysis Using Combustion Ion Chromatography, Jay Sheffer, Metrohm USA

High Throughput Mass Spectrometry Applications in Drug Discovery and Development

Chair: Debopreeti Mukherjee, Merck & Co., Inc.

1:30 84 Acoustic Ejection Mass Spectrometry for Ultrahigh-Throughput Analysis of Pharmaceutical Targets, Hang Hu, Ophelia Ukaegbu, Umme Ayesa, Joseph Gouker, Jarrod Laro, Jane Wen, David McLaren, Michael Wleklinski, Erik Regalado, Emmanuel Appiah-Amponsah Merck & Co., Inc., Chang Liu, SCIEX

2:00 85 Acoustic Ejection Mass Spectrometry in High-Throughput Screening, Xiujuan Wen, David McLaren, Merck & Co., Inc., Chang Liu, SCIEX

2:30 Break

3:00 86 New-Generation Automated Ambient Mass Spectrometry Platform for High-Throughput Experimentation in Early Drug Discovery, Nicholas Morato, Veronica Feng, Kai-Hung Huang, Kitmin Chen, Beinan Yang, Christina Ferreira, Andrew Mesecar, R. Graham Cooks, Purdue University, Carleen Klumpp-Thomas, National Center for Advancing Translational Sciences, Adam Gloeckner, Matt Galbraith, Hamilton Robotics, Csaba Hajdu, Michael Morris, Steven Pringle, Julia Balog, Waters Corporation

3:30 87 Advancing Cancer Research: Broad-Spectrum Cancer Target Identification Using High-Sensitivity Immunopeptidomics, Darshit Shah, Regeneron Pharmaceutical Inc.

New Detection Approaches in Separation Science
Sponsored by ACS Division of Analytical Chemistry
Chair: James Grinias, Rowan University

1:30 88 Quantitative Determination of Biomass Pyrolysis Products Using Micropyrolysis and GC-Polyarc-FID, Charles Mullen, United States Department of Agriculture
2:00 89 Machine Learning vs. Theoretical Computational Prediction of Gas Phase Vacuum Ultraviolet/Ultraviolet (GC-VUV) Absorption Spectra, Kevin Schug, Linh Ho Manh, Jay Rosenberger, Victoria Chen, University of Texas-Arlington
2:30 Break
3:00 90 Simple Interfacing of Capillary Electrophoresis to Mass Spectrometry through Vibrating Sharp Edge Spray Ionization, Lisa Holland, West Virginia University
3:30 91 Light Scattering Applications to Biologics and AAV Characterization, Gurusamy Balakrishnan, Bristol Myers Squibb

Forensic Microscopy: Fusing Theory & Practice
Chair: Michelle D. Miranda, Farmingdale State College, SUNY

1:30 92 Microscopy and Microanalysis of Aluminum Powders Used in Improvised Explosive Devices (IEDs), JoAnn Buscaglia, JenaMarie Baldaino, Kayla Moquin, United States Federal Bureau of Investigation, Jack Hietpas, John Jay College of Criminal Justice
2:00 93 Seldom Believe What Your Client Tells You: Make Sure to Inquire Carefully and Look More Closely, Preferably Before You Start, Thomas Kubic, John Jay College of Criminal Justice
2:30 Break
3:00 94 A Microscopical Approach to Problem Solving in Law and Industry, Chris Palenik, Microtrace
3:30 Panel Discussion

Nitrosamines: Formation, Control, and Acceptable Intakes
Chair: Leonardo Allain, Merck & Co., Inc.

1:30 95 Something in the Air: The Contribution of Nitrogen Oxides to the Formation of Nitrosamines from Vulnerable Active Pharmaceutical Ingredients, Joerg Schlingemann, EMD Serono
2:00 96 Nitrites and NOx Everywhere: Impact in Nitrosamine Formation in Drug Products, Leonardo Allain, Merck & Co., Inc.
2:30 Break
3:00 97 Strategies for Overcoming Challenges in LC-MS Analysis of Nitrosamines in Pharmaceutical Products, Jinjian Zheng, Merck & Co., Inc.
3:30 98 Approaches to Establishing Acceptable Intakes for NDSRIs, Mark Powley, Merck & Co., Inc.

Spectroscopy at Interfaces
Chair: Kenneth L. Knappenberger, Pennsylvania State University

1:30 99 How Does Interfacial Water Structure Change with Increasing Surface Charge Density?, Paul Cremer, Pennsylvania State University
2:00 100 Near Infrared Vibrational Second Harmonic Generation (NIR-vSHG): A New Nonlinear Vibrational Spectroscopy of Interfaces, Eric Borguet, Temple University
2:30 Break
3:00 101 Single Molecule FRET Imaging and Deep Learning Reveal Concentration Dependence of Aggregation Pathways during Aβ42 Aggregation, Sara Sohail, Swarthmore University, Janghyun Yoo, Hoi Sung Chung, NIDDK/NIH
3:30 102 Characterizing Materials Interfaces Using Second Harmonic Generation, Kenneth Knappenberger, Pennsylvania State University

Next Generation Innovations in Biotechnology
Chair: Shirley Fischer-Drowos, Widener University

1:30 103 Bacterial Model Membrane Systems Featuring Phosphatidylethanolamine and Phosphatidylglycerol as Predominant Lipids, Aarshi Singh, Tiffany Ye, Nicholas Lima, Nathan Wittenberg, Lehigh University
1:50 104 Investigation of the Effects of Overexpression of Human Jumping Translocation Breakpoint (JTB) Protein Using In-Solution Digestion-Based Proteomics, Taniya Jayaweera, Madhuri Jayathirtha, Danielle Whitham, Costel Darie, Clarkson University
2:10 105 Extractables and Leachables Study on Self-Amplifying RNA-LNPs Manufacturing, Bin Sun, Cytiva
2:30 Break
3:00 106 Mass Spectrometry-Based Degradomics Analysis of Breast Milk for Early Detection of Breast Cancer, Kaya Johnson, Pathea Bruno, Brian Pentecost, Costel Darie, Clarkson University, Kathleen Arcaro, University of Massachusetts-Amherst
3:20 107 Method Development Approach to Separating Oligonucleotides Under UV and MS Detection, Peter Pellegrinelli, Ben Libert, Chuping Luo, Stephanie Schuster, AMT
3:40 108 Chemical Impurity Analytical Method Development in Biopharmaceutical R&D, Kedene Clarke, GSK

KEYNOTE LECTURE
Monday, November 18, 4:15pm

(#109) Role of Quality and Analytical in Supporting Industry Growth in Low- and Middle-Income Countries
Dr. Ronald Piervincenzi, CEO, United States Pharmacopeia

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

Tuesday Morning, November 19, 2024

Impact of ICH Q14 on Analytical Procedure Validation
Chairs: Isabelle Vu Trieu, Waters Corporation and Kim Huynh-Ba, Pharmalytik

9:00 110 Mapping Key Elements in the Current ICH and USP Guidances for an Enhanced Workflow for Analytical Procedure Development, Richard Verseput, S-Matrix Corporation
9:30 111 Enhanced Method Development using Empower Chromatography Data System and Quality by Design Software, Margaret Maziarz, Andrea Gheduzzi, Stephanie Harden, Isabelle VuTrieu, Waters Corporation
10:00 Break
10:30 112 Challenges of Developing and Validating Analytical Procedures with the New ICH Q14 Guideline, Trevor Williams, Pharmaceutics International Inc.
11:00 113 Opportunities and Barriers in ICH Q14 Implementation: An ISPE-PQLI Survey, Qinggang Wang, Bristol Myers Squibb

New York/New Jersey Sections of the Society for Applied Spectroscopy Gold Medal Award
Honoring Mark Witkowski, United States Food & Drug Administration
Chairs: Dana Garcia, Deborah Peru, DP Spectroscopy and Training

9:00 114 Using Alternate Light Sources to See the Unseen; Award Presentation, Mark Witkowski, Nicola Ranieri, Douglas Albright, John Lynch, Megan Sterling, United States Food & Drug Administration
9:30 115 Advancing Food and Dietary Supplement Safety with 15 Years of Spectroscopic Methods at FDA/CFSAN, Betsy Yakes, United States Food & Drug Administration
10:00 Break
10:30 116 Pharma in Focus: Spectroscopic Imaging for Physicochemical Insights, Daniel Willett, Huzeyfe Yilmaz, Yeakub Zaker, Snober Ahmed, Changning Guo, Jason Rodriguez, United States Food & Drug Administration
11:00 117 Analysis of Unknown (Unlabeled/Mislabeled) Drug Products for Active Pharmaceutical Ingredients at Remote Sampling Sites by FDA's Satellite Laboratory Program, Adam Lanzarotta, United States Food & Drug Administration

Method Development and Applications of Mass Spectrometry: Bioanalysis
Sponsored by North Jersey Section ACS
Chairs: Anthony Pitts-McCoy, Merck & Co., Inc. and Michelle Gonsalves, PTC Therapeutics

9:00 118 Validation and Application of Volumetric Absorptive Microsampling (VAMS) Dried Blood Method for Phenylalanine Measurement in Patients with Phenylketonuria, Diksha Kaushik, Lan Gao, Neil Smith, Ronald Kong, PTC Therapeutics
9:30 119 Validation of Quantitation of MK-6598 Target Protein and Phenylpyruvate in Tumor Biopsies by LCMSMS to Inform Target Engagement in Phase I Oncology Clinical Trial, Carolina Cabral, Erik Henry Knelson, Stuart Shumway, Omobolaji O. Akala, Michael Lassman, Merck Sharp & Dohme LLC
10:00 Break
10:30 120 Bioanalytical Assessments of a Novel Approach to Overcome Microsampling Challenges in Rodent Studies, HsinPin Ho, Bristol Myers Squibb
11:00 121 Overcoming Bioanalytical Assay Challenges to Support New Generation of Antibody-Drug Conjugates, Ines Santos, Jian Chen, Nicholas Colletti, Yongjun Xue, Jim Shen, Bristol Myers Squibb

Separations for Therapeutic Oligonucleotides and New Modalities
Sponsored by Chromatography Forum of DE Valley
Chair: Kaitlin Grinias, GSK

9:00 122 Characterization of RNA Modifications in the Central Nervous System by LC-MS/MS-Based Epitranscriptomics, Kevin Clark, Tufts University
9:30 123 Analytical Control Strategy for Therapeutic Oligonucleotides, Sujana Pradhan, GSK
10:00 Break
10:30 124 Impact of Nucleic Acids Melting Temperature on their Liquid Chromatographic Behavior, Martin Gilar, Samuel Redstone, Alexandre Gomes, Catalin Doneanu, Waters Corporation
11:00 125 Capillary Gel Electrophoresis Separations of DNA: From Fragments to Plasmids, Lisa Holland, West Virginia University

Leveraging Portable Instruments to Solve Problems at the Sample Site
Chair: Pauline Leary, NOBLE

9:00 126 Experiential Forensic Science Research with Portable Spectrometers, Brooke Kammrath, University of New Haven
9:30 127 Portable Raman Spectrometers, Fluorescence, and Lego Blocks, Richard Crocombe, Crocombe Spectroscopic Consulting, LLC, Brooke Kammrath, University of New Haven, Pauline Leary, NOBLE
10:00 Break
10:30 128 FDA's Satellite Laboratory Operations – Using a Field Deployable Tool Kit for Rapid Analysis at International Mail Facilities, Brandon Reyes, United States Food & Drug Administration
11:00 129 Applications of Handheld Spectroscopy in Hazardous Materials Response, Brandon Gayle, City of Raleigh Fire Department

Data-Driven Discovery and Design for Modern Laboratories with Machine Learning and Artificial Intelligence: From Materials Discovery to Process Optimization
Chairs: Caelin Celani, University of Delaware and Michael George, University of Nottingham

9:00 130 Self-Optimized Development of Pharmaceutical Processes, Clarissa Wilding, Richard Bourne, University of Leeds
9:30 131 Iterative Optimization Technology: A Calibration-Free Modelling Approach for Monitoring Active Ingredient in Pharmaceutical Blends, Md. Nahid Hasan, Duquesne University
10:00 Break
10:30 132 Deconvolution of Non-linear Surfaces Using Gaussian Mixture Models: Applications to Hyperspectral Images, Helder Carneiro, Lottie Murray, Roxanne Radpour, Joseph Smith, Caelin Celani, Matthew Doty, Karl Booksh, University of Delaware.
11:00 133 Scalable Continuous Photochemical, Electrochemical and Thermal Reactions: Reactors and PAT Challenges: Exploring Unlocking Molecular Landscapes with Excitation Emission Matrix (EEM) Fluorescence Spectroscopy, David Tiemessen, University of Nottingham

Developments in Separation Sciences
Sponsored by Amgen
Chair: Mary Ellen McNally, FMC Corporation

9:00 134 Elastic Flow Instability Using Polymer Additives to Improve the Efficiency of Packed High-Pressure Liquid Chromatography Columns, Fabrice Gritti, Waters Corporation, Emily Chen, Sujit Datta, Princeton University
9:20 135 Separation of Permanent Anions, Neutral Compounds, and Weak Acids Using Sequential Elution Liquid Chromatography with Tandem Columns, Lauren Lovejoy, GSK, Joe Foley, Drexel University
9:40 136 Benefits of Inert Liquid Chromatography Column Hardware for Various Applications, Samantha Herbick, Diego Lopez, Shun-Hsin Liang, Melinda Urich, Jamie York, Justin Steimling, Restek Corporation
10:00 Break
10:30 137 UPLC Columns: Past, Present and Future, Thomas Walter, Waters Corp.
10:50 138 Fast RP-UHPLC Separation of Ribooligonucleotide Impurities Using Evosphere MAX C18/AR Monodisperse Fully Porous Particle Columns without Ion-Pair Reagents for Simplified Oligo Separations, Edward Faden, Geoff Faden, MAC-MOD Analytical
11:10 139 Accelerating High Throughput Thermodynamic Solubility Screening in Drug Discovery Using LC-MS, Muhammad Qamar Farooq, Adrian Carranza, Wes Barnhart, Nuria Tamayo, Imad Haidar Ahmad, Amgen

Pharmaceutical Chromatography
Sponsored by Amgen
Chair: Mariann Neverovitch, Bristol Myers Squibb

9:00 140 Analytical Method Development for Chromophore-Lacking Formulation Excipients in Gamma-Irradiated LAIs, Suraj Hettiarachchi, GSK

9:20 141 Advancements Towards a Universal, Sensitive, and Selective Detection Technology for Liquid Chromatography, Alex Hodgson, Dale Harrison, VUV Analytics

9:40 142 Modernization of a Legacy Normal Phase Method on a Modern HPLC System, Elom Pedanou, Lise Gauthier, Paula Hong, Waters Corporation

10:00 Break

10:30 143 Improving Chromatography for Basic Analytes Using a Positive Charge Surface Material, Conner McHale, Advanced Materials Technology

10:50 144 Enhancing Quantitation Accuracy and Minimizing Analyte-to-Analyte Variability for High-Throughput Liquid Chromatography - Charged Aerosol Detection (CAD) Methods, Daipayan Roy, Imad Haidar Ahmad, Wes Barnhart, Troy Handlovic, Amgen

11:10 145 Enhancing LC and LC-MS Separations of Basic Compounds with Novel High pH Stable SPP Columns, Stephanie Schuster, Conner McHale, Peter Pellegrinelli, Mark Haynes, Advanced Materials Technology

High-Performance Thin-Layer Chromatography
Chair: Michael Hicks, Merck & Co., Inc.

9:00 146 Authentication of Powdered Mushroom Fruiting Body by High-Performance Thin-Layer Chromatography, Wilmer Perera, CAMAG Scientific, Inc.

9:20 147 Foraging for Methods: The Right Method for the Right Spec, Khanh Tran, Sidney Sudberg, Anthony Fontana, Alkemist Labs

9:40 148 Decoding Hair: Adapting Scalp Hair to Resemble Body Hair for In-Vitro Skin Models, Ernesta Malinauskyte, TRI Princeton

10:00 Break

10:30 149 USP Standards for Passion Flower (Passiflora incarnata L.): Species and Chemotype Differentiation by HPTLC Analysis, Maria Monagas, United States Pharmacopeia, Mirtha Navarro, Felipe Vargas, University of Costa Rica, Eike Reich, Wilmer Perera, CAMAG

10:50 150 HPTLC Identification Tests for Botanical Dietary Supplements and Herbal Medicines in USP Monographs, Cuiying Ma, United States Pharmacopeia

Tuesday, November 19: E-Poster Student Awardees Session; 11:30am – 12:25pm

151 Identifying and Quantifying Pesticides in Environmental Deposition Using Gas Chromatography High-Resolution Mass Spectrometry, George Belay, Eve Painter, Jennifer Faust, The College of Wooster, Rebekah Gray, Goucher College, Christopher Alaimo, Thomas Young, University of California-Davis

152 Binding of Naphthenic Acids to Dissolved Organic Matter, Ronny Goldshmid, Clarissa Jules, Anne Vazquez, St. John's University

153 Using Raman MCR to Investigate Interfacial Water Signal at the Surface of Vesicles, Phuong Ho, Alexander Lott, Olivia Fiebig, Paul Cremer, The Pennsylvania State University

154 Advancing Environmental Monitoring: Rapid Quantitation of 28 PFAS in Aquatic Insect Tissue Using QuEChERS Extraction Coupled with UPLC-MS/MS, Austin Pelletier, Kaitlyn Campbell, Jess Brandt, Christopher Perkins, Anthony Provatas, University of Connecticut

155 Direct Enantiomer Differentiation of Drug and Drug-like Small Molecules using Noncovalent Copper-Amino Acid Complexation and Ion Mobility-Mass Spectrometry, Benjamin Blakley, Jody May, Emanuel Zlibut, Rashi Gupta, John McLean, Vanderbilt University

156 Ion Selective Electrodes: Quantifying the Upper Limit of Detection, Madeline Honig, Phil Bühlmann, University of Minnesota

157 Glycosaminoglycan Imaging by IR-MALDESI, Tana Palomino, David Muddiman, North Carolina State University

158 Decoding CD107a and CD107b Glycosylation, Valentina Rangel-Angarita, Lea Kim, Keira Mahoney, Stacy Malaker, Yale University

Tuesday, November 19: E-Poster Morning Session; 11:30am – 12:25pm

159 The Applications of Spotfire for a Pharmaceutical Forensics Database, Brittany Handzo, Gabrielle Messe, Bristol Myers Squibb

160 Trends in Novel Psychoactive Benzodiazepine Content of Counterfeit Alprazolam Tablets, Michael Kanwischer, NMS Labs

161 Gas Chromatography-Flame Ionization Detector (GC-FID) System Linearity Effects on Limit of Detection Calculations, James Mizvesky, Nicholas Snow, Seton Hall University

162 Reliable Extraction of Fluorophore Blinking Dynamics from Wide-Field Microscopy Videos, Walker Knapp, Eden Fitsum, Alisha Khodabocus, Sinead McWeeney, Kristin Wustholz, William & Mary

163 Illicit Drug Desorption and Chemical Profiling of Fingerprints using SICRIT Ion Source: A Rapid Analysis Approach, Taylor Hayward, Ciara Conway, Jan-Christoph Wolf, Plasmion GmbH

164 Enhancing Overdose Surveillance: Targeted Method Development for Analyzing Psychoactive Substances in Urine, Anthony Lockhart, Daniel Wene, Nkemdili Nebeolisa, Linbin Zhong, Shawn O'Leary, Tina Fan, New Jersey Department of Health

165 Application of Raman Imaging in Surface Mapping of Nano Carbon Based Composite Membranes, Lingfen Rao, Oindrila Gupta, Sagar Roy, Somenath Mitra, New Jersey Institute of Technology

166 Determination of Toxic and Other Trace Elements in Baby Foods Using ICP-MS, Andrea Palpini, Liyan Xing, PerkinElmer

167 Determination of PFAS in Food Using the Automated FREESTYLE PFAS System, Fred Foster, GERSTEL, Inc.

168 Dumas Method Application for Non-Protein Nitrogen (NPN) Analysis in Milk Products, Michelle Kuzio, Jason Mote, Xylem

169 Headspace Analysis of Whole Milk and Soymilk Using a SERS-Active Fiber, Bezalel Adainoo, Lili He, University of Massachusetts

170 Aroma Profiling of Commercial Poi Products in Fresh and Aged States Using Comprehensive Two-Dimensional Gas Chromatography, Sarah Foster, Katelynn A. Perrault Uptmor, William & Mary, Cynthia Cheung, Chaminade University of Honolulu, Laura Tipton, Jonathan D. Baker, Kahoalii K. Keahi-Wood

171 Synthesis and Characterization of Novel Europium-doped Ceria Nanocrystals (EuCeNCs) for Monitoring Antioxidants, Gloria Popoola, Aqsa khan, Silvana Andreescu, Clarkson University

Tuesday, November 19: E-Poster Afternoon Session; 12:30pm – 1:25pm

172 Dissolution Method Development: Lessons Learned on Tablets with Low Solubility, Sensitive to Discrimination and Metal Chelation, Xiaoyun He, Sandya Raghavendra, Weijia Hou, Gilead Sciences, Inc.

173 Investigation of the Effects of Overexpression of Human Jumping Translocation Breakpoint (JTB) Protein Using In-Gel Digestion-Based Proteomics, Peter Biggers, Taniya Jayaweera, Madhuri Jayathirtha, Danielle Whitham, Costel Darie, Clarkson University

174 East Asian Concertina Book, Arabella Sawaked, Elizabeth Sawaked, Zachary Voras, West Chester University

175 Risk Assessment for Nitrosamine Impurities, Richa Mittal, Sushmeet Singh, CMIC CMO USA

176 Advanced Applications of LUMA GC in Pharmaceutical Analysis, Rafael Acosta, VUV Analytics

177 Withdrawn by the author.

178 Mitigation of Low Endotoxin Recovery (LER) Using CSE170 in Recombinant Human Acid Alpha-Glucosidase for the Treatment of Pompe Disease, Shengjie Bian, Eudean Garces, Steven Tuske, Partha Mukherjee, Saroj Ramdas, Amicus Therapeutics Inc., Qi Chen, Fengkun Du, Youwen Pan, Guoyin Shi, WuXi Biologics Co., Ltd.

179 A New LC-MS/MS Method for Identification and Quantitation of an N-Nitroso impurity (NDSRI) in a Commercial Small Molecule Drug Product Capsules, Partha S. Mukherjee, Krishnaiah Charagondla, Kalyani Ginjupalli, Saroj Ramdas, Amicus Therapeutics Inc., Bing Hu, Simrat Kaur, Paresh Thanki, Tejas Tailor, Bhavin Prajapati, SGS Inc.

180 A New Analytical LC-MS/MS Method for Determination of Eight Standard Nitrosamines (NDMA, NMBA, NDEA, NEIPA, NDIPA, NMPA, NDPA, NDBA) in a Commercial Small Molecule Drug Product Capsules and its API, Krishnaiah Charagondla, Partha S Mukherjee, Kalyani Ginjupalli, Saroj Ramdas, Amicus Therapeutics Inc., Bing Hu, Simrat Kaur, Paresh Thanki, Tejas Tailor, Bhavin Prajapati, SGS Inc.

181 Scaling of Challenging UHPLC Compendial Methods on HPLC Systems, Norris Wong, Elom Pedanou, Paula Hong, Waters Corporation

182 Combining Droplet Microreactor and Mass Spectrometry for Efficient Detection of Antihistamine Drugs in Oral Fluid, Mohamed O. Amin, Bessy D'Cruz, Entesar Al-Hetlani, Kuwait University

183 Chemometrics Assisted GC-FID Analysis of Fatty Acids in Blood Plasma Under Varying Dietary Conditions Towards Clinical Applications Mohamed O. Amin, Nouf Aldhafiri, Entesar Al-Hetlani, Kuwait University

184 Applications of Synthetic Carbon for Pharmaceutical Industry, Hillel Brandes, Olga Shimelis, M. James Ross, MilliporeSigma, Katharina Fach, Merck Darmstadt

185 Deviations of Expected Split Ratio of Active Pharmaceutical Ingredients, Alexander Bulsiewicz, Nicholas Snow, Seton Hall University

186 Extended Retention and Separation capacity of Nitrosamines utilizing a Polar Endcapped Monodisperse Fully Porous Particle (MFPP) HPLC Column, Edward Faden, MAC-MOD Analytical, Mark Woodruff, Fortis Technologies

187 Investigation on In-Vivo Degradation Rate of Compound A in Normal Human Stomach pH Range via Design and Execution of In-Vitro Biorelevant Dissolution to De-Risk a Potential PK Variability due to Varied Degradation Levels, Smriti Gupta, Hyunho Kang, Tina Masiuk, Alena Bensussan, Sanjaykumar Patel, Adrian Goodey, Sebastian Escotet, Andre Hermans, Joshua Palacios, Merck & Co.

188 A Proteomic Investigation to Identify Potential Protein Biomarkers for Breast Cancer Detection Using Sera from Control Donors and Women with Triple Negative Breast Cancer, Nicholas Versaci, Danielle Whitham, Norman Haaker, Brian Pentecost, Costel Darie, Clarkson University

189 The Use of Human Breastmilk as a Bio-Fluid for Protein Biomarker Identification for Breast Cancer, Kathleen F. Arcaro, Brian T. Pentecost, University of Massachusetts Amherst, Lilian Corrice, Danielle Whitham, Pathea Bruno, Norman Haaker, Costel C. Darie, Clarkson University

190 Achieving High Recovery & Reproducibility in High Throughput Sample Preparation Using Silica/Polymer Composite 96-Well SPE Plates, Geoff Faden, MAC-MOD Analytical, David Dunthorne, Colin Pipe, Anthony Edge, Matt James, Gemma Lo, Avantor

191 Scalable and Automatable Benchtop Scale Protein A Based mAb Purification Using AffinEx SPE Columns with Resolvex A200 Sample Processor, Qi Huang, Steven Alo, Heather Eastwood, Tuan-Linh Nguyen, Karsten Liegmann, John Laycock, Tecan SP

192 The Importance of Temperature on Complete Digestion of High-Fat Foods for Metals Analysis, Alicia Stell, Samuel Heckle, Macy Harris, Layla Abu-Al-Halaweh, CEM Corporation

Tuesday Afternoon, November 19, 2024

New for 2024 – EAS is honoring ALL 6 awardees in a special award session 1:15pm – 4:30pm in the Amphitheatre. All registered attendees and exhibitors are invited to attend. A complimentary Mixer will be held in the Exposition Rooms immediately following the Award Session.

EAS Award Session
Chaired by Suzanne Schreyer, Rigaku

1:15pm; 193: EAS YOUNG INVESTIGATOR AWARD
Bio-Inspired Technologies for Monitoring Human and Environmental Health
Honoring Ariel Furst, Massachusetts Institute of Technology
Sponsored by American Microchemical Society

1:45pm; 194: EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN SEPARATION SCIENCE
A Career in Analytical Chemistry
Honoring Nelu Grinberg
Sponsored by Waters Corporation

2:15pm; 195: EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN VIBRATIONAL SPECTROSCOPY
Variety of Vibrational Spectroscopy: From Fundamental Research to Practical Applications for Forensic Purposes and Medical Diagnostics
Honoring Igor Lednev, University at Albany
Sponsored by the Coblentz Society

Break 2:45pm – 3:00pm

3:00pm; 196: EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN MASS SPECTROMETRY
Development of Quantitative Mass Spectrometry Approaches for Analyses of Protein and RNA Modifications
Honoring Benjamin Garcia, Washington University-St. Louis
Sponsored by Restek Corporation

3:30pm; 197: EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN MAGNETIC RESONANCE
Probes with a Purpose: NMR Instrumentation for Biological Semisolids and Partially Ordered Samples
Honoring Rachel Martin, University of CA - Irvine
Sponsored by Bruker BioSpin & New Era Enterprises

4:00pm; 198: EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN THE FIELDS OF ANALYTICAL CHEMISTRY
Spectroscopic Approaches for Tracking Degradation of Organic Semiconductors Important for Organic Optoelectronic Devices
Honoring Jeanne Pemberton, University of Arizona
Sponsored by Bristol Myers Squibb

Wednesday Morning, November 20, 2024

Molecular Puzzles: Navigating Analytical Challenges in Peptide, Protein, and Oligonucleotide Drug Products
Chairs: Yongchao Su, Merck & Co., Inc. and Kang Chen, United States Food & Drug Administration

9:00 199 Visible Light Photodegradation of Therapeutic Proteins: Mechanisms, Excipient Effects, and Preventive Strategies, Garth Simpson, Purdue University

9:30 200 Surface-Mediated Spontaneous Emulsification of an Acylated Peptide, Semaglutide, Ken Qian, Eli Lilly and Company

10:00 Break

10:30 201 CryoEM - A Powerful Multi-Attribute Characterization Tool for Nanoparticle Formulations, Mandy Janssen, Sheng Wang, Brent Wood, Giovanna Scapin, Eric Bushong, Brianna Fisher, Kalyn Kallio, NanoImaging Services

11:00 202 Weighing in the Biophysical Characterization Power: From Discovery to In-Depth Understanding to Biologics Product, Jing Song, Merck & Co., Inc.

The Research from our Emerging Forensic Scientists
Sponsored by New Jersey Association of Forensic Scientists
Chair: Monica Joshi, West Chester University of PA

9:00 203 Use of Digital Representations of Skeletal Remains for Forensic Analysis, Katie Steigerwalt, Matthew Kieber-Emmons, Carol Ritter, Cedar Crest College, David Webb, Kutztown University

9:30 204 Assessment of Blood and Semen Detection and DNA Collection from Swabs up to Three Months after Deposition on Five Different Cloth Materials, Emily Kryvorutsky, Francisco Medina-Paz, Brandon Kuba, Sara Zapico, New Jersey Institute of Technology, Gabriela Roca, SERATEC mbH

10:00 Break

10:30 205 Differentiating Black Powder Manufacturers through Post Blast Residue Utilizing SEM-EDS and FTIR-DRIFTS, Damian Niescior, Ken Hand, Georgia Arbuckle, Kimberlee Moran, Rutgers University

11:00 206 Evaluation of Urine Cannabinoids by LC/MS/MS in a Population of CBD Users, Kourtney Albert, Arcadia University

Predictive Sciences for Chromatographic Method Development
Sponsored by North Jersey Section ACS
Chair: Pankaj Aggarwal, Merck & Co., Inc.

9:00 207 Machine Learning Structure-Based Prediction of Chiral Stationary Phases for Chromatographic Enantioseparation from 3D Molecular Conformations, Christopher Welch, Indiana Consortium for Analytical Science & Engineering

9:30 208 Application of Retention Prediction to LC Separation Problems, Martin Gilar, Waters Corporation

10:00 Break

10:30 209 Fuel for the Engine - High Throughput Retention Measurement to Enable Predictive Models for Liquid Chromatography, Dwight Stoll, Sarah Rutan, Trevor Kempen, Bob Piro, Gustavus Adolphus College

11:00 210 Structure and Graph Based Machine Learning Prediction of Retention Times for LC Method Development of Pharmaceuticals, Jonathan Fine, Pankaj Aggarwal, Amanda Mann, Armen Beck, Merck & Co., Inc.

Challenges Managers Face Today
Chair: Denis Swijter, ALMA

9:00 211 Building Bridges: Turning Differences into Strengths, Scott Hanton, Lab Manager Magazine

9:30 212 Supporting Diversity and Inclusion in the Workplace, Dwayne F. Henry, Montgomery College

10:00 Break

10:30 213 How to Manage Conflict, May Adaeze Chinda, University of Ghana Medical Centre

11:00 214 Finding the Holy Grail: Engagement, Tarshae Drummond, Fayetteville State University

The Very Latest Developments in Atomic Spectrometry
Chair: Steven Ray, University at Buffalo, SUNY

9:00 215 Exploring the Analytical Capabilities of LIBS-ICPMS for Geological, Energy, Pharmaceutical, and Medical Applications, C. Derrick Quarles Jr., Elemental Scientific, Benjamin T. Manard, Oak Ridge National Laboratory

9:30 216 Standard-Free Absolute Quantitation of Drug Metabolites via Elemental F and Cl Detection by Plasma-Based Mass Spectrometry, Kaveh Jorabchi, Samuel White, Grace Hahm, Zahra Afsharsaveh, Georgetown University, Matthewy Cerny, Pfizer, Inc.

10:00 Break

10:30 217 Challenges and Opportunities in Single-Particle Inductively-Coupled Plasma Mass Spectrometry (sp-ICP-MS), Antonio R. Montoro Bustos, Monique E. Johnson, George C. Caceres, Karen E. Murphy, Michael R. Winchester, National Institute of Standards and Technology

11:00 218 Ditch the Argon! Plasma-Based Atomic Spectrometry Using Ambient Air, Steven Ray, University at Buffalo, SUNY

Chemical Data Science: Artificial Intelligence and Machine Learning Applied to Analytical Chemistry
Chair: Barry Lavine, Oklahoma State University

9:00 219 Transmission Infrared Spectroscopy and Machine Learning for Forensic Analysis of Automotive Paint, Barry Lavine, Haoran Zhong, Elizabeth Donkor, Collin White, Oklahoma State University, Thomas Hancewicz, TMH Associates

9:30 220 Conformal Prediction Applied to Raman Spectra of Analgesics, Karl Booksh, University of Delaware

10:00 Break

10:30 221 The Use of Near Infrared Spectroscopy and Machine Learning to Assess the Quality of 3D Printing Tablets, Stephen Hoag, Keith Freel, Yihan Wang, Ahmed Ibrahim, University of Maryland-Baltimore, Sharon Flank, Jon Schupp, Infratrac, Inc.

11:00 222 Next Generation Machine Learning Technologies to Accelerate Pharmaceutical Process Research & Development, Joseph Smith, Merck & Co., Inc

Developments in Food and Cannabis Science
Chair: Anthony Provatas, University of Connecticut

9:00 223 Automated Solvent Extraction Method of PFAS from Difficult Food and Food Packaging Matrices, Alicia Stell, Benedict Liu, CEM Corporation

9:20 224 A High-Efficiency Approach to Quantitating Pesticides in Challenging High-Pigmented Food Matrices with GC/MS/MS Using a New Electron Ionization (EI) Source for Maximized Uptime, Anastasia Andrianova, Samuel Haddad, Limian Zhao, Agilent Technologies

9:40 225 Non-Invasive Raman Spectroscopy for the Authentication of Food Products, Alexander Rzhevskii, Thermo Fisher Scientific

10:30 226 Replicating Water and Fat-Soluble Vitamins Analyses on a Modern HPLC System, Kimberly Martin, Lise Gauthier, Elom Pedanou, Paula Hong, Waters Corporation

10:50 226 A Illicit Drug Desorption and Chemical Profiling of Fingerprints using SICRIT Ion Source: A Rapid Analysis Approach, Jan-Christoph Wolf, Ciara Conway, Taylor Hayward, Plasmion GmbH

Perspectives on Macromolecule Analysis
Chair: Costel Darie, Clarkson University

9:00 227 Understanding the Role of CD68 in the Tumor Microenvironment, Valentina Rangel-Angarita, Ryan Chen, Lea Kim, Taryn Lucas, Keira Mahoney, Stacy Malaker, Yale University

9:20 228 Peptidomic Analysis of Breast Milk and Sera from Women with Breast Cancer and Equivalent Controls to Identify Potential Biomarkers for Early Diagnosis, Pathea Bruno, Danielle Whitham, Isabella Pelkey, Brian T. Pentecost, Costel C. Darie, Clarkson University, Kathleen F. Arcaro, University of Massachusetts-Amherst

9:40 229 Proteomics Investigation of Human Breast Milk with Invasive Ductal Carcinoma Breast Cancer and Match Control for Early Detection of Breast Cancer: A Mass Spectrometry Approach, Aneeta Arshad, Costal C. Darie, Clarkson University, Brian T. Pentecost, Kathleen F. Arcaro, University of Massachusetts-Amherst

10:00 Break

10:30 230 Integration of Innovative Biochemical and Instrumental Methods to Enable Structural Elucidation and Spatially Resolve Labile Carbohydrates, Tana Palomino, David Muddiman, North Carolina State University, Juhi Samal, University of Alabama-Birmingham, Ana Sheridan, Ashley Brown, The University of North Carolina at Chapel Hill, Tatiana Segura, Duke University

10:50 231 Optimizing Surface Plasmon Resonance (SPR) Characterization of the Binding Between Individual Tandem Repeats of MUC16 (CA125) and Clinically Relevant Antibodies, Eliza Hanson, Chien-Wei Wang, Rebecca Whelan, University of Kansas

11:10 232 Developing a Method to Monitor the Estrogen-Inducible Proteins in Fishes from the Great Lakes upon Exposure to Environmental Contaminants, Krishan Weraduwage, Taniya Jayaweera, Bernard Crimmins, Sujan Fernando, Thomas Holsen, Costel Darie, Clarkson University

Wednesday, November 20: E-Poster Session: 11:30pm – 12:25pm

233 Development and Qualification of a Greener High pH Generic HPLC Method, Matthew Swoyer, Kaitlin Grinias, GSK

234 Electron Transfer Reactions of Transition-Metal Complexes for Solar Energy Conversion and Storage, Annie Shen, Bryn Mawr College, Michael Eberhart, New Jersey Institute of Technology

235 Sensing Copper (II) Ions with Coumarin Dyes, Revathi Variar, Jingqiu Hu, West Chester University

236 Assessing Algal Toxin Contamination in Connecticut Freshwater Systems Utilizing Liquid Chromatography Tandem Mass Spectrometry, Anthony Provatas, James Stuart, University of Connecticut, Slawomir Piela, Drexel University

237 Qualitative Analysis of Polycyclic Aromatic Hydrocarbons in Vehicle exhaust and Roadway Surfaces Utilizing GC-MS/MS, Anthony Provatas, Conner Kocot, Abigail Manka, University of Connecticut CESE

238 A Green Chemistry Methodology for the Degradation of Malathion, Michael Eckel Santos, Marius Pelmus, Sergiu Gorun, Seton Hall University

239 Precise Water Analysis in Cannabis: Karl Fischer (KF) Titration Method, Michelle Kuzio, Tom Szakas, Xylem

240 An Automated Dynamic Headspace Approach for the Determination of Ignitable Liquid Residues from Mock Arson Evidence Megan Harper-Kerr, GERSTEL, Inc.

241 Investigating Odor Signatures of Electronic Storage Devices, Samuel Friday, Marisia Fikiet, Alyssa Marsico, Brooke Kammrath, University of New Haven, Jon Naples, Connecticut State Police, Pauline Leary, NOBLE

242 Achiral Separation of Fluorofentanyl Derivatives on Chiral Stationary Phases in Varying Mobile Phase Modes, John Ferraro, Weston Umstead, Daicel Chiral Technologies

243 Analysis of Volatile Organic Compounds from Submerged Animal Tissue Decomposing at Varied Temperatures, Virginia Weina, Katelynn Perrault Uptmor, William & Mary

244 Analysis of Green Gunshot Residues Using Scanning Electron Microscopy with Energy-Dispersive X-Ray Spectroscopy and Comprehensive Two-Dimensional Gas Chromatography, Grace Saunders, Katelynn Perrault Uptmor, William & Mary

245 Chemical Fingerprint of Ignitable Liquid Residues by DART-MS: More Than Volatile Organic Compounds (VOC), Mengliang Zhang, Ohio University, Shruthi Perna, Ngee Sing Chong, Middle Tennessee State University

246 The Role of Diphenylamine in Enhancing Fluorescence Analysis of Smokeless Powder and Gunshot Residue for Forensic Purposes, Cody Silverman, Igor Lednev, University at Albany-SUNY

247 Free Tools to Support Liquid Chromatography Teaching, Learning, and Method Development, Dwight Stoll, Gustavus Adolphus College

248 2.7-um Superficially Porous Particles for Chiral Chromatography in HPLC and SFC, Melissa Wilcox, Regis Technologies

249 Enhancing Basic Thin Layer Chromatographic Analysis: Application-Driven Capabilities of the TLC Explorer, Petra Lewits, Michaela Oberle, Markus Burholt, MilliporeSigma

250 Evaluation of Bidentate End-Capping Silylation Reagents for HPLC, Norikazu Nagae, Ryuji Koyama, Tomoyasu Tsukamoto, ChromaNik Technologies Inc., Scott Silver, Pyvot

251 In-Process LCMS Analysis of Polysorbate 80 Biodegradation, Jixin Liu, Kate McEvoy, Wenyi Yee, Croda, Inc.

252 A "Trimmed-Down" Look into Using Analytical Techniques for Lipid and Protein Composition in Aging Indian Hair, Nusrat Islam, Ernesta Malinauskyte, Vanessa Castro, Daniel Strzeszewski, Lijing Xu, TRI Princeton

253 Analysis of Chloro-Thioethers Photodegradation by Fluoro-Phthalocyanines in Homogenous and Heterogenous Systems, Sean Scally, Sergiu Gorun, Marius Pelmuş, Seton Hall University

Wednesday Afternoon, November 20, 2024

High Throughput Analytical Experimentation: An Automated Approach
Sponsored by LRIG Philadelphia
Chair: Sharon V. Matamoros, GSK

1:30 254 Automated Biorelevant Solubility Workstation for Long-Acting Injectable Drug Development, Michael Rerick, Luis Herran, GSK

2:00 255 Enhancing the Automated Screening of Physicochemical Properties of the Discovery Portfolio, Jordan De Jesus Silva, Susana Morais, Alexander S. Chin, Dorothy Levorse, Devan McCoy, Merck & Co., Inc.

2:30 256 Development of Novel Technologies as Enabled by Pre-Competitive Collaborations: The Enabling Technologies Consortium, Rahul Sangodkar, Amgen

3:00 257 Leveraging an Automated Standardized Approach to LC Method Development, Scott Hartzell, Eli Lilly and Company

Sub-Micron Infrared and Raman Spectromicroscopy
Chair: Samuel Tenney, Brookhaven National Laboratory

1:30 258 Materials for Inhaled Aerosol Treatment of Disease: Optical Photothermal Infrared Microscopy (O-PTIR) as an Advanced Characterization Method for Assessing the Emitted Dose of Complex Dry Powder Inhaler Formulations, Mark Banaszak Holl, Sheikh Tanzina Haque, Blessy Joseph, University of Alabama – Birmingham, Dipesh Khanal, University of Sydney, Elizabeth Bielski, Bryan Newman, Huzeyfe Yilmaz, Snober Ahmed, United States Food & Drug Administration

2:00 259 Applications of Combined O-PTIR and Raman in the Analysis of Microplastics from Environmental Samples, Bangshuai Han, Moayad Yacoub, Ball State University, Samuel Tenney, Brookhaven National Laboratory

2:30 260 O-PTIR Submicron Spectroscopy and Imaging of Bone Tissue Mineralization, William Querido, Temple University

3:00 261 Spatially Resolved Spectroscopy for MOF-Based Resist Development, Andrea Kraetz, Michael Tsapatsis, Johns Hopkins University, Prerna Prerna, Ilja Siepman, University of Minnesota, Mueed Ahmad, Stony Brook University, J. Anibal Boscoboinik. Samuel Tenney, Brookhaven National Laboratory

Forensic Analysis: From Lab to Crime Scene
Chair: Sharla Wood, Bristol Myers Squibb

1:30 262 Forensic Soil Analysis by Particle Correlated Raman Spectroscopy (PCRS): Comparison to Traditional Methods, Jasmine Kaur, Joshua Christensen, Drew Kuroda, Ella Galvan, Marisia Fikiet, Virginia Maxwell, Brooke Kammrath, University of New Haven, Ethan Groves, Christopher Palenik, Microtrace, Peter De Forest, Forensic Consultants

1:50 263 Towards Determining the Limit of Detection for a Universal Body Fluid Identification Method for Forensic Purposes, Riley Alpuché, Ben Taubner, Nathaniel Cady, Igor Lednev, University at Albany, SUNY

2:10 264 An Evaluation of the Forensic Readiness of Comprehensive Two-Dimensional Gas Chromatography Towards Organic Trace Analysis, Katelynn Perrault Uptmor, Emma Macturk, Barbara Grace Saunders, Virginia Weina, William & Mary

2:30 265 What is in a Fingermark? A Nontargeted Analysis Using Comprehensive Two-Dimensional Gas Chromatography, Emma Macturk, Katelynn Perrault Uptmor, William & Mary

2:50 266 Discrimination of a Self-Reference Algorithm Threshold with ROC Curve to Distinguish Between Human and Animal Blood Using Raman Spectroscopy for Forensic Purposes, Alexis Weber, SupreMEtric, Harrison Dickler, Igor K. Lednev, State University of New York-Albany

3:10 267 Forensic Fingerprinting of the Unseen: Revealing the Dark Secrets of PFAS with High-Resolution Ion Mobility, Frederick Strathmann, Thomas Lubinsky, MOBILion Systems

Leveraging Modeling for Chromatographic Analysis
Chair: Kate Jackson, Colgate Palmolive

1:30 268 Digitally Enabled Generic Analytical Framework Accelerating the Pace of Liquid Chromatography Method Development for Vaccine Adjuvant Formulations, Mohamed Hemida, Rodell C. Barrientos, Caleb Kinsey, Nathan Kuster, Mayank Bhavsar, Armen Beck, Heather Wang, Andrew Singh, Pankaj Aggarwal, Arthur Arcinas, Malini Mukherjee, Emmanuel Appiah-Amponsah, Erik L. Regalado, Merck & Co., Inc.

1:50 269 Improved Assay Development of Pharmaceutical Modalities Using Feedback-Controlled Liquid Chromatography Optimization, Andrew Singh, Fatima Naser Aldine, Heather Wang, Rodell Barrientos, Michelle Wong, Pankaj Aggarwal, Erik Regalado, Imad Haidar Ahmad, Merck & Co., Inc., Devin Makey, University of Michigan

2:10 270 Does pH Matter? Comparing Multidimensional Design Spaces of Volatile and Non-Volatile Buffer Systems, Arnold Zoeldhegyi, Imre Molnar, Molnar-Institute for Applied Chromatography, Krisztian Horvath, University of Pannonia, Robert Kormany, Egis Plc

2:30 271 The Relevance of Modeling in Pharmaceutical Submissions, Imre Molnár, Arnold Zoeldhegyi, Molnár-Institute

2:50 272 Could Light Ruin your RPLC Robustness – Lessons from API Method Development, Anna Calkins, Jonathan Shackman, Elizabeth Yuill, Bristol Myers Squibb

3:10 273 Reduction of Wet Experiments by Use of Drylab for Simulation and Prediction of Chromatographic Separations, Xiaole Shao, Boehringer Ingelheim

Data Science Solutions for Modern Day Problems
Chair: Robert Vetrecin

1:30 274 Deep Learning to Enhance Investigative Lead Information from Automotive Clear Coats, Barry Lavine, Collin White, Douglas Heisterkamp, Oklahoma State University

1:50 275 Shift Invariant Tri-Linearity Algorithms for Fast, Flexible Blind Source Separation in Hyphenated Chromatography, Neal Gallagher, Eigenvector Research, Inc., Paul-Albert Schneide, BASF SE, Rasmus Bro, University of Copenhagen

2:10pm 276 Expanding the Utility of a Virtual Method Development Tool, Melinda Urich, Justin Steimling, Jamie York, Tim Yosca, Samantha Herbick, Chris Nelson, Restek Corporation, John Garrett, Analytical Innovations

2:30pm 277 Feature Extraction Algorithm for Conventional and Comprehensive Two-Dimensional Gas Chromatography Coupled with Mass Spectrometry, Leandro Wang Hantao, Carlos Alberto Teixeira, Guilherme Post Sabin, Amilton Moreira Oliveira, Luidy Darllan Barbosa, University of Campinas

2:50pm 278 Streamlining Chromatographic Method Evaluation and Ensuring Data Quality through Advanced Tools Farrel Borden, Gary Sharman, Mitcheell Maestre, Agustín Barba, Nicola Tonge, Mestrelab Research

Applications of Analytical Science in Nanotechnology
Chair: Caelin Celani, University of Delaware

1:30 279 Time-Resolved Spectroscopy for Quantitative Characterization of Surface-Modified TiO2, Michael Uzu, University of Delaware

1:50 280 Understanding the Degradation and Strain Effects of Thin GaSe, Lottie Murray, Matthew Doty, University of Delaware

2:10 281 Fluorescent Dyed Gold Core-Silicon Shell Nanoparticles for Biological Applications, Briana M. Mohan, Bhanu P.S. Chauhan, Amana Awwad, Qiaxian Johnson, William Paterson University

2:30 282 Silver Nano Raspberries Stabilized by Cyclic Silanes, Asmaa Lakhal, Saadia Chaudhry, Arleen Ruiz, Bhanu P. S Chauhan, William Paterson College

2:50 283 Decoupling Wavelength Dependence for T-ray Imaging Rescuing the Semiconductor Yield, Anis Rahman, Applied Research & Photonics