

# 2017 EAS Invited Technical Sessions

*Preliminary List as of April 21, 2017*

Note: List does **not** include contributed oral or poster Sessions – these will be posted in the EAS Preliminary Program. Contributed abstract submission deadlines are **May 26 for oral papers** and **September 1 for poster papers**. Submit at [www.eas.org/submit](http://www.eas.org/submit)

## AWARD SESSIONS

### EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN THE FIELDS OF ANALYTICAL CHEMISTRY

*Sponsored by Bristol-Myers Squibb*

**Honoring Janusz Pawliszyn, University of Waterloo**

Chair: Nicholas Snow, Seton Hall University

*Growing Up with SPME*, Nicholas Snow, Seton Hall University

*Providing Rugged Methodology for Regulated Industries*, Mary Ellen McNally, DuPont Crop Protection

*Whole-Column Imaged Capillary Isoelectric Focusing (cIEF): From Academic Idea to Industrial Gold Standard*, Jiaqi Wu, Protein Simple

*Medical and Pharmaceutical Applications of Solid Phase Microextraction*, Barbara Bojko, Nicolaus Copernicus University

### EAS YOUNG INVESTIGATOR AWARD

**Recent Advances in 2D-LC, Part 1: Fundamentals, Instrumentation, and Column Technology**

**Honoring Dwight Stoll, Gustavus Adolphus College**

Chair: William Barber

*Moving into the Mainstream – Reflections on Recent Developments in Two-Dimensional Liquid Chromatography*, Dwight Stoll, Gustavus Adolphus College

*Three-Dimensional and Higher Dimensional Separations*, Mark Schure, Kroungold Analytical

*Recent Developments in Active Temperature Control for Improved Chromatographic Performance*, Stephen Groskreutz, University of Pittsburgh

*A Research Adventure Behind Vacuum-Jacketed Chromatographic Columns: Curiosity, Theory, Development, and Applications*, Fabrice Gritti, Waters

### EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN CHEMOMETRICS

*Sponsored by Eigenvector Research*

**Honoring Barry Lavine, Oklahoma State University**

Chair: Steven Brown, University of Delaware

*Mapping Polyethylene Reactor and Product Space Using Multivariable Analysis of Digital Distributions*, Paul DesLauriers, Chevron Phillips Chemical Company

*Stacking the Deck in Calibration: Better Models and Better Transfers with Stacked Calibration Methods*, Steven Brown, University of Delaware

*Investigation of Meteor and Meteor Impact Samples by Raman Spectroscopy and Multivariate Curve Resolution*, Karl Booksh, University of Delaware

*Multivariate Curve Resolution, Genetic Algorithms and Cross Correlation Library Searching in the Forensic Examination of Automotive Paints*, Barry Lavine, Oklahoma State University

## AWARD SESSIONS

### EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN MAGNETIC RESONANCE

*Sponsored by Bruker BioSpin and New Era Enterprises*

**Honoring Bernhard Blümich, RWTH Aachen University**

Chair: Songi Han, University of CA-Santa Barbara

*Shrinking NMR: From the Laboratory Floor via the Tabletop to the Pocket?*, Bernhard Blümich, RWTH Aachen University

*Compact NMR in Clinical Diagnostics*, David Cistola, Texas Tech University

*Automation of NMR with Machine Learning*, Yi-Qiao Song, Schlumberger-Doll Research

*Structure and Function in Metal Organic Frameworks are Informed by Portable Magnet Relaxometry, Thanks to Bernhard Blümich*, Jeffrey Reimer, University of California-Berkeley

### EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN SEPARATION SCIENCES

*Sponsored by Agilent Technologies*

**Honoring Christopher Welch, Welch Innovation, LLC**

Chair: Mirlinda Biba, Merck & Co.

*The Practice and Consequences of Ultrafast LC and SFC*, Daniel Armstrong, University of Texas-Arlington

*High-Speed Enantioselective Chromatography as the Second Dimension in Multiple Heart-Cutting and Comprehensive 2D-RPLC Analysis*, Erik Regalado, Merck & Co.

*Innovative Approaches in High-Throughput Chromatographic Analysis in Support of Pharmaceutical Development Research*, Kerstin Zawatzky, Merck & Co.

*Recent Progress and Emerging Challenges in Pharmaceutical Separation Science*, Christopher Welch, Welch Innovation, LLC

### EAS AWARD FOR OUTSTANDING ACHIEVEMENTS IN MASS SPECTROMETRY

**Honoring Scott McLuckey, Purdue University**

Chair: Alice Pilo, Merck & Co.

*Gas-Phase Ion/Ion Reactions: Oxidation and the Dehydroalanine Effect*, Alice Pilo, Merck & Co.

*Top-Down Proteomics for Clinical Assay Development*, James Stephenson, Thermo Fisher Scientific

*Characterization and Optimization of Ion Trapping Fields in Toroidal Coordinates*, Stephen Lammert, PerkinElmer

*The Study of Protein Folding and Unfolding via Theta-Tip Nano-Electrospray Ionization*, Scott McLuckey, Purdue University

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## AWARD SESSION *continued*

### NEW YORK SECTION OF THE SOCIETY OF APPLIED SPECTROSCOPY GOLD MEDAL AWARD

Honoring: **Richard Van Duyne, Northwestern University**  
Chair: Kathryn Lee, rap-ID

*Nanoscale Chemical Imaging with Tip-Enhanced Raman Spectroscopy*, Richard Van Duyne, Northwestern University

*Translating SERS into a Robust Detection Platform for Uranium in Complex Matrices*, Amanda Haes, University of Iowa

*Polymer-Enabled Analytical SERS Sensing*, Christy L. Haynes, University of Minnesota

*Imaging Mass Spectrometry on the Nanoscale with Cluster Ion Beams*, Nick Winograd, Penn State University

### AMERICAN MICROCHEMICAL SOCIETY BENEDETTI PICHLER AWARD

Honoring: **Somenath Mitra, NJ Institute of Technology**  
Chair: Robert Vetrecin

*Session speakers to be announced*

## BIOANALYSIS

### Analysis of Peptides and Proteins in Biological Samples in Support of Drug Discovery and Development

Chair: Wenying Jian, Janssen

*Analytical Strategies and Challenges for Peptide Quantification Using LC-MS/MS in Support of GLP TK and Clinical PK Studies*, Yang Xu, Merck & Co.

*Assessing Drug-Target Engagement in Tissue Biopsies*, Eugene Ciccimaro Jr., Bristol-Myers Squibb

*Considerations for Assay Platform and Reagent Selection to Quantify Endogenous Protein Biomarker; a FGF21 Case Study*, Yue Zhao, Bristol-Myers Squibb

*Subunit-Level Analyses of Monoclonal Antibodies from In-Life Samples: A Whole-Molecule LC-MS Method for Quantitation, Quality Attributes, and Biotransformation*, John Kellie, GlaxoSmithKline

### Vibrational Characteristics of Biologics

Chairs: Anna Luczak, Varsha.Ganesh, Bristol-Myers Squibb

*Plaque Detection Using Resonance Raman Spectroscopy*, Robert Alfano, City University of New York

*Concomitant Raman Spectroscopy and Dynamic Light Scattering for Therapeutic Protein Characterization*, Chen Zhou, Eli Lilly

*Use of Raman and Raman Optical Activity for the Structural Characterization of a Therapeutic Monoclonal Antibody Formulation Subjected to Heat Stress*, Geetha Thiagarajan, Merck & Co.

*Ligand-Receptor Binding Investigated by Tip-Enhanced Raman Spectroscopy*, Lifu Xiao, University of Notre Dame

*Vibrational Spectroscopic Imaging Applications to Investigate Exogenous Agent Perturbation and Spatial Distribution in Skin*, Qihong Zhang, Rutgers University

## CHROMATOGRAPHY

**Recent Advances in 2D-LC, Part 2: Solving Real-World Problems in the Pharmaceutical and Chemical Industries, sponsored by the Chromatography Forum of the Delaware Valley**

Chair: William Barber

*Fast Chiral Chromatography as the Second Dimension in 2-D HPLC*, Christopher Welch, Welch Innovation, LLC

*Characterization of Synthetic Polymers Using Ultra-high Pressure Two-Dimensional Liquid Chromatography*, Lu Bai, Dow Chemical

*Expanding the Biologics CMC Analytical Toolkit with Two Dimensional Liquid Chromatography*, Douglas Richardson, Merck & Co.

*Application of 2D-LC-MS in Real-World Pharmaceutical Analysis*, Cadapakam (CJ) Venkatramani, Genentech

**Building the Future in Sample Preparation with Young Investigators, sponsored by the Chromatography Forum of the Delaware Valley**

Chair: Mary Ellen McNally, DuPont Crop Protection

*Improving Metabolite Coverage in Untargeted LC-MS Metabolomics*, Dajana Vuckovic, Concordia University

*Advances in Bioanalytical Sample Preparation*, Jared Anderson, Iowa State University

*The Role of Sample Preparation in Precision Medicine*, Marcel Musteata, Albany College of Pharmacy and Health Sciences

*What's the Matter with Sample Prep? Novel Approaches and Solutions*, Roy Helmy, Merck & Co.

**Emerging Frontiers in High-Throughput Analysis for Process Research & Development**

Chair: Wes Schafer, Merck & Co.

*Enabling High-Throughput Experimentation through High-Throughput Analysis*, Wes Schafer, Merck & Co.

*Reactivity-Based High-Throughput Analysis of Heavy Metals*, Kazunori Koide, University of Pittsburgh

*Asymmetric Reaction Screening with Chiroptical Sensors*, Christian Wolf, Georgetown University

## CULTURAL HERITAGE

*Organized by the New York Conservation Foundation*

**Vibration Science and Technology in Cultural Heritage I**

Chair: William Wei, Netherlands Institute for Cultural Heritage

*Session speakers to be announced*

**Vibration Science and Technology in Cultural Heritage II**

Chair: Andrew Lins, Philadelphia Museum of Art

*Session speakers to be announced*

**Vibration Science and Technology in Cultural Heritage III**

Chair: William Wei, Netherlands Institute for Cultural Heritage

*Session speakers to be announced*

**Vibration Science and Technology in Cultural Heritage IV**

Chair: John Scott, New York Conservation Foundation

*Session speakers to be announced*

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## ENVIRONMENTAL ANALYSIS

### **The Challenge of Testing for Mutagenic Impurities While Considering the Total Exposure**

Chairs: James Stuart, University of Connecticut, Landon Greene, Bristol-Myers Squibb

*Capturing Chemical Exposures: The Exposome and Human Health*, Gary Miller, Emory University

*Early Life Exposure to Environmental Chemicals and Health Trajectories*, Manish Arora, Icahn School of Medicine at Mount Sinai

*Volatile Genotoxic Impurity Determination in Oligonucleotide API at Sub-ppm Level*, Dora Visky, Celgene Corporation

*Novel Approaches to Identify Metabolite-Related Mutagenic Reactions*, James Rusling, University of Connecticut

### **Monitoring Water Pollution to Prevent Future Flints**

Chair: Satinder Ahuja, Ahuja Consulting

*Impact of Flint Water Crisis on Public Safety*, Ni Zhu, Virginia Tech

*Combined Effect of Warming and Pollutants on Sex Determination*, Bethany Decourten, University of North Carolina-Wilmington

*Coal Use as a Cause of Water Quality Impairment*, Larry Cahoon, University of North Carolina-Wilmington

*Sustainable Pathways to Metals Contamination*, Rakesh Sharma, Delhi University

### **Quality Data for Monitoring Pollution and Climate Change, organized by The Coblenz Society**

Chair: Brandye Smith-Goettler, Merck & Co.

*Simulation of the Entire Pathway from Atmospheric CO<sub>2</sub> into Oceans into Microalgal Biomass*, Frank Vogt, University of Tennessee

*Exploring the Multidimensionality of High-Resolution Photoluminescence Spectroscopy for the Environmental Analysis of Polycyclic Aromatic Compounds*, Andres Campiglia, University of Central Florida

## FORENSIC ANALYSIS

### **Cannabinoids**

Chair: Michelle Peace, Virginia Commonwealth University

*The Natural State*, Aron Lichtman, Virginia Commonwealth University

*The Evolution of Synthetic Cannabinoids*, Aron Lichtman, Virginia Commonwealth University

*These Aren't Your Grandfather's Cannabinoids*, Justin Poklis, Virginia Commonwealth University

*Today's Marijuana and MJ Products*, Michelle Peace, Virginia Commonwealth University

### **Breaking Bad Chemistry: The Forensic Response to Clandestine Labs**

Chair: Thomas Blackwell, US Drug Enforcement Administration

*Clandestine Labs: A Walk Through Time*, Ed Kovacs, US Drug Enforcement Administration

*Chemistry of Clandestine Labs*, Jarrod Wagner, Oklahoma State University

## FORENSIC ANALYSIS (continued)

### **Research from our Emerging Forensic Scientists**

Chair: Monica Joshi, West Chester University

*Session speakers to be announced*

## LABORATORY ANALYSIS

### **In- or Out-Sourcing. That is the Question**

Chair: Dennis Swijter, ALMA

*Comparative Review of Keeping Special Microbiology in a Hospital Lab vs. Out-Sourcing to Reference Labs*, Margaret Blaetz, Best Care Laboratories

*Lab Workload Strategies: The In-Sourcing vs. Outsourcing Question*, Kelley Copeland, Pace Analytical

*Learnings from the 2016 National Burn Repository Report*, Pascual Laguerre, Cintas Corporation, Brian Foy, DuPont

*Best Ways to Interact with an Outsourcing Partner*, Scott Hanton, Intertek

## MASS SPECTROMETRY

### **Desorption Mass Spectrometry**

Chair: Barbara Larsen, DuPont

*Fundamentals and Applications of Matrix-Assisted Ionization: Zerp Energy Input Ionization*, Charles McEwen, University of Sciences

*Imaging Mass Spectrometry in Drug Development: Visualizing Tissue with a Molecular Lens*, Reid Groseclose, GlaxoSmithKline

*Improving Quantitation through a Fundamental Understanding of the MALDI Sample Preparation Process*, Kevin Owens, Drexel University

*Industrial Applications of Bruker™ MALDI-TOF Biotyper™ for Micro-organism Identification* Suzanne Singles, DuPont

### **Innovations and Applications in Mass Spectrometric Analysis**

Chair: Jim Shen, Bristol-Myers Squibb

*Mechanistic Study of the Gas-Phase In-Source Hofmann Elimination of Doubly Quaternized Cinchona-Alkaloid Based Phase-Transfer Catalysts by (+)-Electrospray Ionization/Tandem Mass Spectrometry*, Huaming Sheng, Merck & Co.

*Implementation of an Agilent 6230B LC-TOF for the Dual Work Flow HRMS Analysis of ADCs and Small Molecules in a Walk-Up Environment*, Michael Peddicord, Bristol-Myers Squibb

## MICROSCOPY

### **Forensic Microscopy XI "What is it? Who does it?"**

Chair: Thomas Kubic, John Jay College

*The Forensic Microscopy of Dyed Beaver Furs*, Michelle Miranda, SUNY - Farmingdale

*Microscopy of Explosives*, Peter Diaczuk, Penn State University

*Forensic Analysis of Blue Glass Chips by Microspectroscopy and X-Ray Spectroscopy*, Tiffany J. Millet, John Jay College, Mircea Comenescu, Graduate Center - City University of New York

*More Micro Raman Spectroscopy of Organic Gun Shot Residues and Explosive Residues*, Jennifer Leonard, Graduate Center - City University of New York



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## MICROSCOPY *continued*

### **Industrial Applications of Atomic Force Microscopy (AFM)**

Chairs: Amanda Mann, Matthew Lamm, Merck & Co.

*Oil Reservoir Properties at the Nano-Scale: Using AFM in a Bulk Characterization Industry*, Shannon Eichmann, Aramco Services Company

*Atomic Force Microscopy of Polymer Systems: From Morphology to Properties to Chemical Imaging and Spectroscopy*, Gregory Meyers, Dow Chemical

*AFM in Pharmaceutical Formulation Development*, Matthew Lamm, Merck & Co.

*Atomic Force Microscopy and Nano-IR Characterization of Composites*, William Haseltine, Solvay

## NMR SPECTROSCOPY

### **Solid-State NMR of Natural Products: Life without Labels**

Chair: Youngchao Su, Merck & Co.

*Nanometer-Scale NMR Characterization of Functional Polymer Systems and Pharmaceutical Dispersions*, Klaus Schmidt-Rohr, Brandeis University

*Electron Decoupling with Dynamic Nuclear Polarization and Frequency Tunable Gyrotrons*, Alexander Barnes, Washington University-St. Louis

*Multinuclear Quantitative Solid-state NMR of Crystalline and Disordered Pharmaceutical Solids*, Joe Lubach, Genentech

*Solid-State NMR Crystallography of Pharmaceuticals Utilizing Proton-Detected Techniques under Ultrafast Spinning*, Xingyu Lu, Merck & Co.

### **New Frontiers in Solid Analysis Spectroscopy**

Chair: Lydia Breckenridge, Bristol-Myers Squibb

*Laser Induced Breakdown Spectrometry vs. X-Ray Fluorescence*, Sharla Wood, Bristol-Myers Squibb

*Nuclear Magnetic Resonance*, Yongchao Su, Merck & Co.

*Laser Induced Breakdown Spectrometry/Laser Ablation*, Matthieu Baudelet, University of Central Florida

*Matrix-Assisted Laser Desorption Ionization*, Sarah Trimpin, Wayne State University

### **NMR Small Molecules**

Chair: Dewey Barich, GlaxoSmithKline

*Session speakers to be announced*

## PHARMACEUTICAL ANALYSIS

### **Challenges of Lifecycle Management for Method Validation**

Chairs: Kim Huynh-Ba, Pharmalytik and Karen Lucas, Janssen

*Lifecycle Management of Analytical Methods for Biotechnology Products: A Regulatory Perspective*, Rashmi Rawat (*Invited*), US Food & Drug Administration

*Lifecycle Management of Methods in Animal Health*, John Hayes, Merck & Co.

*Lifecycle Management of Analytical Methods for Cleaning Verification Support*, Mariann Neverovitch, Bristol-Myers Squibb

*Lifecycle Management: USP Perspectives*, Gregory Martin, Complectors Consulting

### **Analytical Challenges in Assessment of Drug Formulation Performance and In-Vitro Drug Release**

Chair: Xujin Lu, Bristol-Myers Squibb

*Dissolution Testing from Biorelevant to Quality Control - Challenges and Gaps*, Jian-Hwa Han, Abbvie

*Linking Dissolution Method Development and Clinical Relevance - When is a Method Appropriately Discriminating*, Andre Hermans, Merck & Co.

*Using In-Vitro Dissolution to Support Post Approval Changes - Global Regulatory Expectatio*, Amy Bu, Bristol-Myers Squibb

*Bridging Biopredictive and QC Methods - Framework and Approaches*, David Curran, GlaxoSmithKline

## SPECTROSCOPY

### **Spectroscopic Applications of PAT in the Field of Biologics and Vaccines, organized by The Coblentz Society**

Chair: Brandye Smith-Goettler, Merck & Co.

*Process Control Using Real Time Molecular Weight Light Scattering*, Bhunit Patel, Merck & Co.

*Raman-Based Nutrient and Metabolite Control in Bioprocessing Optimizes Product Quality and Peak Viable Cell Density*, Karen Esmonde-White, Kaiser Optical Systems

*To be announced*, John Bobiak, Bristol-Myers Squibb

### **Spectroscopy for Counterfeit Detection, organized by The Coblentz Society**

Chair: Brandye Smith-Goettler, Merck & Co.

*Determination of Adulterated Neem and Flaxseed Oil Compositions by FTIR Spectroscopy and Multivariate Regression Analysis*, Sayo Fakayode, North Carolina A&T State University

*Field-Deployable Applications of Raman Spectroscopy for Screening of Unapproved and Counterfeit*, Jason Rodriguez, US Food & Drug Administration

### **Ultrasensitive Spectroscopy, organized by NY/NJ SAS**

Chair: Gene Hall, Rutgers University

*Session speakers to be announced*

