# Technical Program

## 2017 Eastern Analytical Symposium & Exposition

EAS is pleased to announce that **Professor Janusz Pawliszyn**, University of Waterloo, will be the Plenary Speaker for EAS 2017. Join us to hear Prof. Pawliszyn give the Plenary Lecture titled "Think Big but Design Small, a Path to Modern Analytical Chemistry," on **Monday, November 13 at 4:30pm** in the Amphitheatre. This presentation will be followed by a time of networking and complimentary refreshments. We encourage all registrants of EAS to attend this special event.

**Monday Morning, November 13, 2017**

### EAS Award for Outstanding Achievements in Magnetic Resonance

**Honoring Bernhard Blümich, RWTH Aachen University**  
**Sponsored by Bruker BioSpin and New Era Enterprises**  
**Chair: Songi Han, University of CA-Santa Barbara**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00</td>
<td>Presentation of the EAS Award for Outstanding Achievements in Magnetic Resonance</td>
</tr>
<tr>
<td>9:05</td>
<td>1 Shrinking NMR: From the Laboratory Floor via the Tabletop to the Pocket?, Bernhard Blümich, RWTH Aachen University</td>
</tr>
<tr>
<td>9:30</td>
<td>2 Compact NMR as a Screening Tool for Diabetes Prevention, David P. Cistola, Paul L. Foster School of Medicine</td>
</tr>
<tr>
<td>10:00</td>
<td>Break</td>
</tr>
<tr>
<td>10:20</td>
<td>3 Porous Media, Magnetic Resonance and Machine Learning, Yi-Qiao Song, Schlumberger</td>
</tr>
<tr>
<td>10:50</td>
<td>4 Structure and Function in Metal Organic Frameworks are Informed by Portable Magnet Relaxometry, Thanks to Bernhard Blümich, Jeffrey A. Reimer, University of California-Berkeley</td>
</tr>
</tbody>
</table>

### New York / New Jersey Section of the Society for Applied Spectroscopy Gold Medal Award

**Honoring Richard P. Van Duyne, Northwestern University**  
**Session Chair: Kathryn Lee, rap.ID Inc.**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00</td>
<td>5 Nanoscale Chemical Imaging with Tip-Enhanced Raman Spectroscopy, Richard P. Van Duyne, Northwestern University</td>
</tr>
<tr>
<td>9:30</td>
<td>6 Translating SERS into a Robust Detection Platform for Uranium in Complex Matrices, Amanda J. Haes, University of Iowa</td>
</tr>
<tr>
<td>10:00</td>
<td>Break</td>
</tr>
<tr>
<td>10:20</td>
<td>7 Polymer-Enabled Analytical SERS Sensing, Christy L. Haynes, Victoria M. Szlag, Seyoung Jung, Theresa M. Reineke, Rebeca Rodriguez, University of Minnesota</td>
</tr>
<tr>
<td>10:50</td>
<td>8 Imaging Mass Spectrometry on the Nanoscale with Cluster Ion Beams, Nicholas Winograd, Pennsylvania State University</td>
</tr>
</tbody>
</table>

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

**Chairs: James Stuart, University of Connecticut and Landon Greene**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00</td>
<td>9 Capturing Chemical Exposures: The Exposome and Human Health, Gary W. Miller, Emory University</td>
</tr>
<tr>
<td>9:30</td>
<td>10 Early Life Exposure to Environmental Chemicals and Health Trajectories, Manish Arora, Icahn School of Medicine at Mount Sinai</td>
</tr>
<tr>
<td>10:00</td>
<td>Break</td>
</tr>
<tr>
<td>10:20</td>
<td>11 Volatile Genotoxic Impurity Determination in Oligonucleotide API at Sub-ppm Level, Dora Visky, Celgene Corporation</td>
</tr>
<tr>
<td>10:50</td>
<td>12 Novel Approaches to Identify Metabolite-Related Mutagenic Reactions, James F. Rusling, University of Connecticut</td>
</tr>
</tbody>
</table>

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

**Chair: Mary Ellen McNally, DuPont Crop Protection**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00</td>
<td>13 Improving Metabolite Coverage in Untargeted LC-MS Metabolomics, Dajana Vuckovic, Dmitri Sitnikov, Parsram Ramrup, Concordia University</td>
</tr>
<tr>
<td>9:30</td>
<td>14 Development of Nucleic Acid Preservation and Extraction Methods, Jared L. Anderson, Kevin D. Clark, Omprakash Nacham, Marcelino Varona, Iowa State University</td>
</tr>
<tr>
<td>10:00</td>
<td>Break</td>
</tr>
<tr>
<td>10:20</td>
<td>15 Sample Preparation and Precision Medicine, Marcel Musteata, Albany College of Pharmacy and Health Sciences</td>
</tr>
<tr>
<td>10:50</td>
<td>16 What’s the Matter with Sample Prep? Novel Approaches and Solutions, Roy Helmy, Merck &amp; Co.</td>
</tr>
</tbody>
</table>

### Development & Optimization of Analytical Methods

**Chair: Judy Lin, Novartis**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:20</td>
<td>18 Analytical Method Development for Multicomponent Drugs, Challenges and Solutions, Prasad Panzade, Yuliya Yarkho, Apotex Inc.</td>
</tr>
<tr>
<td>9:40</td>
<td>19 System Suitability Failures Encountered in Pharmaceutical Analysis by UHPLC, Xiande (Andy) Wang, Jessica Wysocki, Qingjun (Mike) Liu, Rosie Tran, Dave Thomas, Janssen Pharma, J&amp;J</td>
</tr>
</tbody>
</table>
10:00  Break
10:40  21 Size Exclusion Chromatography of Biopolymers and Synthetic Polymers with Common Reversed-Phase and HILIC Columns, Joe P. Foley, Drexel University, Anna M. Caltabiano, GlaxoSmithKline
11:00  22 Titration for Early Drug Discovery and Development, Lori Spafford, Metromh

Industrial Applications of Atomic Force Microscopy (AFM), sponsored by The Dow Chemical Company
Chairs: Amanda Mann, Matthew Lamm, Merck & Co.

9:00  23 Oil Reservoir Properties at the Nano-Scale: Using AFM in a Bulk Characterization Industry, Shannon L. Eichmann, David Jacobi, Mohammad H. Haque, Aramco Services Company, Nancy A. Burnham, Worcester Polytechnic Institute

9:00  Break
10:50  26 Atomic Force Microscopy and Nano-IR Characterization of Composites, William Haseltine, Solvay

Monitoring Water Pollution to Prevent Future Flints
Chair: Satinder Ahuja, Ahuja Consulting

9:00  27 Learned from the Flint Water Crisis: Communicating Science and Influencing Public Discourse Using Science, Christina Devine, Ni Zhu, Virginia Tech
9:30  28 Combined Effects of Increased Temperature and Endocrine Disrupting Pollutants on Sex Determination, Survival, and Development across Generations, Bethany DeCourten, Susanne M. Brander, University of North Carolina-Wilmington

9:00  Break
10:20  29 Coal Use as a Cause of Water Quality Impairment, Larry Cahoon, University of North Carolina-Wilmington
10:50  30 Waste to Wealth: Sustainable Advancement in Greener Analytical Pathways for Remediation of Metal Contaminated Waste-Water, Rakesh K. Sharma, University of Delhi

Funding Analytical Research in Challenging Times: NSF and Beyond
Chairs: Sharon Neal, University of Delaware, Kelsey D. Cook, National Science Foundation

9:00  31 Opportunities and Suggestions for Securing NSF Funding, Lin He, Michelle Bushey, Kelsey D. Cook, National Science Foundation
9:20  32 The NSF Proposal Review Process – An Inside/Outside Perspective, Zeev Rosenzweig, University of Maryland-Baltimore County
9:40  33 The National Science Foundation Merit Review Criteria & Programs that Support Chemistry Education, Dawn Rickey, National Science Foundation

9:00  Break
10:20  34 Interpreting and Writing Reviews, Lisa A. Holland, West Virginia University
10:40  35 Fostering Collaborations in Times of Budget Uncertainties: A NIST Perspective, Carlos A. Gonzalez, National Institute of Science & Technology
11:00  36 Panel Discussion

New Frontiers in Solid Analysis Spectroscopy
Chair: Lydia Breckenridge, Bristol-Myers Squibb

9:00  37 LIBS and XRF: Complimentary Solid-State Analysis Techniques in the Pharmaceutical Lab, Sharla Wood, Lydia Breckenridge, Nancy Lewen, Bristol-Myers Squibb
9:30  38 Ultrafast Magic Angle Spinning NMR of Small Molecule and Peptide Therapeutics, Yongchao Su, Xingyu Lu, Merck & Co.

9:00  Break
10:20  39 LIBS and LA-ICP-MS for Forensic Anthropology, Mauro Martinez, Matthieu Baudelet, University of Central Florida
10:50  40 New Ionization Processes in Mass Spectrometry Provide Missing Link between ESI and MALDI, Experimentally and Fundamentally, Sarah Trimpin, Wayne State University

Monday Poster Session: PROTEIN & PEPTIDE ANALYSIS

12:00-2:00  41 Improvement in Resolution and Throughput on Size Exclusion Chromatography Analysis for Monoclonal Antibodies by Using a 2 Micron Diol Column, Ernest J. Sobkow, YMC America
12:00-2:00  42 Reduce Peptide Fibrillation Risk by Flow Chemistry, Allison Green, Hao Luo, François Lévesque, Bangping Xiang, Ping Zhuang, John Naber, Merck & Co.
12:00-2:00  43 Structural Characterization of Biologics by 2D-UHPLC-High Resolution Tandem Mass Spectrometry, Yun Wang, Richard Huang, Ekaterina Deyanova, Yuan Cheng, Pradhyot Nandi, Paul Stetsko, Stephen Carl, Olafur Gudmundsson, Guodong Chen, Bristol-Myers Squibb
Monday Poster Session: ADVANCES WITH MASS SPECTROMETRY

12:00-2:00  44 Influencing the Selectivity of Small Proteins and Peptides on the Raptor™ ARC-18, Thi Do, Restek Corp.
12:00-2:00  45 Prediction of Long Term Peptide Chemical Stability, Jameson R. Bothe, Yuhang Jiang, Yogita Krishnamachari, Paul Walsh, John Lena, Claudia Neri, Merck & Co.
12:00-2:00  46 Composition Determination of Copolymer of Vinylpyrrolidone (VP) and Poly(ethylene glycol) Methacrylate (PEG-MA): A New Technique for “Gentle” Whitening, Zheng Li, Ashland
12:00-2:00  47 Rapid Characterization of Insulin Modifications and Sequence Variations by Proteinase K Digestion and UHPLC-ESI-MS, Rong-Sheng Yang, Weijuan Tang, Huaming Sheng, Fanyu Meng, Merck & Co.
12:00-2:00  48 Expanding the Analytical Toolbox for Protein Aggregation Studies, Nicole M. Schiavone, Erik Guetschow, Alexey Makarov, Merck & Co.
12:00-2:00  49 Protein Purification and Reconstitution of Biological Clock in Test Tube to Determine Robustness, Manpreet Kaur, Yong I. Kim, New Jersey Institute of Technology
12:00-2:00  50 Development of a Platform for Peptide Stability Assessment on Solid Substrates, Margaret Roeder, Jameson Bothe, Yash Kapoor, Paul Walsh, Justin Pennington, Merck & Co.

Monday Poster Session: GREEN ANALYSIS

12:00-2:00  51 Towards a Simultaneous Elemental and Molecular Chemical Imaging Platform via a Combination of Optical and Mass Spectrometries, Jacob T. Shelley, Sunil P. Badal, Montwaun D. Young, Jessica R. Hellinger, Rensselaer Polytechnic Institute
12:00-2:00  52 Direct, Sensitive Detection of a Broad Range of Analytes from Surfaces with Flowing Atmospheric Pressure Afterflow (FAPA) Mass Spectrometry, Sunil P. Badal, Montwaun D. Young, Jessica R. Hellinger, Jacob T. Shelley, Rensselaer Polytechnic Institute
12:00-2:00  53 Using Optimization Algorithms to Determine Isotope Ratios from Tandem Mass Spectrometry, William Simon, Princeton University
12:00-2:00  54 Fragmentation Mechanisms of Protonated Benzoic Acid and Related Compounds: Competitive Generation of Protonated Carbon Dioxide or Protonated Benzene, Sihang Xu, Athula Attygalle, Julius Pavlov, Stevens Institute of Technology
12:00-2:00  55 Analysis of Products from the Liquid Phase Reaction of Cinnamaldehyde with Pd/C in the Presence of Lewis Acid Salts, Amanda B. Childs, Lindsey A. Weich, Cedar Crest College
12:00-2:00  56 Benefits of ICP-MS with 10 Times Higher Sensitivity and 1/2 of Argon Consumption, Iouri Kalinitchenko, Oliver Buettel, Analytik Jena US

Monday Poster Session: NUCLEAR MAGNETIC RESONANCE

12:00-2:00  57 Metals Impurities: Efficient USP 232 Quantification, Thomas Rettberg, Vikas Padhye, LGC Standards
12:00-2:00  58 Acid Number of Crude Oils and Petroleum Products by Catalytic Thermometric Titration Using ASTM D8045, Lori Spafford, Metrom
12:00-2:00  59 The Development of a High-Throughput UHPLC Method for Determination of the Emitted Dose Uniformity (EDU) and Aerodynamic Particle Size Distribution (APSD) by Andersen Cascade Impaction (ACI) for Dry Powder Inhaler (DPI), Jagruti A. Patel, Josephine Bermudez, Merck & Co.
12:00-2:00  60 Withdrawn by the author.
12:00-2:00  61 Sustainable Imaging Technology for Thermal Printing, Terri Powell, Brian Einsla, John Roper, The Dow Chemical Company
12:00-2:00  62 How Not To Do It: (Mis)Adventures in Developing an Environmentally Freezing Point Depression Experiment, Jacob M. Newman, Touro College - Lander College for Men

Monday Poster Session: HPLC TECHNIQUES

12:00-2:00  63 Spin-Lattice Relaxation of Pharmaceutical Polymorphs by High-Resolution Solid-State NMR, Robbie J. Iuliucci, Washington and Jefferson College, Brooke Liningar, Sarah Stuchell, Jordan Hosfelt, Rosalynn Quijones-Fernández, Deben Shoup, Gracey Behnke, Taylor Maddox, Marshall University
12:00-2:00  64 Chemometric Application Development for Benchtop Permanent Magnet NMR Systems Operating at 42, 60, and 80 MHz – Demonstration of Equivalency with Supercon 300 MHz NMR, John C. Edwards, Process NMR Associates
12:00-2:00  65 1H qNMR Analysis of Alcoholic Beverages - Detailed Chemical Fingerprint Information for Quality Control and Process Understanding, John C. Edwards, Process NMR Associates
12:00-2:00  66 Polymer Analysis Applications of Thermo Fisher Scientific picoSpin NMR Spectrometers, Daniel Frasco, Thermo Fisher Scientific

Monday Poster Session: HILIC

12:00-2:00  67 Affecting Selectivity and HILIC Retention on a FluoroPhenyl Stationary Phase, Shane Stevens, Restek Corp.
12:00-2:00  68 Unique Chirally Modified Carbohydrate Based Chiral Stationary Phases to Improve Chiral Separations, Matthew Przybycie, David Kohler, ES Industries
12:00-2:00  69 A Guide for HPLC Troubleshooting: How to Diagnose and Solve Chromatographic Problems, Imad Haidar Ahmad, He Yu, Hao Luo, Ping Zhuang, Merck & Co.
Monday Afternoon, November 13, 2017

EAS Award for Outstanding Achievements in the Fields of Analytical Chemistry
Honoring Janusz Pawliszyn, University of Waterloo
Sponsored by Bristol-Myers Squibb
Chair: Nicholas H. Snow, Seton Hall University

2:00  73 Growing Up with SPME, Nicholas H. Snow, Seton Hall University
2:30  74 Providing Rugged Methodology for Regulated Industries, Mary Ellen P. McNally, Stephen J. Platz, DuPont Crop Protection
3:00  Break
3:20  75 Whole-Column Imaged Capillary Isoelectric Focusing (cIEF): From Academic Idea to Industrial Gold Standard, Jiaqi Wu, Protein Simple
3:50  76 Medical and Pharmaceutical Applications of Solid Phase Microextraction, Barbara Bolko, Nicolaus Copernicus University
4:30  Break
4:35  77 Plenary Lecture “Think Big but Design Small, a Path to Modern Analytical Chemistry” by Janusz Pawliszyn, University of Waterloo

Ultrasensitive Spectroscopy, organized by NY/NJ SAS
Chair: Gene S. Hall, Rutgers University

2:00  78 Engineering Plasmonic Nanostructures for Ultrasensitive SERS Applications, Laura Fabris, Supriya Atta, Ted V. Tsoulos, Manjari Bhamidipati, Rutgers University
2:30  79 From Research to Routine: Surface-Enhanced Raman Spectroscopy as a Practical Tool in Art Analysis, Marco Leona, Metropolitan Museum of Art
3:00  Break
3:20  80 The Resonance Raman Spectra of Salmon Oil, Fran Adar, Horiba Instruments, Gene S. Hall, Rutgers University

3:50  81 The Raman Spectra of Cis and Trans Fatty Acids, Gene S. Hall, Rutgers University, Fran Adar, Horiba Instruments

Forensic Microscopy XI “What is it? Who does it?”, sponsored by the New York Microscopical Society
Chair: Thomas Kubic, John Jay College

2:00  82 Forensic Science and the Amazing Multicolor Fur Coat: Microscopy of Dyed Beaver Hair, Michelle D. Miranda, Farmingdale State College
2:30  83 Microscopic Changes in Markings Made by a Tavor Rifle, Peter Dierczuk, Pennsylvania State University, Andrew J. Winter, Centenary University
3:00  Break
3:20  84 Forensic Analysis of Blue Glass Chips by Microspectroscopy and X-Ray Spectroscopy, Tiffany J. Millet, Graduate Center - City University of New York, Mircea Comenescu, John Jay College
3:50  85 The Microscopic and Spectroscopic Analysis of Organic Gunshot Residues and Explosives, Jennifer Leonard, Graduate Center - City University of New York

Solid-State NMR of Natural Products: Life without Labels
Chair: Yongchao Su, Merck & Co.

2:00  86 Quantitative and Selective 13C NMR for Determining the Composition of Wood and Cork, Klaus Schmidt-Rohr, Pu Duan, Xiaoyan Cao, Brandeis University
2:30  87 Electron Decoupling with Frequency Agile Gyrotrons and Fluorescent Polarizing Agents for DNP in Human Cells, Alexander Barnes, Washington University-St. Louis
3:00  Break
3:20  88 Multinuclear Quantitative Solid-state NMR of Crystalline and Disordered Pharmaceutical Solids, Joe Lubach, Genentech
3:50  89 Solid-State NMR Crystallography of Pharmaceuticals Utilizing Proton-Detected and Multidimensional Techniques, Xingyu Lu, Chengbin Huang, David Hesk, Anthony Leone, R. Thomas Williamson, Wei Xu, Yongchao Su, Merck & Co.

Advancements in Chromatography & Electrophoresis
Chair: Joe P. Foley, Drexel University

2:00  90 Peak Capacity and Peak Capacity per Unit Time in Capillary and Microchip Electrophoresis, Joe P. Foley, Donna M. Blackney, Erin J. Ennis, Drexel University
2:20  91 Spiral Design Rotors: A Significant Advance in Countercurrent Chromatography, Martha Knight, Rodrigo A. Lazo-Portugal, CC Biotech LLC
2:40  92 Experimental Evaluation of Microfluidic LC Column Performance: Straight vs. Serpentine Channels, Martin Gilar, Thomas S. McDonald, Fabrice Gritti, Waters, Inc.
2017 EAS Final Program

3:00 Break


3:40 94 Evaluating Surfactants Using Potentiometric Titration, Kerri-Ann Blake, Metrohm USA

Monitoring Pollution and Climate Change, organized by The Coblentz Society
Chair: Brandye Smith-Goettler, Merck & Co.

2:00 95 Modeling the Transformation of Inorganic Environmental Pollutants into Microalgal Biomass, Frank Vogt, Mohammed F. Hasan, University of Tennessee

2:30 96 Exploring the Multidimensionality of High-Resolution Photoluminescence Spectroscopy for the Analysis of Organic Pollutants in the Gulf of Mexico, Andres Campiglio, University of Central Florida

3:00 Break

3:20 97 Optical Characterization of Individual Aerosol Particles for Defense and Environmental Monitoring, Vasanthi Sivaprakasam, Naval Research Laboratory

3:50 98 Panel Discussion

Analytical Challenges in Assessment of Drug Formulation Performance and In-Vitro Drug Release
Chair: Xujin Lu, Bristol- Myers Squibb

2:00 99 Dissolution Testing from Biorelevant to Quality Control - Challenges and Gaps, Jian-Hwa Han, Abbvie

2:30 100 Linking Dissolution Method Development and Clinical Relevance – When is a Method Appropriately Discriminating?, Andre Hermans, Merck & Co.

3:00 Break

3:20 101 Using In-Vitro Dissolution to Support Post Approval Changes - Global Regulatory Expectations, Xin (Amy) Bu, Bristol-Myers Squibb

3:50 102 Approaches to the Development of Biorelevant and QC Dissolution Methods, Michael D. Likar, Ling Zhang, Pfizer

Increasing High-Throughput: Sample Preparation to Engineering
Chair: Mary Lynn Grayeski, Marywood University

2:00 103 Automated Forced Degradation Screening for Genotoxic Risk Assessment of Small Molecule Pharmaceutical Candidates, Kaitlin M. Grinias, John Campbell, Kenneth Wells, GlaxoSmithKline

2:20 104 Mitigating Risk for Oral Solid Dosage (OSD) Extraction Using Design of Experiment (DoE) to Define an Alternate Homogenization Sample Preparation Process, Adriene Malsbury, Khanh Ha, Jeff Dai, William Fish, Bristol-Myers Squibb


3:00 Break


4:00 108 SPE is LC: Using Automation and Chromatographic Principles to Achieve High Performance SPE (SmartSPE), Mark Hayward, Kim Gamble, ITSP Solutions, Jonathan Ho, Tom Moran, Shimadzu

Tuesday Morning, November 14, 2017

EAS Award for Outstanding Achievements in Separation Sciences
Honoring Christopher J. Welch, Welch Innovation, LLC
Sponsored by Agilent Technologies
Chair: Mirlinda Biba, Merck & Co.

9:00 109 The Practice and Consequences of Ultrafast LC and SFC, Daniel Armstrong, University of Texas-Arlington

9:30 110 High-Speed Enantioselective Chromatography as the Second Dimension in Multiple Heart-Cutting and Comprehensive 2D-RPLC Analysis, Erik L. Regalado, Merck & Co., Chandan L. Barhate, Daniel Armstrong, University of Texas - Arlington, Christopher J. Welch, Welch Innovation, LLC

10:00 Break

10:20 111 Innovative Approaches in High-Throughput Chromatographic Analysis in Support of Pharmaceutical Development Research, Kerstin Zawatzky, Merck & Co., Christopher J. Welch, Welch Innovation, LLC

10:50 Presentation of the EAS Award for Outstanding Achievements in Separation Sciences

10:55 112 Pharmaceuticals, Separations and Separation Science, Christopher J. Welch, Welch Innovation, LLC

American Microchemical Society Benedetti-Pichler Award
Honoring Somenath Mitra, NJ Institute of Technology
Session Chair: Robert Vetrecin

9:00 113 Approaches to Modify Silica Particles for HPLC, Luis A. Colón, Joseph R. Ezzo, Amaris C. Borges-Muñoz, Josmely Vélez-González, University at Buffalo, The State University of New York


10:00 Break
10:20  115 Microfluidic High-Throughput Screening Consumables that Leverage Existing Laboratory Tools, Vincent T. Remcho, Oregon State University

10:50  116 Carbon Nanotube Based Chromatography, Sample Preparation and Membrane Separations, Somenath Mitra, NJ Institute of Technology

Research from our Emerging Forensic Scientists, sponsored by NJ Association of Forensic Scientists
Chair: Monica Joshi, West Chester University

9:00  117 Determination of Gunshot Residue Settling Velocity, Cassidy Schultheis, Stephanie Wetzel, Duquesne University, Allison Laneve, Stephanie Horner, RJ Lee Group


10:00 Break

10:20  119 Evaluation and Preservation of Urine in Forensic Toxicology, Meaghan M. Ringel, Arcadia University, Karen S. Scott, Shanan S. Tobe, Gail A.A. Cooper, Office of the Chief Medical Examiner

10:50  120 Using SPME-GC/MS to Detect Volatile Compounds Remaining from the Storage of Dead Mice, Angelica D. Wilz, Thomas A. Brettell, Thomas Pritchett, Cedar Crest College

11:20  121 Application of Gold and Silica Nanoparticles for Explosives Detection, Alexandra P. Sterner, Monica Joshi, Gaea Lawton, West Chester University

Integrating Solid State NMR Experiment and Prediction
Chair: Dewey Barich, GlaxoSmithKline

9:00  122 Characterization of Solid Pharmaceutical Compounds and their Dosage Forms Using Solid-State NMR of Quadrupolar Nuclei and Plane-Wave DFT Calculations, Robert Schurko, David A. Hirsh, Sean T. Holmes, Austin A. Peach, University of Windsor

9:30  123 Multinuclear Solid-State NMR Investigation of Atorvastatin Calcium, Steve Bai, Sean T. Holmes, University of Delaware

10:00 Break


10:50  125 Developing Accurate Crystallography without Diffraction, James Harper, University of Central Florida

Transforming Multivariate Data into Knowledge
Chair: Suzanne Schreyer, Rigaku Analytical Devices

9:00  126 Root Cause Investigation of Contaminants in Raw Materials and Active Pharmaceutical Ingredients, Olga Laskina, Kathryn Lee, Oliver Valet, Markus Lankers, rap.iD Inc.

9:20  127 In-Vivo, Glucose Detection using Mid-Infrared Laser Spectroscopy and Multivariate Analysis, Alexandra Werth, Sabbir Liakat, Claire Gmachl, Princeton University

9:40  128 Integrating Instrument Standardization Methods into Data Preprocessing Schemes, Barry M. Wise, Robert T. Roginski, Benjamin Kehimkar, Eigenvector Research

10:00 Break

10:20  129 Applications of FT-NIR in Hot Melt Extrusion Process Monitoring, Herman He, Scott Martin, Thermo Fisher Scientific, Anh Vo, Jiaxiang Zhang, Michael Repka, University of Mississippi

10:40  130 Validation of ATR Correction and Reverse ATR Correction Algorithms, Improved by Optimized Corrections, Gregory M. Banik, Michelle Dsouza, Keith Kunitsky, Robin O’Connor, Bio-Rad Laboratories

11:00  131 CLS & PCR Analysis of Liquids, Elucidating the Connection between Physics and Chemometrics, Howard Mark, Mark Electronics

Innovative Analytical Approaches in Biotechnology
Chair: Dil Ramanathan, Kean University

9:00  132 Quantification of Oleic Acid in Biologics Solutions Enables Early Detection of Host Cell Protein Mediated Polysorbate 80 Degradation, Meng Xu, Zhihua Liu, Dilusha Dalpathado, Joseph Valente, Mark Bolgar, Bristol-Myers Squibb

9:20  133 Effective Determination of Pharmaceutical Impurities by Two-Dimensional Liquid Chromatography (2D-LC), Chris Desjardins, Zhimin Li, Paula Hong, Patricia McConville, Waters, Inc.

9:40  134 Sol-Gel Capillary Microextraction with Niobia-, Antarla-, and Zirconia-based Sorbents Providing Selective Enrichment of Phosphopeptides and Neurotransmitters for Online HPLC Analysis, Abdul Malik, Sheshanka Kesani, MinhPhuong Tran, Abdullah Alhendal, Mohanraja Kumar, University of South Florida

10:00 Break


11:00  137  Fast Isotope Ratio Mass Spectrometry (FIRMS): A Tandem Mass Spectrometry Technique for the Rapid and Semi-Comprehensive Evaluation of Isotope Ratios, Fredrick M. Ochieng, Brian A. Logue, South Dakota State University, Paul J. Hinker, South Dakota School of Mines and Technology


Spectroscopy for Counterfeit Detection, organized by The Coblentz Society
Chair: Brandye Smith-Goettler, Merck & Co.

9:00  139  Chemometric Approach to Purity Analysis and Quality Assurance of Pure and Adulterated Natural and Essential Oils, Sayo O. Fakayode, University of Arkansas-Fort Smith, Brianda Elzey, North Carolina Agricultural & Technical State University, David Pollard, Winston-Salem State University, Carol M. Babyak, Appalachian State University

9:30  140  Field-Deployable Applications of Raman Spectroscopy for Screening of Unapproved and Counterfeit Drugs, Jason D. Rodriguez, United States Food & Drug Administration

10:00  Break

10:20  141  Portable Raman Spectroscopy for Rapid Identification of Unknown Precious Gemstones, Kristen A. Franq, Dawn Yang, B&W Tek

10:50  142  Biotherapeutics Counterfeit Determination, Ishan Barman, John Hopkins University

Modern Advances in Gas Chromatography
Chair: James Stuart, University of Connecticut

9:00  143  Study of VOC Exposure at Fuel Stations with a Portable GC System, Anika Poli, Douglas R. Adkins, Patrick R. Lewis, Defiant Technologies

9:20  144  High-Throughput Implementation of Gas Chromatography with Automated Sample Preparation and Universal Carbon Response Calibration, Marcelo Figueira, Reetam Chakrabarti, Marie Devlin, The Dow Chemical Company

9:40  145  Fast Gas Chromatography of Residual Solvents in Pharmaceutical Excipients Using a Novel Vacuum Ultraviolet Spectroscopy Detector, Lindsey Shear-Laude, Jack Cochran, VUV Analytics

10:00  Break


10:40  147  Guidelines on Selecting, Determining, and Interpreting Analytical Detection Limits, Ephraim M. Govere, Pennsylvania State University

Vibration Science and Technology in Cultural Heritage I, organized by the New York Conservation Foundation
Chair: Andrew Lins, (retired) Philadelphia Museum of Art

9:00  148  Considerations of the Potential for Damage to Individual Works of Art caused by Vibration during Construction/Demolition Projects, Andrew Lins, (retired) Philadelphia Museum of Art

9:30  149  A Blueprint for Managing Construction Vibration Risk Near Sensitive Structures, Douglas Rudenko, Mohammad Sharifinassab, Vibra-Tech Engineers

10:00  Break

10:20  150  Vibration Risk Assessment for Immovable Artworks in Churches during a Tunneling Work, Anna Henningsson, Disent AB

10:50  151  Vibration Protocols to Protect Museum Collections during Major Demolition Works: Experiences from Liverpool’s Library Project, Siobhan Watts, UK National Trust, David Crombie, Tracey Seddon, National Museums Liverpool

Tuesday Poster Session: GRADUATE STUDENT AWARDS, sponsored by Merck & Co.

12:00-2:00  152  Infrared Spectroscopy Based Approach to Assess Metabolic Profile and Damage in Cardiac Tissue, Saumya Tiwari, Rohit Bhargava, University of Illinois at Urbana-Champaign, Jai Raman, Oregon Health and Science University

12:00-2:00  153  A Quantitative Mass Spectrometry Imaging Workflow Using IR-MALDESI and MSIReader, Mark T. Bokhart, Ken Garrard, David C. Muddiman, North Carolina State University, Elias Rosen, Corbin Thompson, Craig Sykes, Angela DM Kashuba, University of North Carolina-Chapel Hill, Jeffrey Manni, JGM Associates

12:00-2:00  154  An Integrated Platform of Three LC-MS-MS Methods for the Quantification of Urinary Metabolites Differentially Expressed in Respiratory Illnesses, Mona M. Hamada (Khamis), Hanan Awad, Kevin Allen, Darryl J. Adamko, Anas El-Aneed, University of Saskatchewan

12:00-2:00  155  A Sweet Promise from Solid-State Nanopores: Polysaccharide-Sugar Analysis Challenge, Buddini Iroshika Karawdeniya, Y.M. Nuwan D.Y. Bandara, Jonathan W. Nichols, Robert B. Chevalier, Jason R. Dwyer, University of Rhode Island

Tuesday Poster Session: UNDERGRADUATE STUDENT AWARDS, sponsored by Merck & Co.

12:00-2:00  156  Investigation of Photoanodic Water Oxidation Surface Species on Hematite Using SI-SECM, Mihail R. Krumov, Burton H. Simpson, Joaquin Rodriguez-Lopez, University of Illinois at Urbana-Champaign
12:00-2:00  Efficient Method for the Identification of Common Herbicides in Rain Water and from Air Filters by UPLC-MS/MS, Steven L. Kolakowski, James D. Stuart, Christopher R. Perkins, Anthony A. Provatas, University of Connecticut

12:00-2:00  Comparison of GC Column Conditions Using the Mahalanobis Distance, Alexandra Clifford, Edward J. Soares, Amber M. Hupp, The College of the Holy Cross

12:00-2:00  Electrochemical Characteristics of a Class of Pyrenequinones, Rebecca Kubena, Luxi Shen, Héctor D. Abruna, Cornell University

Tuesday Poster Session: HPLC APPLICATIONS

12:00-2:00  Analysis of Plasma Free Metanephrine, Normetanephrine, and 3-Methoxytyramine by Hydrophilic Interaction Liquid Chromatography, Connor Flannery, Restek Corp.

12:00-2:00  Automated Online Desorption and Analysis of DNP Derivatives of Airborne Aldehydes and Ketones Using a New Robotic Autosampler, Fred D. Foster, Jackie Whitecavage, Kurt Thaxton, John Staff, GERSTEL

12:00-2:00  Method Development on a Combined Reverse Phase and SFC HPLC System, Peter C. Ratsep, John R. D’Alessio, Shimadzu Scientific Instruments

12:00-2:00  Resolving the Issues in Challenging Analysis of a Compound without a Chromophore and a Compound with a Reactive Primary Amino Group, Van Truong, Hao Luo, Bing Ma, Merck & Co.

12:00-2:00  Analysis and Derivatization of Water-Sensitive Activated Carboxylic Acids Using Reversed-Phase Liquid Chromatography, Maor F. Baruch, Michael Puppolo, James Choi, Niharika Chaganti, Chen Zhou, Hovione

Tuesday Poster Session: MASS SPECTROMETRY Biotransformations

12:00-2:00  LC-MS Method Development for the Detection of Phosphate Lipids, Junling Gao, Pei Huo, Wendy Zhao, Yan Lin, Merck & Co.

12:00-2:00  Simultaneous Determination of M12 and M17, Unique Human Metabolites of a BTK Inhibitor (BMS-896142) Using LC-MS-MS: Assay Development, Qualification, and Case Studies, Yulia A. Kim, Ang Liu, Jian Wang, Weiping Zhao, Ihab Girgis, Wenyi Li, Bristol-Myers Squibb

12:00-2:00  Rapid and Sensitive Quantification of Desmosine in Body Fluids Using Stable-Isotope Labeling and MALDI-MS2, Prateek Kumar N. Rathod, Manjeet Kaur, Hsin-Pin Ho, Marissa Louis, Kevin J. Mark, Jong-Il Lee, Emmanuel Chang, York College-City University of New York Graduate Center, Basant Dhital, Gregory Boutis, Brooklyn College -City University of New York Graduate Center

12:00-2:00  Mass Spec Profiling and Antimicrobial Efficacy of Asparagus Officialis, Bombax Malabarica and Moringa Oleifera Plant Extracts, Lindsey Bodnar, John Mikhail, Yassel Hernandez, Rachana Bhatt, Anima Ghosal, Dil Ramanathan, Kean University

Tuesday Poster Session: PHARMACEUTICAL FORMULATIONs

12:00-2:00  Analytical Validation, Separation and Stability Study of Multi Compound Formulations – Challenges and Approach, Shiladitya Sen, Charles River Laboratories

12:00-2:00  Sensitive UV-HPLC Method for the Analysis of the Docusate and Related Compounds, Michael Breslav, Rajesh Darji, Gail Reed, Johnson & Johnson Consumer Inc.

12:00-2:00  Data Integrity for Analytical Instrument Benchtops, Leticia Quinones, George Bouziotis, Robert Falana, Robert Reba, Bristol-Myers Squibb
2017 EAS Final Program

Tuesday Afternoon, November 14, 2017

EAS Award for Outstanding Achievements in Chemometrics Honoring Barry Lavine, Oklahoma State University
Sponsored by Eigenvector Research
Chair: Steven Brown, University of Delaware

Emerging Frontiers in High-Throughput Analysis for Process Research & Development
Chair: Wes Schafer, Merck & Co.

12:00-2:00  178 Finding the Solution to Analytical Sample Preparation: An Automation Story, Alexandra Andrews, Margaret Roeder, Edward Mularz, Jameson Bothe, Elizabeth Pierson, Merck & Co.

12:00-2:00  179 Analysis of the Moisture Content in Lyophilized Proteins by Near-Infrared Spectroscopy, Ewa Kowalczyk, Seton Hall University, Mary Krause, Ming Huang, Robert Wethman, John Wasylyk, Bristol-Myers Squibb

12:00-2:00  180 Applying USP 921 to your Moisture Determination Lab and Karl Fischer Titrations, Bruce Herzig, MilliporeSigma

12:00-2:00  181 Development and Implementation of Novel Automated Micro-Titration Instrument for Physical Characterization in Early Stage of Pharmaceutical Development, Steve Wang, Merck & Co.

12:00-2:00  182 The 48 Siblings of Ibuprofen, Jens Boertz, Omar Mneimne, LGC Standards

3:00  189 Asymmetric Reaction Screening with Chiroptical Sensors, Christian Wolf, Georgetown University

3:30  190 Enabling Modern Catalysis in Drug Discovery and Development with High-Throughput Experimentation Chemistry and (Ultra!) Fast Analysis, Spencer Dreher, Merck & Co.

Breaking Bad Chemistry: The Forensic Response to Clandestine Labs
Chair: Thomas Blackwell, US Drug Enforcement Administration

2:00  191 Clandestine Labs: A Walk Though Time, James DiSamo, Edward J. Kovacs III, US Drug Enforcement Administration

2:30  192 Investigating One Pot Methamphetamine Clandestine Laboratories, Jarrad Wagner, Oklahoma State University

3:00  193 Break

3:20  194 Laboratory Analysis of Clandestine Labs, Noel Vadell, US Drug Enforcement Administration

NMR Analysis of Complex Systems: Computer Assisted Analysis and Pulse Sequence Development
Chair: Gary E. Martin, Merck & Co.

2:00  195 Unequivocal Determination of Complex Molecular Structures with Anisotropic NMR Measurements, Yizhou Liu, Josep Sauri, Gary E. Martin, R. Thomas Williamson, Merck & Co., Emily Mevers, Jon Clardy, Harvard University, Mark W. Peczuh, University of Connecticut, Henk Hiemstra, University of Amsterdam

2:30  196 Towards Unbiased and more Efficient NMR Based Structure Elucidation: A Powerful Combination of CASE Algorithms and DFT Calculations, Alexei V. Buevich, Merck & Co., Mikhail E. Elyashberg, Advanced Chemistry Development


3:00  198 Discovery of Unique Hydrogen Bonding Motif in Nucleosides Leads to a Novel Protecting-Group Free Selective 3’ Nucleoside Functionalization Chemistry, Mikhail Reibarkh, Merck & Co.

**Surface Science and Spectroscopy**  
Chair: Andrew Teplyakov, University of Delaware

2:00 201 Recent Advances in Raman Microscopy for Pharmaceutical and Life Science Applications, Alexander Rzhevskii, Thermo Fisher Scientific

2:20 202 Applications of Nanoscale IR Spectroscopy and Imaging in Pharmaceutical Science, Curtis Marcott, Light Light Solutions, Eoghan Dillon, Kevin Kjoller, Craig Prater, Ansasys Instruments

2:40 203 Confocal Raman Microscopy Characterization of Waterborne Coatings, Dana Garcia, Wenjun Wu, Arkema Inc.

3:00 Break

3:20 204 Mapping the Surface Concentration of Coatings on Metal and Glass Surfaces using FTIR Reflectance Spectroscopy, Mary Thomson, Peter Melling, Resmspec Corp., Robert Kertayasa, Rolink LLC

3:40 205 Probing Nanoscale Hydrophobicity and Chemical Distribution of Surface Modified Polyethersulfone (PES) Membranes, Wanyi Fu, Wen Zhang, New Jersey Institute of Technology

4:00 206 The Interactions between Amine-Rich Poly [oxo-norbornene]-Coated Gold Nanoparticles and Phospholipid Membranes, Zeev Rosenzweig, University of Maryland Baltimore County, Zheng Zheng, David Boschert, Karen Lienkamp, University of Freiburg, Bo Zhi, Christy L. Haynes, University of Minnesota

4:20 207 Sustainable Magnetically Retrievable Nanoadsorbents for Selective Removal of Pb2+ and Pd2+ Ions from Different Charged Wastewaters, Sripama Dutta, University of Delhi

**Applications Using Matrix Assisted Laser Desorption Ionization Mass Spectrometry**  
Chair: Barbara S. Larsen, DuPont

2:00 208 Fundamentals and Applications of Matrix-Assisted Ionization: Zero Energy Input Ionization, Charles N. McEwen, Khao Hoang, University of Sciences, Milan Pophristic, MSTM, LLC

2:30 209 Imaging Mass Spectrometry in Drug Development: Visualizing Tissue with a Molecular Lens, Reid Groseclose, GlaxoSmithKline

3:00 Break

3:20 210 Improving Quantitation through a Fundamental Understanding of the MALDI Sample Preparation Process, Kevin G. Owens, Drexel University

3:50 211 Industrial Applications of the Bruker™ MALDI-TOF Biotyper, Suzanne K. Singles, Barbara S. Larsen, DuPont Corporate Center for Analytical Sciences

---

**Performance Testing and Impurity Analysis of Pharmaceutical Products**  
Chair: Leonel Santos, United States Pharmacopeia

2:00 212 Analyzing Multi Component Dissolution Samples Using Chemometrics and In-Situ Fiber Optic UV Spectrophotometry, Andrew Kielt, Ishai Nir, Jeff Seely, Distek

2:20 213 Novel Instrument Solution for Content Uniformity Sample Preparation, Ishai Nir, Andrew Kielt, Jeff Seely, Distek

2:40 214 Use of Biphasic Dissolution to Improve Bioprediction for an Amorphous Low Solubility Crystallizer, Gregory Johnson, Wei Xu, Merck & Co.

3:00 Break

3:20 215 Development of Solution Based Certified Reference Materials for the Analysis of Pharmaceutical Impurities in Monograph Testing Methods, Uma Sreenivasan, Sarah Ajaz, Zoe Ruan, Maysa Bakir, Nicholas Hauser, Cerilliant Corporation - MilliporeSigma


---

**The Depth & Breath of Vibrational Spectroscopy**  
Chair: Jim Rydzak, Specere Consulting

2:00 218 See Through Barrier Using Raman Spectroscopy with Large Sampling Volume, Jun Zhao, Jack Zhou, Katherine Bakeev, B&W Tek

2:20 219 Using a New Horizontal Transmission Cell for FT-IR Characterization of Edible Oils, Gene S. Hall, Rutgers University

2:40 220 Reagent Free Near-Infrared (NIR) Spectroscopic Analysis of Moisture in Lyophilized Products, Kyle Hollister, Metrohm USA

3:00 Break


2017 EAS Final Program

Technical Program

Wednesday Morning, November 15, 2017

EAS Award for Outstanding Achievements in Mass Spectrometry
Honoring Scott McLuckey, Purdue University
Chair: Alice Pilo, Merck & Co.

9:00 228 Gas-Phase Ion/Ion Reactions: Oxidation and the Dehydroalanine Effect, Alice Pilo, Merck & Co., Zhou Peng, Scott McLuckey, Purdue University

9:30 229 Top-Down Proteomics for Clinical Assay Development, James Stephenson, Thermo Fisher Scientific

10:00 Break


10:50 Presentation of the EAS Award for Outstanding Achievements in Mass Spectrometry

10:55 231 Towards Selective Cleavage of Proteins: Progress towards Gas-Phase Enzymes, Scott McLuckey, Purdue University

EAS Young Investigator Award, Recent Advances in 2D-LC, Part 1: Fundamentals, Instrumentation, and Column Technology
Honoring Dwight Stoll, Gustavus Adolphus College
Sponsored by The Dow Chemical Company
Chair: William Barber, Chromatography Forum of Delaware Valley

9:00 Presentation of the EAS Young Investigator Award

9:05 232 Moving into the Mainstream – Reflections on Recent Developments in Two-Dimensional Liquid Chromatography, Dwight Stoll, Gustavus Adolphus College

9:30 233 Orthogonality Measurements for Multidimensional Chromatography in Three and Higher Dimensional Separations, Mark R. Schure, Kroungold Analytical, Joe M. Davis, Southern Illinois University - Carbondale

10:00 Break


The Cannabinoids Story - From Research, Medical Use, and Abuse, sponsored by NJ Association of Forensic Scientists
Chair: Michelle R. Peace, Virginia Commonwealth University

9:00 236 Turning Over a New Leaf: The Endogenous Cannabinoid System, Aron H. Lichtman, Virginia Commonwealth University

9:30 237 Unintended Consequences of Preclinical Cannabinoid Research: Emergence of Synthetic Cannabinoids, Aron H. Lichtman, Virginia Commonwealth University

10:00 Break

10:20 238 These Aren’t Your Grandfather’s Cannabinoids, Justin L. Poklis, Virginia Commonwealth University

10:50 239 Today’s Marijuana and Marijuana Products, Michelle R. Peace, Virginia Commonwealth University

NMR Spectroscopy of Unique Materials and Unusual Applications
Chair: Neil Jespersen, St. John’s University

9:00 240 Water Exchange Dynamics in Hollow Colloids Studied by Diffusion Nuclear Magnetic Resonance, Emilia V. Silletta, Theodore Hueckel, Stefano Sacanna, Alexej Jerschow, New York University


9:40 242 Dynamics and Solvation Structure of Lithium Ions in Li-Ion Battery Electrolyte, Mohaddese Mohammadi, Evgeny Nimerovsky, Alexej Jerschow, New York University

10:00 Break

### Quality Control of Pharmaceutical Products
**Chair: Jason Shen, Celgene**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00</td>
<td>Thermogravimetric Analysis of Dilute Aqueous Solutions, Charles Potter, TA Instruments</td>
</tr>
<tr>
<td>9:40</td>
<td>A Practical Approach of Determining the Cause of ICH Accelerated Stability Failure of Solid Dosage Formulations through Scientifically Designed Forced Degradation Studies and Selecting Optimum Packaging to Prevent Stability Failures, Alith S. Nair, Bilcare Research</td>
</tr>
<tr>
<td>10:00</td>
<td>Break</td>
</tr>
<tr>
<td>10:20</td>
<td>3-D Raman Imaging: A Method to Study the Effects of Lubrication on the Microstructure of Tablets, Shashwat Gupta, Savitha Panikar, Fernando Muzzio, Rutgers University</td>
</tr>
<tr>
<td>10:40</td>
<td>Ion Pairing Chiral Separation of Two Positively Charged Amphiphilic Diastereomeric Degradation Products in Tablet Formulation, Preeti Patel, Dawn Kou, Larry Wigman, Genentech</td>
</tr>
<tr>
<td>11:00</td>
<td>Proposed United States Pharmacopeia Validated Method for Analysis of Chlorpheniramine Maleate and Its Organic Impurities in Over the Counter Tablets and Extended Release Tablets Using Silica Hydride HPLC Columns, Joshua E. Young, Bill Ciccone, MicroSolv Technology Corporation, Richard B. Nguyen, United States Pharmacopeial Convention, Joseph J. Pesek, Maria T. Matyska, San Jose State University</td>
</tr>
</tbody>
</table>

### Challenges of Lifecycle Management for Method Validation
**Chairs: Kim Huynh-Ba, Pharmalytik and Karen Lucas, Janssen**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00</td>
<td>Lifecycle Management of Analytical Test Methods to Support OTC Products, David Mitchell, Johnson &amp; Johnson</td>
</tr>
<tr>
<td>10:00</td>
<td>Break</td>
</tr>
<tr>
<td>10:20</td>
<td>Lifecycle Management of Analytical Methods for Cleaning Verification Support, Mariann Neverovitch, Antonio Fernandez, Elizabeth Moroney, Bristol-Myers Squibb</td>
</tr>
<tr>
<td>10:50</td>
<td>Lifecycle Management: USP Perspectives, Gregory Martin, Complectors Consulting</td>
</tr>
</tbody>
</table>

### Vibrational Characteristics of Biologics
**Chairs: Anna Luczak, Varsha Ganesh, Bristol-Myers Squibb**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00</td>
<td>Resonance Raman Scattering in Cancer Tissue, Arterial Plaques, and Resonance Stimulated Raman Scattering in Carotene- Methanol Solution, Robert Alfano, City University of New York</td>
</tr>
<tr>
<td>9:30</td>
<td>Characterization of Therapeutical Protein Stability and Aggregation at High Concentration via Concomitant DLS and Raman Spectroscopy, Chen Zhou, Eli Lilly, John Carpenter. University of Colorado</td>
</tr>
<tr>
<td>10:00</td>
<td>Break</td>
</tr>
<tr>
<td>10:20</td>
<td>Applications of Drop Coat Deposition Confocal Raman Spectroscopy in BioPharmaceuticals, Ravikalyanaraman, Bristol-Myers Squibb</td>
</tr>
<tr>
<td>10:50</td>
<td>Ligand-Receptor Binding Investigated by Tip-Enhanced Raman Spectroscopy, Lily Xiao, Zachary Schultz, University of Notre Dame</td>
</tr>
<tr>
<td>11:20</td>
<td>Confocal Raman Microscopy Tracks Fluvenamic Acid Delivery Using Lipophilic versus Hydrophilic Penetration Enhancers, Qihong Zhang, Yelena Pyatski, Richard Mendelsohn, Carol R. Flach, Rutgers University-Newark</td>
</tr>
</tbody>
</table>

### Characterization and Control of mAb, Protein & Peptide Therapeutics
**Chair: Mike Hicks, Merck & Co.**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00</td>
<td>Capillary Nanogel Electrophoresis for Analyses of Proteins and Biological Therapeutics, Lisa A. Holland, Cassandra L. Crippenfield, Srikant Gattu, Lloyd Bwanali, West Virginia University</td>
</tr>
<tr>
<td>9:20</td>
<td>Fast, High Resolution Size Exclusion Chromatography of Monoclonal Antibodies (mAbs) and Antibody Drug Conjugates (ADCs), Stacy L. Shollenberger, Phu T. Duong, Atis Chakrabarti, Keegan Gike, Tosoh Bioscience</td>
</tr>
<tr>
<td>9:40</td>
<td>Determination of pH-Induced Oligomerization of a Lipidated Peptide by IMS-MS, Elizabeth E. Pierson, Nicholas A. Pierson, Justin P. Pennington, Merck &amp; Co.</td>
</tr>
<tr>
<td>10:00</td>
<td>Break</td>
</tr>
<tr>
<td>10:20</td>
<td>An Immuno-Analytical Separation Instrument for the Determination of Bioactive Peptides in Biosamples, Norberto Guzman, Princeton Biochemicals</td>
</tr>
<tr>
<td>10:40</td>
<td>Chemical Identification of Subvisible Particles in Protein-Based Formulations and Impact of Silicone Oil on the Protein Aggregation, Olga Laskina, Oliver Valet, Markus Lankers, rap.lD Inc.</td>
</tr>
<tr>
<td>11:00</td>
<td>Generation of Mouse and Rabbit Monoclonal Antibodies, Q. Julia Zhao, Bowen Bioscience</td>
</tr>
</tbody>
</table>

### Vibration Science and Technology in Cultural Heritage III, organized by the New York Conservation Foundation
**Chair: William Wei, Cultural Heritage Agency of the Netherlands**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00</td>
<td>Protecting a Cultural Icon: Moving the Liberty Bell with Minimal Vibration, Karie Diethorn, Independence National Historical Park</td>
</tr>
<tr>
<td>9:30</td>
<td>Strategy of Measurement and Data Analysis for the Monitoring during the Transport of Paintings, Matthias Läuchli, Nathalie Bäschin, Museum of Fine Arts Bern, Cornelius Palmbach, Bern University of the Arts</td>
</tr>
</tbody>
</table>
10:00  Break
10:20  267  Transport of Pastel Paintings: Fatigue Damage due to Vibrations, Leila Sauvage, Rijksmuseum
10:50  268  Conundra in Analysis of Damage Causation, John C. Scott, Conservator of Art and Architecture

Wednesday Poster Session: PHARMACEUTICAL API

12:00-2:00  269  Handheld LIBS for Pharmaceutical Raw Material Identification: Delivering Solutions that Maximize Value, Qun Li, Katherine A. Bakeev, Dan Liu, Jack Zhou, B&W Tek
12:00-2:00  270  Characterization on Non-Compendial Reference Standards for Impurities: How Good is Good Enough?, Christian Zeine, Omar Mneimne, LGC Standards
12:00-2:00  271  Considerations for Designing Stable Certified Reference Materials, Lesley S. Owens, Brian W. Alexander, Paul R. Gaines, Thomas J. Kozikowski, James A. King Jr., Inorganic Ventures
12:00-2:00  272  Identify Complicated Impurity Profiles in the Stability Indicated HPLC Method Development, Yan Wang, Apotex Pharmaceutical

Wednesday Poster Session: GAS CHROMATOGRAPHY

Bridge to Hotel
12:00-2:00  273  New GC Inlet Liner Deactivation Exhibits Excellent Response for Active Compounds, Cathy S. Hetrick, Linx Waclaski, Brian Jones, Mark Badger, Restek Corp.
12:00-2:00  274  Measurement of Polychlorinated Biphenyls in Serum by HRGC-ID-HRMS, Songyan Du, Norman Patterson, David Riker, New Jersey Department of Health
12:00-2:00  275  Improved Quantitation for EPA Method 8015C Diesel Range Organics, Tom J. Mancuso, Dawn May, Perkin Elmer
12:00-2:00  276  Flavors, Odors, and Contaminants in Alcoholic Beverages Using Vacuum Assisted Sorbent Extraction and GC-MS Analysis, Victoria L. Noad, Daniel B. Cardin, Entech Instruments
12:00-2:00  277  Improve the Precision of Headspace Gas Chromatography Method for Analytes with High Boiling Points Using Internal Standard, Antonio Oliveira, Merck & Co.

Wednesday Poster Session: SENSORS & SURFACE SCIENCE

12:00-2:00  278  Cyanalyzer: The Development of a Medical Laboratory Device for the Rapid Diagnosis of Cyanide Exposure, Brian A. Logue, Randy Jackson, South Dakota State University
12:00-2:00  279  Oxidoreductases Enhanced by Green Procedures. Applications to Biosensors, Eugene Kang, Uday-Kiran Bijja, Mihaela Leonida, Fairleigh Dickinson University
12:00-2:00  280  Controlling Surface Modification Through the Use of Mixed Azide-Terminated Self-Assembled Monolayers, Ruth M. Mandel, Mackenzie G. Williams, Andrew V. Teplyakov, University of Delaware
12:00-2:00  281  Photosensitized Lipid Peroxidation Accelerates Vesicle Rupture on SiO2 Surfaces: A QCM-D Study, Nathan J. Wittenberg, Ashley Baxter, Lehigh University
12:00-2:00  282  Fabrication and Modification of Silicon Nitride Based Nanopore and Optical Sensors, Y.M. Nuwan D. Y Bandara, Buddini Iroshika Karawdeniya, Julie C. Whelan, Jonathan W. Nichols, Robert B. Chevalier, Jason R. Dwyer, University of Rhode Island

Wednesday Poster Session: ENVIRONMENTAL ANALYSIS

12:00-2:00  283  A Simple, Fast, and Robust Analytical Method for the Determination of Ethylenethiourea in Mancozeb Technical and Formulation Products, Xiaoyan Wang, Frank J. Zawacki, FMC Corp.
12:00-2:00  284  Structural Characteristics of Unique Bacterial Poly(hydroxalkanoate) Biopolymers Derived from Cheap, Renewable Substrates Using NMR Techniques, Gary D. Strahan, Richard D. Ashby, Daniel K. Y. Solaiman, United States Drug Administration
12:00-2:00  285  Analysis of Polycyclic Aromatic Hydrocarbons in Avian Dry Blood Spots by Ultra-Performance Liquid Chromatography Utilizing Simple Liquid Extraction and Phospholipid Solid-Phase Extraction Preparation, Benjamin S. Reale, Andre Jang, Sreya Julakanti, James D. Stuart, Christopher R. Perkins, Anthony A. Provatas, University of Connecticut
12:00-2:00  286  Accelerated Solvent Extraction of Polycyclic Aromatic Hydrocarbons from Avian Bill Horns and Subsequent Analysis by UPLC-UV, Anthony A. Provatas, Alexander V. Yevdokimov, Son Nguyen, John Ciurylo, Eric Noi, James D. Stuart, Christopher R. Perkins, University of Connecticut
12:00-2:00  287  Quantitation of Pharmaceutical and Personal Care Products in Water Using a Laminar Flow Tandem Mass Spectrometer, Jamie S. Foss, Sharanya Reddy, PerkinElmer
12:00-2:00  288  Analysis and Identification of Ozone-Squalene Particulate Phase By-Products, Breeann Coffaro, Clifford Weisel, Rutgers University, Christine Ho, Bridgewater-Raritan High School
12:00-2:00  289  Real-Time Monitoring of Biodiesel Production with Compact NMR Spectroscopy, Bernhard Blümich, Kawarpal Singh, Sharoff Pon Kumar, RWTH Aachen University
Wednesday Poster Session: SPECTROSCOPY

12:00-2:00 290 Comparison of Singlet Oxygen Assay Performance in Isotropic and Microheterogeneous Solvents, Johanna Herman, Sharon Neal, University of Delaware

12:00-2:00 291 Dynamic Fluorescence Measurements of Rose Bengal Photooxidation, Yinan Zhang, Sharon L. Neal, University of Delaware

12:00-2:00 292 Detection of PPM Concentration of Iodate by UV Spectrophotometry, Eric D. Oliver, Thermo Fisher Scientific

12:00-2:00 293 UV/VIS and Fluorescence Studies on the Binding of Bovine and Human Serum Albumins with Novel Anticancer Drug Candidates, Angie Li, Karen Chen, Aireen Romu, Vijaya Korlipara, Enju Wang, St. John’s University

12:00-2:00 294 Spectroscopic Response of Novel Ru(II) Complexes to DNA and Other Polyanions, Madison Reimer, Chelsea McKain, Gregory Ostner, Armando Seitllari, Elise Megehee, Enju Wang, St. John’s University

12:00-2:00 295 Determining the Utility of Carbon-Fluorine Vibrational Frequencies as Local Structural Probes, Charvanaa Dhoonmoon, Casey H. Londergan, Haverford College

12:00-2:00 296 The Application of Far Infrared Microspectroscopy in the Analysis of Artists’ Pigments, Ronald Rubinovitz, Thermo Fisher Scientific, David W. Schiering, Anthony W. Didomenico, Czitek, Beth Price, Kate Duffy, Philadelphia Museum of Art

12:00-2:00 297 Chiral Process Monitoring Using Fourier Transform Molecular Rotational Resonance Spectroscopy, Justin L. Neill, BrightSpec, Luca Evangelisti, University of Bologna, Brooks H. Pate, University of Virginia, Yuan Yang, Frank Gupton, Virginia Commonwealth University

12:00-2:00 298 Conformity Analysis by FT-NIR: A Rapid Method for Non-Targeted Adulterant Screening and Overall Process Monitoring, Jason E. Erickson, Bruker Optics

12:00-2:00 299 Applications of Fourier Transform Molecular Resonance Rotational Spectroscopy (FT-MRR) in Residual Solvents Analysis, Shelby S. Fields, Justin L. Neill, Matthew T. Muckle, Roger Reynolds, BrightSpec

12:00-2:00 300 An Exploration of 2D-LC-SERS: A Novel Detection Modality for Multidimensional Chromatography, Melanie D. Davidson, Navya Kesavan, Christa L. Brosseau, Saint Mary’s University

Wednesday Afternoon, November 15, 2017

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

2:00 301 Fast Chiral Chromatography as the Second Dimension in 2-D HPLC, Christopher J. Welch, Welch Innovation, LLC


3:00 Break

3:20 303 Expanding the Biologics CMC Analytical Toolkit with Two Dimensional Liquid Chromatography, Douglas Richardson, Yuetsan Chen, Jun Heo, Bhumit Patel, Jayesh Desai, David Pollard, Merck & Co.

3:50 304 Application of Multidimensional Chromatography in Real World Pharmaceutical Analysis, C.J. Venkatraman, Mohammad Al-Sayah, Ila Patel, Larry Wigman, Jacob Kay, Meenakshi Goel, Genentech, Shu Rong Huang, University of Washington

Innovations and Applications in Mass Spectrometric Analysis, organized by the North Jersey Mass Spectrometry Discussion Group
Chair: Jim Shen, Bristol-Myers Squibb

2:00 305 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.


3:00 Break

3:20 307 Application of LC-HRMS in a Regulated CRO Laboratory, Lian Shan, Q2 Solutions

3:50 308 Implementation of Electron-Based Dissociation on Biomolecules Structure Elucidation, Zhidan Liang, Wendy Zhong, Merck & Co.

Forensics in Focus
Chair: Matthew Wood, Ocean County Sheriff Department

2:00 309 Analysis of Pesticide Residues in Cannabis Regulated by Oregon State Using LC-MS/MS, Jamie S. Foss, Sharanya Reddy, PerkinElmer
## Spectroscopic Applications of PAT in the Biopharmaceutical and Chemical Industries, organized by The Coblentz Society

**Chair:** Brandye Smith-Goettler, Merck & Co.

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors/Institutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>3:00</td>
<td>Break</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3:20</td>
<td>312</td>
<td>Harnessing Emerging IR and Raman Technologies to Obtain the Best Chemical Information from Pharmaceutical Products, Thomas Tague Jr., Bruker Corporation</td>
<td></td>
</tr>
<tr>
<td>3:40</td>
<td>313</td>
<td>Complimentary Micro EDXRF and Micro Raman To Characterize Children’s Crystal Accented Watches, Gene S. Hall, Rutgers University</td>
<td></td>
</tr>
</tbody>
</table>

**In- or Out-Sourcing? That is the Question**

**Chairs:** Dennis Swijter, ALMA, and Scott Hanton, Intertek

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors/Institutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:00</td>
<td>314</td>
<td>Downstream Process Control Using Real Time Molecular Weight with Light Scattering, Bhumit Patel, Adrian Gospodarek, Mark Brower, Douglas Richardson, David Pollard, Merck &amp; Co., Michael Larkin, Sophia Kendrick, Izhar Medalsy, Wyatt Technology</td>
<td></td>
</tr>
<tr>
<td>2:30</td>
<td>315</td>
<td>Raman-Based Nutrient and Metabolite Control in Bioprocessing Optimizes Product Quality and Peak Viable Cell Density, Karen Esmonde-White, Maryann Cuellar, Alexander Pitters, Sean Gilliam, Ian Lewis, David Strachan, Herve Lucas, Bruno Lenain, Kaiser Optical Systems</td>
<td></td>
</tr>
<tr>
<td>3:00</td>
<td>Break</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3:50</td>
<td>317</td>
<td>Simultaneous Monitoring of Reactions by NMR, Raman, IR, and NIR, Xiaoyun Chen, Donald Eldred, Xianghui Wang, Siyu Tu, Li Cui, Paul LaBeaume, Mark Rickard, Jing Liu, Hsu Chiang, Kwan Skinner, The Dow Chemical Company</td>
<td></td>
</tr>
</tbody>
</table>

## Analysis of Peptides and Proteins in Biological Samples in Support of Drug Discovery and Development, sponsored by MicroSolv Technology Corporation

**Chairs:** Wenying Jian, Janssen

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors/Institutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:00</td>
<td>322</td>
<td>Merck Strategy on Handling Hybrid Assay Coupling Immunoaffinity Purification with LC-MS/MS for Peptide Quantification in Regulated Bioanalysis to Support GLP TK and Clinical PK Studies, Yang Xu, Merck &amp; Co.</td>
<td></td>
</tr>
<tr>
<td>3:00</td>
<td>Break</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3:20</td>
<td>324</td>
<td>Considerations for Assay Platform and Reagent Selection to Quantify Endogenous Protein Biomarker, a FGF21 Case Study, Yue Zhao, Bristol-Myers Squibb</td>
<td></td>
</tr>
<tr>
<td>3:50</td>
<td>325</td>
<td>Subunit-Level and Intact Analyses of Monoclonal Antibodies from In-Life Samples: LC-MS Methods for Pharmacokinetic Quantitation, Critical Quality Attributes, and Biotransformation, John Kellie, GlaxoSmithKline</td>
<td></td>
</tr>
</tbody>
</table>

**Go with the Flow: Flavonoids, Formulations and Volatiles in Foods**

**Chair:** Kate Jackson, Colgate-Palmolive Co.

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors/Institutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:00</td>
<td>326</td>
<td>UHPLC-HRMS Analysis of Theobromine in Theobroma Cacao and Chocolates, Katarina Mladenovic, Yuriko Root, Dil Ramanathan, Kean University</td>
<td></td>
</tr>
<tr>
<td>2:20</td>
<td>327</td>
<td>Incorporating Rheological and Tribological Techniques in the Food Industry, James P. Eickhoff Jr., Charlotte Reppich, Anton Paar</td>
<td></td>
</tr>
<tr>
<td>2:40</td>
<td>328</td>
<td>Quantitative Headspace Measurement of Volatiles to Semi-Volatiles in Dairy Products using Vacuum Assisted Sorbent Extraction (VASE) and GCMS Analysis, Daniel B. Cardin, Victoria L. Noad, Entech Instruments</td>
<td></td>
</tr>
<tr>
<td>3:00</td>
<td>Break</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3:30</td>
<td>329</td>
<td>Naked-Eye Electrochemical E.coli. Detection, Kwok-Fan Chow, Sachintha Wijesinghe, Jung-Min Oh, University of Massachusetts Lowell</td>
<td></td>
</tr>
<tr>
<td>3:40</td>
<td>330</td>
<td>UHPLC-HRMS Analysis of Aechmea Magdalenae Rhizome’s Antibacterial Activity against E. coli Using Phospholipids as an Indicator, Mina E. Giron, Quintin Ferraris, Anima Ghosal, Yuriko Root, Dil Ramanathan, Kean University</td>
<td></td>
</tr>
</tbody>
</table>

**In- or Out-Sourcing? That is the Question**

**Chairs:** Dennis Swijter, ALMA, and Scott Hanton, Intertek

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors/Institutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:00</td>
<td>318</td>
<td>Comparative Review of Keeping Special Microbiology in a Hospital Lab vs. Out-Sourcing to Reference Labs, Margaret E. Biaetz, East Coast Clinical Consultants</td>
<td></td>
</tr>
<tr>
<td>2:30</td>
<td>319</td>
<td>Increasing Laboratory Efficiency through In-Sourcing and Out-Sourcing Strategies, Todd Mitchell, Pace Analytical</td>
<td></td>
</tr>
<tr>
<td>3:00</td>
<td>Break</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Memorial Session Honoring Herk Felder, sponsored by the American Microchemical Society
**Chair:** Bruce McPherson

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:00</td>
<td>331</td>
</tr>
<tr>
<td>2:30</td>
<td>332</td>
</tr>
<tr>
<td>3:00</td>
<td>Break</td>
</tr>
<tr>
<td>3:20</td>
<td>333</td>
</tr>
<tr>
<td>3:50</td>
<td>334</td>
</tr>
</tbody>
</table>

---

**DOWNLOAD the show’s official mobile app**

Make sure and download the FREE ultimate show guide for the 56th Annual Eastern Analytical Symposium and Exposition—the official mobile app. Available for iPhone, iPad and Android devices, you can now take advantage of features designed to help you get the most out of attending the event, all from the convenience of your own mobile device.

How to download the app:
- Visit the App Store or Google Play, and search the keyword EAS 2017.
- Or you can scan the QR code on the right.

After downloading the app, you’ll need to login with your Last Name and Registration Number.

The app contains the following:

- **SCHEDULE**: a searchable directory of available sessions, plus your personal list of any sessions you registered for
- **FLOORPLAN**: a viewable map to navigate the show floor with ease
- **SPEAKERS**: a complete listing of all speakers at the event
- **EXHIBITORS**: a searchable list of all exhibiting companies, plus a list of exhibiting companies you were automatically matched with during registration