

FACSS PRESENTS

SciX 2019

Final Program

Subject to Change, Always Check the Mobile App Onsite for the Latest

ABOUT THE PROGRAM

SciX 2019 is the annual meeting of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). This event is a comprehensive, intimate and all-inclusive meeting where the newest, most innovative research in the analytical sciences is presented. Meet up with old and new friends, learn, and network while attending multiple days of oral presentations, workshops, poster sessions, the SciX technical exhibition hall, and a plethora of social events.

SUNDAY, OCTOBER 13

6:15 pm – 7:15 pm Welcome and Keynote Presentation

Chair: Garth Simpson



Keynote Lecture

The Convergence of Measurement and Data Sciences: A Great Exchange

Rohit Bhargava

University of Illinois

7:15 pm Welcome Mixer and SAS Sunday Night Student Poster Session

MONDAY, OCTOBER 14

7:45 am – 9:30 am Plenary Session

Chair: Mary Kate Donais

8:00 am RSC Theophilus Redwood Award/2018 Coblentz Society Craver Award



Polymer-enabled Plasmonic Sensing

Christy L. Haynes,

University of Minnesota

8:30 am



Ellis R. Lippincott Award
From Bond-selective Chemistry to Bond-selective Imaging: My 30 Years' Path to Tackle Missions Impossible

Ji-Xin Cheng, Boston University

9:00 am



Spectroscopy's Emerging Leader in Molecular Spectroscopy Award
Decoding the Molecular Pathology of Cancer with Vibrational Spectroscopy

Ishan Barman, Johns Hopkins University

9:45 am – 10:45 am Poster Session and Break

10:50 am – 12:30 pm Morning Symposia

AES-01**Electrokinetic Fundamentals**

Chair: Aliaksei Boika, Karina Torres Castro

- 10:50 AM Gigantic Dielectrophoresis of Proteins in Solution
Dmitry Matyushov
- 11:10 AM Exploiting Dielectrophoresis to Separate Single Walled Carbon Nanotubes
Alexandra Ros
- 11:30 AM AC Electrokinetic Phenomena in Electroanalysis
Aliaksei Boika
- 11:50 AM Strategies for dynamic particle manipulation and assessment employing insulator-based dielectrophoresis
Blanca Lapizco-Encinas
- 12:10 PM A Parallelized in Flow Electrorotation Platform with Individual Control on the Trapping and Release of Single Cells
Kevin Keim

AWD-01**RSC Theophilus Redwood Award Honoring Christy Haynes**

Chair: Christy Haynes

- 10:50 AM Tunable Chiroptical Properties in Metamaterials and Nanocrystals
Vivian Ferry
- 11:10 AM Studies of Biomolecules with Multiphoton Microspectroscopy
Janina Kneipp
- 11:30 AM Plasmon-enhanced Single-molecule Fluorescence in Living Bacterial Cells
Julie Biteen
- 11:50 AM Nanoscale Battery Materials Induce DNA Damage in Bacteria
Tian (Autumn) Qiu
- 12:10 PM Breakdown of Plastics in the Environment: The Impact of Weathering on the Fate and Transformation of Aquatic Plastic Debris
Melissa Maurer-Jones

BIM-01**Biomedical Spectroscopy and Imaging for Cancer**

Chair: Michael Schmitt

- 10:50 AM Fluorescence Lifetime Spectroscopy and Imaging in Clinical Applications
Laura Marcu
- 11:10 AM Hyperspectral SRS Imaging for Label-free Molecular Subtyping of Glioblastomas
Zhiwei Huang
- 11:30 AM Multiplex SRS Imaging Cytometry Reveals Novel Metabolic Signatures in Drug-resistant Cancer Cells
Ji-Xin Cheng
- 11:50 AM Exploring Raman Spectroscopy for the Identification of Vulval Squamous Cell Carcinoma and Vulval Intraepithelial Neoplasia
Nick Stone
- 12:10 PM Nonlinear Multimodal Imaging for Intraoperative Tumor Diagnosis
Michael Schmitt

FORENS-01**Nuclear Forensics**

Chair: Dallas Reilly, Greg Klunder, Robert Lascola

- 10:50 AM Infrared Spectroscopic Method for Uranium Isotopic Analysis
Alicia Strange Fessler
- 11:10 AM Inferring Nuclear Fireball Properties from Experimental Data
Batikan Koroglu
- 11:30 AM Resonance Ionization Mass Spectrometry for Actinide Isotope Analysis
Brett Isselhardt

- 11:50 AM Elemental and Isotope-ratio Mass Spectrometry with a Solution-cathode Glow Discharge Ionization Source
Garett MacLean
- 12:10 PM Laser-induced Spectrochemical Assay for Uranium Enrichment
George Chan
- IR-02 Nanoscale IR Spectroscopy I: Recent Advances**
Chair: Andrea Centrone
- 10:50 AM Unlocking the Potential of Photothermal Infrared Microscopy on Spatial Resolution, Sensitivity, and Richness of Information
Xiaoji Xu
- 11:10 AM Tapping-mode PTIR: A Versatile IR Nanoscopy Method for Challenging Samples
Georg Ramer
- 11:30 AM Tapping Mode AFMIR: A Versatile Tool to Characterize Drug-loaded Polymeric Nanoparticles
Ariane Deniset-Besseau
- 11:50 AM Correlative Nanoscopy for Organic, Inorganic and Hybrid Material Analysis
Tobias Gokus
- 12:10 PM Nanoscale Spectroscopy and Imaging (s-SNOM and AFM-IR) Using a Femtosecond Difference Frequency Generation Laser Source
Qichi Hu
- IR-12 Forefront of Molecular Spectroscopy**
Chair: Isao Noda
- 10:50 AM Understanding of Biodegradable Polymer Blend Thin Films Using 2D Correlation Analysis and Chemical Images
Young Mee Jung
- 11:10 AM Effective Use of Spectral Database Software with Two-dimensional Correlation Spectroscopy (2D-COS)
Isao Noda
- 11:30 AM Application of NIR Spectroscopy to Physical Chemistry
Yukihiro Ozaki
- 11:50 AM Raman Hyperspectroscopy for Forensic Purposes and Medical Diagnostics
Igor Lednev
- 12:10 PM Advances in Balanced Detection Interferometric Cavity Assisted Photothermal Spectroscopy
Bernhard Lendl
- LIBS-01 Fundamentals**
Chair: Alessandro Digiacomo
- 10:50 AM Time-resolved Characterization of Laser Induced Plasmas with Dual-comb Spectroscopy
Jason Jones
- 11:10 AM Modeling Equilibrium Chemistry in Laser Induced Plasmas and Plasma Chemical Reactors
Igor Gornushkin
- 11:30 AM What Are We Looking At? An Atypical View of the LIP
Jonathan Merten
- 11:50 AM Probe Volume and Energy Balance in Laser-induced Breakdown Spectroscopy
Jörg Hermann
- 12:10 PM On the Plasma Phase Immediately After the Laser Matter Interaction
Alessandro De Giacomo
- NANO-01 Carbon-based Nanomaterials: Synthesis, Properties, and Applications**
Chair: Wei Zhao
- 10:50 AM Resolving Carbon Nanotube Structures by DNA
Ming Zheng

- 11:10 AM Magnetic Brightening of Hidden Fine Structures in Carbon Nanotube Quantum Defects
HAN Htoon
- 11:30 AM Carbon-based Functional Nanomaterials for Electrochemical Energy Technologies
Shaowei Chen
- 11:50 AM Carbon Nanomaterials in Energy Storage: From 1D to 3D
Jie Liu
- 12:10 PM Tip-enhanced Raman spectroscopy investigation of transition complex immobilization on 2D carbon nanosheet
Marie Richard-Lacroix
- PMA-03 Biopharmaceutical Raw Material Characterization**
Chair: John Bobiak
- 10:50 AM Determination of Amino Acid Glycation and Vitamin Degradation in Chemically Defined Media Powders by HPLC
Lisa Bareford
- 11:10 AM Evaluation of Cell Culture Media Using Absorption and Transmission Fluorescence Excitation Emission Matrix (A-TEEM) Spectroscopy
Alvin Togonon
- 11:30 AM Digital Image Processing for Quantitative Analysis
Kevin Cantrell
- 11:50 AM Protein Mobility Evaluated by Fourier-transform Fluorescence Recovery After Photobleaching (FT-FRAP)
Andreas Geiger
- 12:10 PM Warehouse Verification of Incoming Materials in Pharma with Mobile Raman
Keith Carron
- RAM-11 Food Security**
Chair: Roy Goodacre
- 10:50 AM Detection of Multiple Food Bacteria by SERS
Karen Faulds
- 11:10 AM Confirmatory, Non-invasive and Non-destructive Raman-based Diagnostics of Biotic and Abiotic Stresses on Plants
Dmitry Kurouski
- 11:30 AM Emerging Approaches for Representative Food Analysis Using Raman Spectroscopy
Nils Kristian Afseth
- 11:50 AM Raman Spectroscopic Measurements of Salmon Meat Composition Using 1000 nm Excitation
Mary Lewis
- 12:10 PM Vibrational Spectroscopy with Chemometrics: A Rapid Screening Tool to Determine Authenticity of Extra Virgin Olive Oil
Didem Aykas
- SPEC-03 Society for Archaeological Sciences Session on Chemistry in Art and Archaeology I**
Chair: Mary Kate Donais, Andrew Zipkin
- 10:50 AM Spectroscopic Mapping of the Vinland Map and Related Manuscripts: New Analytical Tools Offer New Evidence
Richard Hark
- 11:30 AM When Heritage Meets Science - Integrated Approaches and International Cooperation
Antonio Candeias
- 11:50 AM Novel Biotechnological Approaches for Cultural Heritage: Challenges and Perspectives
Ana Teresa Caldeira
- 12:10 PM Spectroscopic Characterization of Historic Fabrics from a Turn of the Century New England Mill
Mary Kate Donais

SPSJ-01	VUV/FUV/DUV I <i>Chair: Yukihiro Ozaki, Yusuke Morisawa</i>
10:50 AM	Standoff Deep UV Raman Imaging Spectrometer for Trace Explosives: Photonic Crystal Narrow Wavelength Devices <i>Sandy Asher</i>
11:10 AM	DUV Raman Spectroscopy for Probing Protein Aggregates: Spontaneous Refolding of Amyloid Fibrils <i>Igor Lednev</i>
11:30 AM	UV Photochemistry and Photophysics of Tryptophan in Azurin <i>Judy Kim</i>
11:50 AM	Synchrotron-based UV Resonance Raman Investigation of DNA Structure and Interactions <i>Barbara Rossi</i>
12:10 PM	Spectroscopic Characterization of Individual Wide-gap Semiconductor Nanoparticles <i>Yuika Saito</i>

1:30 pm – 3:10 pm **Afternoon Symposia**

AES-02	Electrokinetic Applications <i>Chair: Jeffrey Moran, Anna Nielsen</i>
1:30 PM	Breaking the Diagnostic Barrier for Hemoglobinopathies in Low-resource Settings with Electrophoresis <i>Umut Gurkan</i>
1:50 PM	Self-electrophoretic Microswimmers for Wastewater Treatment and Remediation <i>Jeffrey Moran</i>
2:10 PM	Electrophysiology of Biosorbent: Cupriavidus Necator <i>Anthony Giduthuri</i>
2:30 PM	Electrokinetic Determination of Solution Phase Kinetic Properties at Microfluidic Liquid Interfaces <i>Md Nazibul Islam</i>
2:50 PM	Perspectives on Selected Dielectrophoresis Platforms for Particle Separations <i>Rodrigo Martinez-Duarte</i>
ATOM-01	Low Pressure Glow Discharge Spectroscopies <i>Chair: Jorge Pisonero</i>
1:30 PM	Selection of Analytical Lines in Glow Discharge Optical Emission - New Opportunities with a State-of-the-art Spectrometer <i>Arne Bengtson</i>
1:50 PM	A Critical Review of the Analytical Potential of Pulsed Radiofrequency Glow Discharge Time-of-flight Mass Spectrometry <i>Nerea Bordel</i>
2:10 PM	Glow Discharge Optical Emission Spectroscopy with Compressed Sensing Encoding in the Spectral Dimension <i>Gerardo Gamez</i>
2:30 PM	Elemental analysis of multi-layered structures using GD-OES and Micro-XRF <i>Matthieu Chausseau</i>
2:50 PM	The Continued Development of a New DC/RF/Pulsed-RF Glow Discharge Lamp and Supply <i>Kim Marshall</i>
AWD-13	Ellis R. Lippincott Award Honoring Ji-Xin Cheng <i>Chair: Ji-Xin Cheng</i>
1:30 PM	Stimulated Raman Imaging with Chemical Tags <i>Wei Lu</i>
1:50 PM	Retinal Oximetry by Visible Light Optical Coherence Tomography <i>Ji Yi</i>
2:10 PM	High-resolution spectroscopic imaging for understanding myelofibrosis <i>Rohith Reddy</i>

- 2:30 PM Revealing Subcellular Structures with Live-cell and 3D Fluorescence Nanoscopy
Fang Huang
- 2:50 PM Dispersion-based Spectroscopic Imaging: Principles and Applications in Biomedicine
Francisco Robles
- BIM-02 Spectroscopic Approaches to Tackle Infectious Diseases**
Chair: Jürgen Popp
- 1:30 PM Finally, a Slam Dunk SERS Application: Metabolic Responses for Fast Antibiotic Susceptibility Testing
Lawrence Ziegler
- 1:50 PM Plasmonic Nanostructures for Pathogen Fingerprinting and Killing
Wei-Chuan Shih
- 2:10 PM Raman Spectroscopic Characterization of Leukocyte in Scenario of Infection and Inflammation
Anuradha Ramoji
- 2:30 PM Phosphorescent Liquid Bandages for the Identification of Inflammatory Bacterial Infections
Haley Marks
- 2:50 PM Raman Spectroscopic Phenotyping - Identification of the Infection Causing Bacteria and Quantification of the Antibiotic Susceptibility
Jürgen Popp
- IR-03 Nanoscale IR Spectroscopy II: Fundamentals and Applications**
Chair: Andrea Centrone, Georg Ramer
- 1:30 PM Thermal Effects in Photo-induced Force Microscopy (PiFM)
Eric Potma
- 1:50 PM Exploration of the Origin of Photo-induced Force in Tapping Mode Nanoscale Infrared Microscopy
Xiaoji Xu
- 2:10 PM Novel Concepts in Infrared Nano-Imaging – Competing, Confusing, Controversial, or Complementary?
Markus Raschke
- 2:30 PM Characterization 2D Materials and Heterostructures with Infrared Nanospectroscopy (PTIR)
Andrea Centrone
- 2:50 PM Nanoscale Materials Analysis Using AFM-IR
Liang Gong
- LIBS-03 Biomedical and Pharmaceutical Applications**
Chair: Noureddine Melikechi
- 1:30 PM Laser-induced Breakdown Spectroscopy (LIBS) for the Diagnosis of Neurodegenerative Diseases
Rosalba Gaudio
- 1:50 PM Diagnosis of Human Malignancies Using Blood Sample Laser-induced Breakdown Spectroscopy in Combination with Chemometric Methods
Xiaohui Li
- 2:10 PM Bacterial Limit of Detection Reduction Utilizing a Novel Sample Preparation Protocol
Steven Rehse
- 2:30 PM In Situ Analytical Characterization and Chemical Imaging of Tablet Coatings Using Laser Induced Breakdown Spectroscopy
Lanfang Zou
- 2:50 PM From Bench to Bedside: LIBS Imaging Is Entering the Clinic as a New Diagnostic Tool for Respiratory Diseases
Motto-Ros Vincent
- MASS-04 Forensic Applications of Mass Spectrometry**
Chair: Glen Jackson
- 1:30 PM Sourcing of Latent Print Chemical Residue Using 2D-GC-MS
Candice Bridge

- 1:50 PM GC-MS and Product Ion MS-MS Studies on Substituted Cathinone Designer Drugs
Randall Clark
- 2:10 PM Barking up the Wrong Tree: Combating Illegal Trade in Endangered Wood Species with Mass Spectrometry
Rabi Musah
- 2:30 PM Statistical Comparison of Mass Spectra for Seized Drug Identification
Ruth Smith
- 2:50 PM Integrated SERS-PSI-MS Platform Using Gold Nanoparticle-embedded Paper for Trace Detection of Illegal Drugs
Jeremy Driskell
- NANO-02 Nano-facilitated Sensing**
Chair: David Thompson
- 1:30 PM Imaging Nano Particles with X-ray Excited Optical Luminescence
Jeffrey Anker
- 1:50 PM Investigating Antibody-gold Nanoparticle Adsorption Dynamics to Optimize Conjugates for Biosensing
Jeremy Driskell
- 2:10 PM Prospects for Detection of a Wide Variety of Analytes with SERS
Erik Emmons
- 2:30 PM Sensor Surface Temperature and Headspace-sampled SERS Signals
David Thompson
- PMA-01 Solving Industrial Problems Using Vibrational Spectroscopy**
Chair: Andrew Marriott
- 1:30 PM Drug-amino Acid Co-amorphous Formulation Analysis by FTIR Spectroscopy
Mohammed Alsalhi
- 1:50 PM Use of FT-IR Modelling to Determine Isotopic Impurities in the Deuterated Reagent d3-methylamine Hydrochloride
Andrew Marriott
- 2:10 PM ATR-FTIR Imaging to Study the Aggregation of Biopharmaceuticals Through Secondary Structure Analysis
Hannah Tiernan
- 2:30 PM In-column ATR-FTIR spectroscopy for analysis of monoclonal antibody purification
Sergei Kazarian
- 2:50 PM Enantioselective Raman Spectroscopy – a Novel Tool for Enantiomeric Discrimination
Claudia Rullich
- RAM-09 IRDG**
Chair: Karen Faulds
- 1:30 PM What Can We Learn from SERS of Bacteria and Their Metabolites
Bell Steven
- 1:50 PM Elucidation of Two-photon Properties via Surface-enhanced Hyper-raman Scattering of Rhodamine-like Dyes
Jacob Olson
- 2:10 PM SERS Probes to Monitor Communicable and Non-communicable Diseases
Laura Fabris
- 2:30 PM Single-molecule and Single-particle Surface-enhanced Raman Scattering (SERS) in Analytical Chemistry
Alexandre Brolo
- 2:50 PM Determining the Level and Location of Functional Groups on Commercial Graphene Using Tip-enhanced Raman Spectroscopy
Elizabeth Legge

- SPEC-04** **Society for Archaeological Sciences Session on Chemistry in Art and Archaeology II**
Chair: Mary Kate Donais, Andrew Zipkin
- 1:30 PM From Coast to Karoo: A Radiogenic Bioavailable Strontium Isoscape in South Africa for Provenience Studies
Andrew Zipkin
- 1:50 PM Micro- to Nanoscale IR in Heritage Science: the Distribution of Metal Carboxylates in Oil Paint
XIAO Ma
- 2:10 PM Trace Element Analysis of Archaeological Human Enamel and Bone Apatite: Implications for Documenting Biological Sex and Health Status
Beth Scaffidi
- 2:30 PM Strengths and Limitations of Fecal Stanols as a Population Proxy for Cahokia, Illinois and the Jordanian Desert
AJ White
- 2:50 PM Food, Networks, Power: Exploring Ancient Cypriot Foodways Through Organic Residue Analysis
Rebecca Gerdes

- SPR-01** **Nanostructure Implications on Plasmonics**
Chair: Amanda Haes
- 1:30 PM Aluminum Plasmonic Antennas for Surface-enhanced Infrared Absorption Spectroscopy
Jennifer Shumaker-Parry
- 1:50 PM Plasmonic Properties of Non-precious Metal Cu-based Nanostructures
Jingyi Chen
- 2:30 PM Observation of Hot-Carrier Driven Chemical Reaction by TERS
Dmitry Kurouski
- 2:50 PM Plasmonic Properties of Multimetal Layers Nanodisk Array
Benjamin Charron

3:10 pm – 3:50 pm **Poster Viewing and Break**

3:50 pm – 5:30 pm **Afternoon Symposia**

- AES-03** **ACS ANYL-AES Joint Session: Micro/Nano Scale Analytics Driven by Electric Fields**
Chair: Mark Hayes, Lane Baker
- 3:50 PM Thread-based Sensors and Fuel Cells
Frank Gomez
- 4:10 PM Multi-detector approaches for improved resolution in capillary electrophoresis
Christopher Baker
- 4:30 PM DNA Sequence-specific Enrichment Using Isotachopheresis
Juan Santiago
- 4:50 PM Single-particle Analysis of Virus Capsid Assembly by Resistive-pulse Sensing
Stephen Jacobson
- 5:10 PM Electrokinetic Assessment of Bacteriophage Virus
Adriana Coll De Peña

- ATOM-02** **Laser Ablation Based Spectroscopies**
Chair: Jorge Pisonero
- 3:50 PM Laser ionization mass spectrometry for direct atomic analysis of solids
Jose Miguel Vadillo
- 4:10 PM Fast and High Resolved Elemental Analysis Using ns/fs-LA
Jorge Pisonero
- 4:30 PM Novel reference materials for LA-ICP-MS analysis on hair
Mauro Martinez

- 4:50 PM Exploring the Potential of Fast Washout LA with Quasi-simultaneous Multi-isotope Detection for Single Cell Elemental Imaging Using LA-ICP-ToF-MS
Kharmen Billimoria
- 5:10 PM Direct Detection of Single Particles with SIMS and ICP-MS: On Recent Advances and Remaining Challenges
Carsten Engelhard
- AWD-06 Spectroscopy's Emerging Leader in Molecular Spectroscopy Award Symposium Honoring Ishan Barman**
Chair: Ishan Barman
- 3:50 PM Developing Surface Enhanced Deep Raman Spectroscopy for Clinical Applications
Nick Stone
- 4:10 PM Raman Microscopy for High-throughput Molecular Analysis
Katsumasa Fujita
- 4:30 PM Label-free Morphomolecular Microscopic Investigation of Live Leukemic Cells
Rishikesh Pandey
- 4:50 PM Nanoengineered Interfaces for Optical Sensing of Chemicals and Biochemicals
Steve Semancik
- 5:10 PM Quantitative Confocal Raman Microscopy Detection of a Hybrid Phospholipid Bilayer-Based Sandwich Immunoassay within Individual Chromatographic Silica Particles
Jay Kitt
- CTP-01 Commercialization of Analytical Technologies**
Chair: Karen Esmonde-White, Scott Rudder
- 3:50 PM Tips 4 Successful Entrepreneurship: Jump Don't Step!
Scott Rudder
- 4:10 PM Moving Disruptive Innovation to Market
Isao Noda
- 4:30 PM Growing a Company on Customer Specifications
Cheryl Provost
- 4:50 PM Navigating a Successful Pathway to Exit: Strategies for Building Value and Finding the Right Partner
Randy Heyler
- 5:10 PM Speaker Roundtable
Scott Rudder
- IR-04 Advances in Molecular Spectroscopy**
Chair: William Wang
- 3:50 PM A Novel Analytical Technique of Chemical Reaction in a Ultra-thin Film Using pMAIRS
Takeshi Hasegawa
- 4:10 PM Variations in Bone Composition at Sub-micron Resolution
Nancy Pleshko
- 4:30 PM Polarized Infrared Light Reveals Order and Disorder in 2-, 4- and 8-week Post-infarct Rat Heart
Kathleen Gough
- 4:50 PM Submicron Simultaneous IR and Raman Spectroscopy (IR-Raman): Breakthrough Developments in Optical Photothermal IR (O-PTIR) Combined with Raman Provide New Capabilities
Mustafa Kansiz
- 5:10 PM Identification of Unknown Samples Through Simultaneous IR and Raman Measurement and Database Searching: Exploiting Synergies for Complementary and Confirmatory Analysis
Gregory Banik

- IR-11 Nanoscale IR Spectroscopy III: Bio-Applications**
Chair: Andrea Centrone, Liang Gong
- 3:50 PM Understanding the Recorded Signal in Atomic Force Microscopy-infrared Spectroscopy (AFM-IR) Measurements
Rohit Bhargava
- 4:10 PM Nanoscale Chemical Analysis from Single Biomolecules to Living Organisms in Air and Native Liquid Environment
Francesco Simone Ruggeri
- 4:30 PM Infrared Difference-nanospectroscopy to Probe the Light-induced Conformational Changes of Transmembrane Proteins in Individual Membrane Patches
Valeria Giliberti
- 4:50 PM Structural Characterization of Plant Epicuticular Waxes Using AFM-IR
Dmitry Kurovski
- 5:10 PM Nanoscale Chemical Heterogeneity as a Function of Tissue Age for Wild Type Mice Femurs Measured by Photothermal Infrared Spectroscopy (PTIR)
Taeyong Ahn
- LIBS-09 Geology**
Chair: Lutfü Özcan
- 3:50 PM "LIBS and Geology," A Long and Nice Story: What It's Now Possible to Do and How to Do It Well
Cécile Fabre
- 4:10 PM Ultrafast Analysis in Mining Industry for Noble Metals
Lutfü Özcan
- 4:30 PM Fast High-resolution Multi-elemental Mapping of Phosphate Pellets Using Laser Induced Breakdown Spectroscopy
Nawfel Azami
- 4:50 PM In-situ Elemental Rock Testing (In-SERT) Probe: Development Feasibility of a LIBS and Raman Spectroscopy Based Characterization System
Shane Lee
- 5:10 PM Direct Determination of Soils Texture Using Laser-induced Breakdown Spectroscopy and Multivariate Linear Regressions
Christian Goueguel
- MASS-02 Untargeted Metabolomics: Innovations and Applications**
Chair: Amina Bouslimani
- 3:50 PM Unraveling Drug Metabolism Complexity via Untargeted Mass Spectrometry
Alan Jarmusch
- 4:10 PM Contextualizing Host-parasite-microbiome Interactions Using Lc-ms/ms-based Metabolomics and Chemical Cartography
Laura-Isobel McCall
- 4:30 PM Mass Spectrometry Based Machine Learning Approaches to Discover Nutrients That Can Revitalize the Modern Diet
Gabriel Navarro
- 4:50 PM Characterizing the Chemotypic Landscape of Polymicrobial Communities
Vanessa Phelan
- 5:10 PM Scaling Molecular Networks to the Cloud Enables New Visualizations
Mingxun Wang
- PAT-07 Process Analytical in the Petroleum/refineries Industry**
Chair: Toni Miao
- 3:50 PM Process Analytics in the Petrochemical Industry: 30 Years Back and 10 Years Forward
Charles Miller

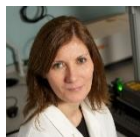
- 4:10 PM Chemometrics in Refinery applications - a new approach
Michael Kleimann
- 4:30 PM Using Infrared Spectroscopy for Alkylation Process Monitoring
Howard Lacheen
- 4:50 PM The Benefits of High-throughput Raman for Process Analysis
Mark Kemper
- 5:10 PM Evaluating the Capability of the Ultraportable, Ergonomic 4300 FTIR for Rapid Delineation of Hydrocarbons in Soil
Natasha Sihota
- PMA-02 Biophysical Characteristics of Biotherapeutics: From Discovery to Development**
Chair: Deniz Temel
- 3:50 PM Raman Spectroscopy in Cancer Pathology Classification
Sarah Shidler
- 4:10 PM Novel Method for Multidimensional Fluorescence Characterization of Protein Binding
Karen Gall
- 4:30 PM Scanning Electron Cryomicroscopy (CryoSEM)-Raman Spectroscopy for Analysis of Complex Drug Products
Huzeyfe Yilmaz
- 4:50 PM An Integrated Data Analysis Approach for Analysis of Biotherapeutics by Native CE-MS
Christopher Brown
- 5:10 PM Monitoring and Control in Upstream and Downstream Bioprocessing Based on Process Raman Spectroscopy
Karen Esmonde-White
- RAM-06 SERS I**
Chair: Roy Goodacre, Colin Campbell, Duncan Graham
- 3:50 PM SERS in Tissue Models
Colin Campbell
- 4:10 PM Multimodal Optical Biosensing Toward Point-of-care Diagnosis and Monitoring
Gerard Cote
- 4:30 PM Reproducible Immunoassay of Multiple Biomarkers Using SERS Mapping on Three-dimensional Nanopillar Arrays
Jaebum Choo
- 4:50 PM Detection of MMP Activity Using Surface Enhanced Raman Scattering to Aid Cancer Detection
Sian Sloan-Dennison
- 5:10 PM Surface-enhanced Raman Scattering Nanosensors for optophysiology: Exploring Neurochemistry in Near-real-time
Gregory Wallace
- SPSJ-02 VUV/FUV/DUV II**
Chair: Yukihiro Ozaki
- 3:50 PM Laser Cooling of (Anti)hydrogen Using Pulsed VUV Radiation
Takamasa Momose
- 4:10 PM Taming DUV Raman Microscopy with Plasmonic Metals
Atsushi Taguchi
- 4:30 PM Investigation for Sigma Orbitals in the Liquids and Solids of Normal- and Cyclo-alkanes Using ATR-FUV
Yusuke Morisawa
- 4:50 PM Electrochemical Attenuated Total Reflectance Spectroscopy in Far- and Deep-ultraviolet Regions
Ichiro Tanabe
- 5:10 PM Attenuated Total Reflection FUV-DUV Spectroscopy of Graphene Nanostructures and Graphene-polymer Nanocomposites with Quantum Chemical Calculations
Krzysztof Bec

TUESDAY, OCTOBER 15

7:45 am – 9:00 am Plenary Session

Chair: Mary Kate Donais

8:00 am Charles Mann Award for Raman Spectroscopy

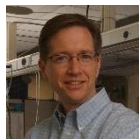


Development of SERS and SESORRS for Multiplexed Bioanalysis

Karen Faulds, University of Strathclyde

8:30 am

ANACHEM Award



Droplet Microfluidics with Mass Spectrometry for High-Throughput Chemistry, Screening, and Sensing

Robert Kennedy, University of Michigan

AES-04 3D Printed Microfluidics: New Materials and New Applications

Chair: R. Scott Martin, Ana Egatz-Gomez

- 9:15 AM Miniaturizing 3D Printed Microfluidics: Materials, Tools, and Trends
Greg Nordin
- 9:35 AM Electron Microscopy Sample Preparation Systems Fabricated by 3D Printing
Michael Roper
- 9:55 AM Realizing the Potential of Polyjet 3D Printing
Andre Castiaux
- 10:15 AM 3D Printed Analytical Tools for Quantitative Studies of Human Health
Cody Pinger
- 10:35 AM 3D Printed Microfluidic Devices for Immunoaffinity Extraction of Preterm Birth Risk Biomarkers
Adam Woolley

AWD-03 Charles Mann Award Symposium Honoring Karen Faulds

Chair: Karen Faulds

- 9:15 AM Mann versus Food
Roy Goodacre
- 9:35 AM SERS Optophysiology for Monitoring Chemical Gradients
Jean-Francois Masson
- 9:55 AM Biosensing Devices for Consumer Focused Healthcare Applications
Kristy McKeating
- 10:15 AM Electrochemically Modulated Liquid Chromatography (EMLC): An Approach to Manipulate Solute Retention and Quantify Fundamental Electrosorption Phenomena
Marc Porter
- 10:35 AM At Last, a Wo-Mann
Duncan Graham

BIM-03 Liquid Biopsies for Biomedical Applications (CLIRSPEC)

Chair: Matthew Baker

- 9:15 AM The Role of Phospholipid Protein Balance in Neurodegenerative Disorders. Analysis of Human Blood Serum Using Raman Spectroscopy in Liquid Biopsies
Joanna Depciuch
- 9:35 AM Plasmonic Point of Care Sensors for the Detection of Disease Specific miRNA in Biofluids
Samuel Mabbott
- 9:55 AM A Triage Blood Test for Brain Cancer: Development of High-throughput ATR-FTIR Technology for Rapid Spectroscopic Serum Diagnostics
Holly Butler
- 10:15 AM Raman Spectroscopy Reveals Distinct Metabolic Patterns in Blood of Crohn's Disease Subjects vs Healthy Controls
Renzo Vanna
- 10:35 AM A Novel Screening Method for Diagnosing Alzheimer's Disease Based on Raman Hyperspectroscopy and Advanced Statistics
Nicole Ralbovsky

CHEM-01 New Frontiers in Chemometrics

Chair: Federico Marini

- 9:35 AM Chemometric Analysis of Mass and Infrared Hyperspectral Imaging Data in the Investigation of Biological Tissues Under Environmental Stressing Conditions
Roma Tauler
- 9:55 AM Spectral-Spatial Exploration of Hyperspectral Imaging Data Sets Using PCA and Wavelet Transform

- Ludovic Duponchel*
 10:15 AM Coupling Variable Selection and Multi-block Predictive Modeling Through the So-covsel Algorithm
Federico Marini
- 10:35 AM Chemical Imaging Measurements of the Tumor Microenvironment Predict Colorectal Cancer Outcome
Saumya Tiwari
- FORENS-02** **Food Forensics**
Chair: Betsy Jean Yakes
- 9:15 AM Determination of the limit of detection of multiple pesticides utilizing gold nanoparticles and surface enhanced Raman spectroscopy (SERS)
Anne-Marie Dowgiallo
- 9:35 AM Determination of Seafood Decomposition by Large Volume Static Headspace Analysis and Chemometrics
Zhengfang Wang
- 9:55 AM Miniature Instruments in the Hands of the Consumer: Are They Making the Right Measurement in the Right Place
Ellen Miseo
- 10:15 AM Opportunities of Food Sensors for Field Applications: From Crop to Your Grocery Store
Luis Rodriguez-Saona
- 10:35 AM A SERS and Mobile Raman Platform for Combating Food Fraud
Keith Carron
- IR-05** **Quantum Cascade Lasers**
Chair: Bernhard Lendl
- 9:35 AM Real-world Applications of Quartz-enhanced Photo Acoustic Gas Sensing
Vincenzo Luigi Spagnolo
- 9:55 AM New Modalities in EC-QCL Spectroscopy for Liquid Sensing
Bernhard Lendl
- 10:15 AM A QCL-based Photoacoustic Sensor for Online Monitoring of N₂O Emissions of Wastewater Treatment Plants
Christoph Haisch
- 10:35 AM Mid-infrared Quantum Cascade Laser Based Spectroscopic Ellipsometry
Markus Brandstetter

- IR-09 Recent Advances in Using Molecular Spectroscopy for PAT**
Chair: Mike George
- 9:15 AM Deep Dive into a Telescope Reaction for the Synthesis of a Pharmaceutical
John Wasyluk
- 9:35 AM A Robust NIR Quantitative Method Against Powder Stream Density for the Inline Monitoring of Drug Content in a Simulated Continuous Process
Natasha Velez
- 9:55 AM In Situ Monitoring of Heterogeneous Hydrosilylation Reactions by Infrared and Raman Spectroscopy
Xiaoyun Chen
- 10:15 AM Lyophilization Process Understanding by In-line Raman Measurement
Dongsheng Bu
- 10:35 AM Chemdetect Mid-ir Analyzer for Online Monitoring of Bioreactor Growth Media and Waste Products
Craig Magee
- MASS-03 Identification of Peptide Isomers with Mass Spectrometry**
Chair: Ryan Julian
- 9:15 AM Lysosomal Degradation of Peptide Isomers and Epimers
Ryan Julian
- 9:35 AM Single-cell Mass Spectrometry Enables Profiling of Anionic and Cationic Metabolites in the Live *Xenopus laevis* (Frog) Embryo
Erika Portero
- 9:55 AM Developing New Approaches for the Better Characterization of Isomeric Peptides: Ion Mobility Separations Enabled by Structures for Lossless Ion Manipulations
Gabe Nagy
- 10:15 AM Coupling Enzymatic and Mass Spectrometry Based Approaches for Non-targeted D-amino Acid Containing Peptide Discovery
David Mast
- 10:35 AM Covalent Ion/Ion Reactions in an Ion Mobility Mass Spectrometer
Ian Webb
- PMA-07 Metabolic Screening and Small Molecule Detection**
Chair: Katherine Hollywood
- 9:15 AM High-throughput Chemical Reaction Screening and Correlative Metabolomics by MRM-profiling
Christina Ferreira
- 9:35 AM Using Mass Spectrometry to Discover New Bile Acids from the Gut Microbiome
Emily Gentry
- 9:55 AM Online Monitoring of Volatile Organic Compounds by Proton Transfer Reaction Mass Spectrometry: Applications Within Synthetic Biology
Katherine Hollywood
- 10:15 AM Development of Near Infrared Spectroscopy for On-line Monitoring of Biomass Quality Characteristics
Timothy Rials
- 10:35 AM Ion Pair Chromatography versus HILIC: Comparison of the Two Separation Techniques for Highly Polar Compounds
Ruchi Mehta
- RAM-03 Nano Raman**
Chair: Andrew Whitley
- 9:15 AM Nanoscale Nonlinear Excitonic Photophysics in 2D Semiconductors
Nicholas Borys
- 9:35 AM TERS Investigation of Combustion-generated Ultrafine Particulate Matter
Marc Chaigneau

- 9:55 AM Stokes and Anti-stokes in Tip-enhanced Raman Spectroscopy: Quantitative Insights into Plasmon Resonance, Near-field Temperature and Spatial Resolution
Marie Richard-Lacroix
- 10:15 AM Recent TERS Adventures at the Solid-liquid Interface: Chemical and Chemical Reaction Imaging
Ashish Bhattarai
- 10:35 AM Forward and Reverse Chemical Nanoscopy at Solid-air and Solid-liquid Interfaces
Patrick El Khoury

RAM-07 SERS II

Chair: Colin Campbell, Roy Goodacre, Duncan Graham

- 9:15 AM Electrochemical SERS for Bacterial Detection
Christa Brosseau
- 9:35 AM Ultrasensitive and Reproducible Detection of inti1 Enabled by Slippery Liquid-infused Porous Surface-enhanced Raman Scattering (SLIPSERS) and Hot-spot Normalization (HSN)
Peter Vikesland
- 9:55 AM SERS as an Analytical Tool for Synthetic Cannabinoid Screening in Oral Fluid
Chiara Deriu
- 10:15 AM Rapid Identification and Quantification of Trace Fentanyl in Drugs of Abuse with Portable Raman
Hao Wang
- 10:35 AM The Detection of Biomarkers Associated with Sepsis Using SERS
Emma O'Connor

SPSJ-03 Near Infrared Spectroscopy I

Chair: Shigeaki Morita

- 9:15 AM Quantitative Analysis of Weakly and Strongly Interacting Three-component Solvent Systems: NIR versus Raman Spectroscopy
Heinz Siesler
- 9:35 AM Anharmonic Quantum Mechanical Simulation of NIR Spectra. Applications in Physical and Analytical Chemistry
Krzysztof Bec
- 9:55 AM Spectral Analysis of Saccharides Focusing on the Anomer Structure
Sae Tanaka
- 10:15 AM Gradient LC-NIR and Its Application
Shigeaki Morita
- 10:35 AM ChemDetect Mid-IR Analyzer for Inline Chemical Identification of Liquid Chromatography Separations
Craig Magee

11:00 am – 11:45 am Poster Session and Break

11:30 am – 12:45 pm Exhibit Hall Activities

“What’s Hot” Vendor Presentations (11:30 am - 1:20 pm)

Complimentary Lunch (12:00 - 12:45 pm)

1:30 pm – 3:10 pm Afternoon Symposia

AES-08 Biological and Pharmaceutical Applications

Chair: Wenwan Zhong, Mike Beauchamp

- 1:30 PM Isolation and concentration of proteins and small complex bioparticles with electric fields
Mark Hayes
- 1:50 PM Capillary Electrophoresis-mass Spectrometry for Top-down Proteomics
Liangliang Sun

- 2:10 PM Silica Fluorination - A Novel Electroosmotic Flow Control Approach
Christopher Harrison
- 2:30 PM Characterization of Molecular and Biomolecular Interactions with Lipid Bilayers Using Nanodisc Affinity Capillary Electrophoresis
Christopher Palmer
- 2:50 PM Monitoring Phosphorylation and Methylation of Histone Peptides Using Host-assisted Capillary Electrophoresis
Wenwan Zhong
- ATOM-03 **Atomic Spectroscopy Techniques for Nuclear Applications****
Chair: Benjamin Manard
- 1:30 PM The Use of Automation to Improve Analytical Precision of Isotopic and Impurity Analysis
Cole Hexel
- 1:50 PM Balancing Actinide Measurement Quality with the Needs of the Data End-user: A Critical Evaluation of ICP-MS Instrumentation and Techniques in the Nuclear Sciences
William Kinman
- 2:10 PM Overview of Laser Ablation-based Optical Spectroscopy Techniques for Radiological Analysis
Kyle Hartig
- 2:30 PM Innovative Sample Preparation Methodologies for ICP-MS Analysis of Nuclear Materials
John Brockman
- AWD-08 **ANACHEM Award Symposium Honoring Robert Kennedy****
Chair: Robert Kennedy
- 1:30 PM Microfluidic Design Advances Immunoblotting to the 21st Century
Amy Herr
- 1:50 PM Microfluidic Strategies for Measuring Adipocyte Signalling
Michael Bowser
- 2:10 PM Microfluidic Devices to Investigate Dynamic Signaling in Pancreatic and Liver Cells
Michael Roper
- 2:30 PM Microfluidic Tools for Epigenetic Profiling and Diagnostics
Ryan Bailey
- 2:50 PM Microfluidic Manipulation of Living Immune Tissue
Megan Catterton
- BIM-04 **Spectroscopy and Precision Medicine****
Chair: Michael Walsh
- 1:30 PM Investigating Scleroderma Skin Biopsies with Spectroscopy
Hari Sreedhar
- 1:50 PM Biofluid Disease Diagnostics: A High-throughput Spectroscopic Method for the Detection of Brain Tumours
James Cameron
- 2:10 PM Use of Raman Spectroscopy for the Study of Radiation Response in Brain Tumour Cells
Iona Hill
- 2:30 PM Fourier Transform Infrared Spectroscopy Reveals Mechanism of Bone Mineral Formation: From Amorphous Precursor to Mature Crystal
William Querido
- 2:50 PM Multi-modal Imaging Analysis on Joint Capsule Tissue from Total Hip Replacement Patient
Songyun Liu

- IR-10** **Recent Advances in Using Molecular Spectroscopy for Pharmaceutical Research**
Chair: Mike George
- 1:30 PM Introducing Selectivity and Improved Sensitivity for In-line Measurements of Stirred Suspensions with
 Ultrasound-enhanced Raman Spectroscopy
Karin Wieland
- 1:50 PM Battling the Myths of Process FTIR Spectroscopy
Dan Wood
- 2:10 PM Process Optimisation for Manufacturing with Light
Mike George
- 2:30 PM Speaker Roundtable
Karin Wieland
- LIBS-02** **LIBS for Industry 4.0**
Chair: Francois Doucet
- 1:30 PM LIBS in the Aluminum Recycling Processes
Amy Bauer
- 1:50 PM LIBS: The Ideal Tool for Industry 4.0
Francois Doucet
- 2:10 PM Experimental Design: A Helpful Tool Before LIBS On-site Analyses of Agricultural Soils
Bruno Bousquet
- 2:30 PM LIBS for Quality Control in the Pharmaceutical Industry: Case of Asbestos in Cosmetic Powders
Herve Sanghapi
- 2:50 PM Temporal-spatial Resolved Laser-induced Breakdown Spectroscopy of T91 Steel of Different Aging
 Grades
Meirong Dong
- LIBS-05** **Archaeology and Anthropology**
Chair: Matthieu Baudelet
- 1:30 PM pXRF and pLIBS for Archaeological Ceramics
Mary Kate Donais
- 1:50 PM Matrix-matched Standards for Anthropology Studies
Matthieu Baudelet
- 2:10 PM Hot Tea Demineralizes Enamel While Cold Tea Protects: Spectroscopic and Microscopic Analysis
Sinai H. C. Manno
- 2:30 PM Speaker Roundtable
Matthieu Baudelet
- RAM-08** **SERS III**
Chair: Duncan Graham, Colin Campbell, Roy Goodacre
- 1:30 PM Charge transfer effects in the detection of proteins
Zachary Schultz
- 1:50 PM Chemically Imaging Cells with Super-resolution SERS
Nathan Lindquist
- 2:10 PM Gold Nanostars Enable Quantification of Cancer Biomarkers at the Single Cell Level
Laura Fabris
- 2:30 PM Self-folding Hybrid Graphene Skin for 3D SERS Imaging of Single Live Cells
Santosh Paidi
- 2:50 PM 3D Time-lapse SERS Imaging of Living Cells for Detection of Alkyne-tagged Drug Uptake
Kazuki Bando

- RAM-17** **Raman Spectroscopy for Security and Forensics Purposes**
Chair: Igor Lednev
- 1:30 PM Point-of-use Raman Solutions for Security and Forensics Purposes: Opportunities and Challenges of Real-world Deployment
Jürgen Popp
- 1:50 PM How Raman Spectroscopy Can Be Used to Assess Selective Drug Detection Using Molecular Imprinted Polymers
Amanda Haes
- 2:10 PM Development of Standoff Deep UV Resonance Raman Determination of Trace Explosives
Sandy Asher
- 2:30 PM New Horizons in Organic Gunshot Residue Analysis
Shelby Khandasammy
- 2:50 PM Standoff Detection of Threat Materials Using a FAST-SHS Raman Hyperspectral Imaging Sensor
Nirmal Lamsal
- SPEC-02** **SAS Session: Microplastics in the Environment I**
Chair: Andrew Whitley, Shelly Moore
- 1:30 PM Microplastics Differ Between Indoor and Outdoor Air masses: Insights from Multiple Microscopy Methodologies
Emily Gaston
- 1:50 PM A Comparison Of multiple Techniques, FT-IR, Py-gcms, and Raman for Polymer Identification in Plastic Marine Debris
Eunah Lee
- 2:10 PM Detection and Analysis of Microplastics Using Raman Spectroscopy
Sarah Shidler
- 2:30 PM Rapid, Automated Analysis of Microplastics Using Laser Direct Infrared Imaging and Spectroscopy
Darren Robey
- 2:50 PM Methods Workshop Held to Advance the Development of Standardized Methods to Measure Microplastics
Shelly Moore
- SPR-02** **Sensing with Plasmonics**
Chair: Amanda Haes, Jean-Francois Masson
- 1:30 PM Pyrolyzed Photoresist Films: Utility of Carbon Substrates in Immunometric Assays Using Surface-enhanced Raman Scattering
Marc Porter
- 1:50 PM 3D Printing for Plasmonic Interfaces and Biosensing
Quan Cheng
- 2:10 PM Going Green with Silver: Development of Sustainable Plasmonic Sensors
Christa Brosseau
- 2:30 PM Sensitive, Selective, and Quantitative Copper Sensor Using Click-chemistry with Gold Nanoparticles
ReJeana Cary
- 2:50 PM The Plasmonic Stability of Gold Nanostars Synthesized Using Good's Buffers
Amanda Haes
- SPSJ-04** **Near Infrared Spectroscopy II**
Chair: Shigeaki Morita
- 1:30 PM Novel Miniaturized Spectrometric Attempts to Monitor Quality of Food and Medicinal Plant Products
Christian Huck
- 1:50 PM Improving Preprocessing of Spectral Data by the VSN (Variable Sorting for Normalization) Algorithm
Federico Marini

- 2:10 PM Relationship Between Bioactivity and Water Structure Analyzed by NIR Spectroscopy
Mika Ishigaki
- 2:30 PM Optimization of Enhanced Near-infrared Spectroscopic Technique for Rapid Chemical Composition Analysis
Kodai Murayama

3:10 pm – 3:50 pm Poster Viewing and Break

3:50 pm – 5:30 pm Afternoon Symposia

AES-06 AES: Leaders in the Field

Chair: Sagnik Basuray, Adam Woolley

- 3:50 PM Precision Medicine Is Advanced by Profiling Cellular-to-molecular Diversity Using Electrophoretic Cytometry
Amy Herr
- 4:10 PM 3D-printed Tools for Quantitative Bioanalysis
Dana Spence
- 4:50 PM Microfluidic Organic Chemical Analyzers for Detection of Solar System Biosignatures
Richard Mathies

ATOM-09 High End ICP-MS Instrumentation

Chair: Johanna Irrgeher

- 3:50 PM SAS Atomic Section Student Award Winner: A Comparative Analysis of Optical Spectrometric Methods and MC-ICP-MS for Stable Isotope Analysis of Magnesium in Geological Samples
Carlos Abad
- 4:10 PM Application of Single Particle Inductively Coupled Plasma-mass Spectrometry (sp-ICP-MS/MS) in the Analysis of Nanoparticles in Hydrocarbons
Jenny Nelson
- 4:30 PM Optimizing ICP-MS/MS for Ultra Trace Analysis of Challenging Elements in Environmental Applications
Daniel Proefrock
- 4:50 PM Sulfur Isotope Analysis at Ultra Trace Levels by EA-MC ICP-MS
Michael Wieser
- 5:10 PM Potential of MC-ICP-CC-MS in Cosmochemistry and Geochronology
Justin Simon

CHEM-03 Chemometrics at Work in Industry

Chair: Neal Gallagher

- 3:50 PM Application of NIR in the Oil/Gas Industry
Randy Bishop
- 4:10 PM Autonomous Calibration
Brian Rohrback
- 4:30 PM Compression is Good for the Goal?
Donal O'Sullivan
- 4:50 PM On-line, real-time monitoring for process control and optimization: processing nuclear materials
Amanda Llnes
- 5:10 PM Modern Tools for Model Development and Maintenance
Paul Cammarata

CTP-03 Solving Developing World Chemistry Challenges: Where Are We Now?

Chair: Diane Parry

- 3:50 PM Spectroscopy and Alternative Plastics from Vegetable Oils
Isao Noda
- 4:10 PM Hardware and Software Tools to Enable High-Quality Portable Mass Spectrometry Analyses
Jacob Shelley

- 4:30 PM Applying Chemistry to Confront International Humanitarian Problems
Ronda Grosse
- 4:50 PM Strategies to Keep Research Moving Amidst Disaster Relief
Ellen Miseo
- 5:10 PM High-speed Quantitation of More Than 30 Bioprocess Media Metabolites/nutrients with Miniature CE-MS
Christopher Brown
- IR-06 Mid-IR Frequency Combs**
Chair: Bernhard Lendl
- 3:50 PM Dual Comb Spectroscopy with Quantum Cascade Lasers: Development, Outlook, and New Possibilities
Raphael Horvath
- 4:10 PM Molecular Spectroscopy with Frequency Combs
Oliver Heckl
- 4:30 PM Electro-optic Dual Optical Frequency Comb Generators: Evolution and Opportunities in Spectroscopy
Pedro Martín Mateos
- 4:50 PM Semiconductor Laser Frequency Combs: From Fundamentals Towards Applications
Johannes Hillbrand
- 5:10 PM Multi-species Chemical Sensing Using QCL Based Dual Comb Spectroscopy
Jonas Westberg
- LIBS-08 LIBS Elemental Imaging**
Chair: Vincent Motto-Ros
- 3:50 PM Combining Spectroscopic and Tomographic Data
Jozef Kaiser
- 4:10 PM Multiscale Quantitative Mineral Analysis by Laser-induced Breakdown Spectroscopy
Elton Soares de Lima Filho
- 4:30 PM Multi-sensor Imaging by LIBS
Jhanis Gonzalez
- 4:50 PM Elemental Imaging by LIBS: Recent Advances and Remaining Challenges
Vincent Motto-Ros
- 5:10 PM Imaging Biochemical Signatures of Stress Events in Human Deciduous Teeth
Bruno Bousquet
- PAT-06 PAT Enabled Flow Chemistry and Continuous Manufacturing**
Chair: Jim Rydzak, Savitha Panikar
- 3:50 PM Process Intensification Tactics in the Quest for Advancing Global Health Access
Katherine Belecki
- 4:10 PM In-line FTIR Technology: Application to Continuous Flow Chemistry
Norman Wright
- 4:30 PM Sampling Devices for In-line near Infrared Spectroscopy Monitoring of Powder Blend Homogeneity in Continuous Manufacturing
Anders Sparen
- 4:50 PM The Tablet Press Feed-frame as a Optimum Point for Monitoring the Quality of a Tablet Product Made Using a Continuous Manufacturing Process
Steve Hammond
- 5:10 PM Development of Categorical Chemometric Models to Support Continuous Drug Product Manufacturing
Caitlin Schram

- PMA-09 **Pharmaceutical Forensics: Applying Analytical Science to Safe Manufacturing, Supply, and Screening****
Chair: Ravi Kalyanaraman, Scott Huffman
- 4:10 PM Colombian Procedure for Handling of Falsified/Altered Products
Miller Lysen
- 3:50 PM USP Technology Review Program for Evaluating Screening Technologies for Medicine Quality Assurance
Stephen Kimatu
- 4:30 PM Combatting the Illegal Trade of Medicines: BMS Strategy Against Counterfeiting, Tampering, Diversion and Theft
Ramon Rivera
- 4:50 PM SERS for the Detection and Analysis of Fentanyl
Li-Lin Tay
- 5:10 PM Development of Pharmaceutical Tablet Authentication System using Spectroscopic Techniques in combination with Multivariate Method
Md Nayeem Hossain
- RAM-12 **Emerging Raman****
Chair: Pavel Matousek, Duncan Graham, Ian Lewis
- 3:50 PM Interference-enhanced Raman Spectroscopy as a Tool for Developing Chip-based Sample Preparation Strategies
Susanne Pahlow
- 4:10 PM Time-gated Raman Mapping Using DMD-based Spectral Multiplexing
Ioan Notingher
- 4:30 PM Raman Fusion Spectroscopy: Multi-wavelength Excitation for Compact Devices
Johannes Kiefer
- 4:50 PM Towards Raman-based cell sorting as a quality control step for highly efficient 3rd generation bio kerosene production
Karin Wieland
- RAM-16 **Stand-off Raman****
Chair: Nathaniel Gomer
- 3:50 PM Standoff Chemical and Explosive Detection of Military Relevant Threats
Jason Guicheteau
- 4:10 PM Standoff Raman and Raman Imaging Using a Monolithic Spatial Heterodyne Raman Spectrometer
S. Michael Angel
- 4:30 PM Underwater Time-gated Standoff Raman Spectroscopic Sensor for Detecting Hazardous Chemicals
Shiv Sharma
- 4:50 PM Advancements in Standoff Detection of Chemical, Explosive and Narcotic Threats Using Raman FAST Hyperspectral Imaging
Matthew Nelson
- 5:10 PM Government Applications for Emerging Standoff Detection Equipment
Michael Shepard
- SPEC-05 **SAS Session: Microplastics in the Environment II****
Chair: Andrew Whitley
- 3:50 PM Increasing the Accessibility for Characterizing Microplastics: Introducing New Application-based and Spectral Libraries of Plastic Particles (SLOPP & Slopp-e)
Bridget O'Donnell
- 4:10 PM Open Specy: An Open Source, Online, Spectra Classification and Sharing Tool
Win Cowger
- 4:30 PM Microplastic Identification Using Non-optimized Discriminant Fusion Classification Based on ATR-FTIR Spectroscopy
John Kalivas

- 4:50 PM Development of Automatic Microplastic Measurement with Surface Z-axis Tracking Mode by μ -RAMAN Imaging Spectroscopy
hyo jin kim
- 5:10 PM Identification of Microplastic Particles Using Vibrational Spectroscopy Coupled to Multivariate Analysis
Maria El Rakwe
- SPR-06** **Rising Stars in Plasmonics**
Chair: Jean-Francois Masson
- 3:50 PM Angstrom Scale Chemical Analysis of Metal-supported Regioisomeric Assemblies by Ultrahigh Vacuum, Tip-enhanced Raman Spectroscopy
Nan Jiang
- 4:10 PM Hot Electron Dynamics in Plasmonic Thermionic Emitters
Matthew Sheldon
- 4:30 PM Point-of-Care Plasmonic Devices for Bacterial Pathogen Detection
Laura Sagle
- 4:50 PM Digital Plasmonic Holography
Ryan Spies
- 5:10 PM Surface Plasmon Resonance Biosensor Design for Domoic Acid Biomarker Detection and Evaluation of Chronic Exposure
Betsy Jean Yakes

7:00 pm SAS Awards Ceremony: Followed by SAS Invite-only Reception at 8:00 pm

WEDNESDAY, OCTOBER 16

7:45 am – 9:00 am Plenary Session

Chair: Mary Kate Donais

8:00 am **Lester W. Strock Award**



Remote LIBS, Raman and Hyperspectral Raman Imaging Using a Monolithic Spatial Heterodyne Spectrometer

S. Michael Angel, University of South Carolina

8:30 am



**AES Electrophoresis Mid-Career Award
Digitizing Endocrine Tissue Secretions into Nanoliter Droplets for Analysis of Hormones and Metabolites at High Temporal Resolution**

Christopher J. Easley, Auburn University

9:15 am – 10:55 am Morning Symposia

ATOM-04 Atmospheric Pressure Glow Discharge Spectroscopies I (Instrumentation)

Chair: R. Kenneth Marcus

9:15 AM A New Ionization Source for Environmental Mass Spectrometry

Charles Wilkins

9:35 AM Factors Effecting Uranium Isotope Ratio Measurements in the Ls-apgd/orbitrap Coupling

R. Kenneth Marcus

9:55 AM SAS Atomic Section Student Award Winner - Elemental Mass Spectrometry of Fluorine: Challenges and Innovations in Ionization and Detection

Joseph Lesniewski

10:15 AM Investigations of Matrix Management Protocols for the Solution Cathode Glow Discharge (SCGD)

Stuart Schroeder

10:35 AM New Approaches for a Combined Atomic and Molecular (CAM) Ionization Source

David Koppelaar

- AWD-05** **Lester Strock Award Symposium Honoring S. Michael Angel**
Chair: S. Michael Angel
- 9:15 AM Exploring the Planets with LIBS, Raman, and Luminescence Spectroscopies: Chemcam, Supercam and SHERLOC on Nasa's Mars 2020 Rover, and More to Come
Roger Wiens
- 9:35 AM Advances in Combined Time-resolved Remote LIBS and Raman Spectroscopy
Shiv Sharma
- 9:55 AM Laser Ablation Spectrochemical Analysis
Rick Russo
- 10:15 AM Characterizing Limiting Noises in Laser Induced Breakdown Spectroscopy: Still- challenging Issues
Nicolò Omenetto
- 10:35 AM Deployment of a LIBS System Using a Remotely Operated Vehicle at Seafloor Hydrothermal Vents
Alan Chave
- AWD-07** **AES Mid-Career Award Symposium Honoring Chris Easley**
Chair: Jason Dwyer, Christopher Harrison
- 9:15 AM Microfluidic Systems for Studying the Gut Microbiome
Charles Henry
- 9:35 AM Electrophoretic Analysis of Small Molecules Released from Islets of Langerhans
Michael Roper
- 9:55 AM Integrating Microfluidic-based Cell Culture with Analysis
R. Scott Martin
- 10:15 AM Selective Assembly and Analysis of Melanoma Cells and Cell Clusters at an Array of Bipolar Electrodes
Robbyn Anand
- 10:35 AM 3D Printed Integrated Microfluidic Devices for Extraction, Fluorescence Labeling, and Separation of Preterm Birth Biomarkers
Anna Nielsen
- BIM-05** **Vibrational Spectroscopy: Toward Clinical Applications**
Chair: Karen Esmonde-White, Fay Nicolson
- 9:15 AM Investigating Term and Preterm Labor Using in Vivo Raman Spectroscopy
Laura Masson
- 9:35 AM Raman Imaging of Breast Microcalcifications from a Relevant Patient Cohort Reveals New Insights into the Vibrational Features of These Important Cancer Signs
Renzo Vanna
- 9:55 AM Red Blood Cell Degradation Evaluated by Raman Spectroscopy
Richard Dluhy
- 10:15 AM Study of Red Cell Concentrate (RCC) Supernatant for the Non-invasive Assessment of Storage-related Changes Using Deep Raman Spectroscopy
Martha Vardaki
- 10:35 AM A tale of diagnostic imaging and commercialization: why understanding each chapter matters
Katherine Cilwa
- CHEM-04** **Chemometric Opportunities in the Forensic Sciences**
Chair: Rabi Musah
- 9:15 AM Food Authentication and Adulteration Detection with Data Fusion of Non-optimized Classifiers
John Kalivas
- 9:35 AM Determining the Strength of Forensic Lubricant Evidence from DART-MS and GC-MS Data
Candice Bridge
- 9:55 AM A Regression-based Algorithm to Maximize the Confidence in Mass Spectral Identifications
Glen Jackson

- 10:15 AM Multi-label Classification Methods for the Forensic Identification of Fauna or Flora Within Mixtures
Samira Beyramysoltan
- 10:35 AM Combining Advanced Statistical Methods and Laser-induced Fluorescence in Forensic Analysis
George Donati
- FORENS05** **Methods for Challenging Forensics Applications**
Chair: Greg Klunder
- 9:15 AM Kinetic and Thermodynamic Models of Evaporation for Forensic Applications
Victoria McGuffin
- 9:35 AM Evaluating the Impact of Preconcentration using Silicon Nanowire Arrays with Ion Mobility Spectrometry
Matthew Mullen
- 9:55 AM Predicting the lifetime of trace explosives materials on surfaces
Michael Papantonakis
- 10:15 AM Adaptive Multivariate Chemical Imaging for High-throughput Detection of Illicit Substances in Mail
Shawna Tazik
- 10:35 AM Near-Infrared Spectroscopy of Gases from Heated Explosives
Greg Klunder
- IR-07** **Time-resolved IR and 2D-IR Spectroscopy**
Chair: Mike George
- 9:15 AM Pulse Radiolysis with Time-resolved Infrared Detection: A Powerful Method for Unraveling the Mechanisms of Redox Processes
David Grills
- 9:35 AM Development and Applications of Quantum Cascade Laser Frequency Comb Spectroscopy for Fast Time-resolved IR Spectroscopy
Raphael Horvath
- 9:55 AM Isolating Protein Amide I Signals in Water Using 2D-IR Spectroscopy
Samantha Hume
- 10:15 AM Time-resolved Resonance Raman Studies of Re(i) Complexes with Blended Intraligand and Metal-to-ligand Charge-transfer States
Keith Gordon
- 10:35 AM Filming Chemical Reactions at the Single-molecule Level Using Electron Beam
Khlobystov Andrei
- LIBS-04** **Molecular Signal in LIBS**
Chair: Michael Gaft
- 9:15 AM Progress in Laser Ablation Molecular Isotopic Spectrometry (LAMIS)
Alexander Bol'shakov
- 9:35 AM LIBS-MLIF method for halogens detection in air ambient conditions
Lev Nagli
- 9:55 AM Molecular Emissions in the Laser-induced Plasma in Simulated Martian Conditions: Calibration Models and New Insights from Plasma Imaging
David Vogt
- 10:15 AM Using Molecular Bands for Geological Purposes: An Exploratory Fluor Study
Cécile Fabre
- 10:35 AM Molecule Formation In Calcium Carbonate And Calcium Hydroxide Libs Plasmas: Model And Experiment
Igor Gornushkin
- PAT-05** **Advances in On-line Process Analysis**
Chair: Alison Nordon
- 9:15 AM Machine Learning and Online Analysis for Advanced Process Control and Optimisation
Aparajith Bhaskar

- 9:35 AM Rapid In-situ Measurement of Parahydrogen Fraction with Raman Spectroscopy and the Use of Parahydrogen for Enhanced Sensitivity Benchtop NMR Spectroscopy
Andrew Parrott
- 9:55 AM Advantages of Measuring Moisture Content with Process Analytical Technology
Adam Hopkins
- 10:15 AM A Digital Science Platform for Process Chemometric Model Maintenance
David Joyce
- 10:35 AM Design and Development of a Samples and Variable Selection Method for a Robust Partial Least Squares (PLS) Regression
Rajesh Morampudi
- PMA-08 Artificial Intelligence in Pharma**
Chair: Steve Buckley, Peter Harrington
- 9:15 AM The Role of Ai-powered Computational Pathology to Advance Biomarker Discovery in Pharma
Vipul Baxi
- 9:35 AM Machine Learning for Characterizing and Authenticating Natural Medicines
Peter Harrington
- 10:15 AM Machine Learning Implementation in Practical Environments
Steve Buckley
- 10:35 AM Limit of Detection Calculations in Multivariate Model Applications
Doug Steinbach
- RAM-01 Low Frequency Raman**
Chair: Anjan Roy
- 9:15 AM Time-resolved (Ten Milli-second) Low Frequency Raman Spectroscopy: A Method of Evaluating Dynamic Behaviour in Drug Formulations
Keith Gordon
- 9:35 AM Low-frequency Raman Spectroscopy of Modern and Ancient Pigments
Timothy Korter
- 9:55 AM Quantification of Crystalline Active Pharmaceutical Ingredients by Transmission Low-frequency Raman Spectroscopy
Motoki Inoue
- 10:15 AM Novel Method for Solubility Determination of Crystalline Drugs in Polymeric Matrices Using Hot Melt Extrusion and Terahertz-Raman Spectroscopy
Ecaterina Bordos
- 10:35 AM THz-raman Measurements of Crystallinity and Form in Pharmaceuticals and Drug Development
Anjan Roy
- RAM-13 Biomedical Raman (CLIRSPEC)**
Chair: Nick Stone
- 9:15 AM Multimodal, Label-free Detection of Ganglion Cells for Diagnosing Hirschsprung Disease
James Chan
- 9:35 AM Unique Nano-assemblies Built of "Off-the-shelf" Components for Raman Theranostics
Priyanka Dey
- 9:55 AM Using Cholesterol Modified Nanoparticles as Agents for Cardiovascular Disease Systems
Fatima Ali
- 10:15 AM Breast Tumors Tissue Phantom: Mimicking and Modelling the Raman Spectra from Different Breast Cancers
Rishikesh Pandey
- 10:35 AM Assessing Liver Health for Transplant
Colin Campbell

11:00 am – 11:45 am Poster Viewing

11:30 am – 12:45 pm Exhibit Hall Activities

“What’s Hot” Vendor Presentations (11:30 am - 1:20 pm)

Complimentary Lunch (12:00 - 12:45 pm)

1:30 pm – 3:10 pm Afternoon Symposia

AES-05 Biosensors

Chair: Erin Henslee, Rucha Natu

1:30 PM TBD

1:50 PM Detecting Single Nucleotide Polymorphism with Giant Magnetoresistive Biosensor
Todd Klein

2:10 PM Microfluidic Platform for Biomarker Detection; from Maternal Disease to Cancer
Zeinab Ramshani

2:30 PM A rapid and low cost peptide sensor for Pb²⁺ detection by direct interface capacitance measurement
Jie Wu

2:50 PM Borrowing from Packed Bed Reactors: A flow-through, nano-porous, shear-enhanced electrode for electrochemical spectroscopy - A sensitive and selective Biosensor
Sagnik Basuray

ATOM-05 Atmospheric Pressure Glow Discharge Spectroscopies II (Applications)

Chair: R. Kenneth Marcus

1:30 PM Analysis of Nanoparticles Using Novel Approaches to Solution-cathode Glow Discharge Atomic Emission Spectrometry
Steven Ray

1:50 PM Developments in Solution-cathode Glow Discharge for Elemental Analysis of Aqueous Samples
Michael Webb

2:10 PM Liquid-electrode Plasma Induced Vapor Generation Method
Zhenli Zhu

2:30 PM Plasmas in Contact with Liquids: Physicochemical Processes at the Plasma-liquid Interface
Selma Mededovic Thagard

2:50 PM Elemental Analysis in the Petroleum Industry Using Plasma Techniques
Laura Poirier

CHEM-05 Unraveling Sample Matrix Effects with Chemometrics

Chair: John Kalivas

1:30 PM The Development of Chemometric Functional Libraries
Leonardo Ramirez-Lopez

1:50 PM Local Calibration Using Multivariate Curve Resolution Methods
Hamid Abdollahi

2:10 PM Quantification of Mixtures in Presence of Interferences and Matrix Effects by Multivariate Curve Resolution
Roma Tauler

2:30 PM Identifying Matrix Matched Samples by Leveraging Spectral Calibration Model Regression Vectors
John Kalivas

2:50 PM Modeling and Performance Evaluation of a Real-time Molecular Chemical Imaging (MCI) Surgical Endoscope
Arjun Bangalore

- CTP-04 **Deviations from the Beer-lambert Law: New Perspectives and Solutions****
Chair: Jürgen Popp, Thomas Mayerhöfer
- 1:30 PM The Bouguer-beer Lambert Law (re-)viewed from a Wave Optics Perspective
Thomas Mayerhöfer
- 2:10 PM Beyond the Beer-lambert Approximation, Considerations for Quantitative Chemical Analysis at the Nanoscale with the PTIR Technique
Andrea Centrone
- 2:30 PM A Comparison of Computational Approaches to Remove "Artefacts" in IR Spectroscopy
Shuxia Guo
- 2:50 PM Infrared Spectroscopic Imaging - From a Simple Combination of Spectroscopy and Microscopy to New Design Concepts
Rohit Bhargava
- FORENS-03 **Forensic Analysis in the Lab and at the Crime Scene****
Chair: Igor Lednev
- 1:30 PM Forensic Science R&D Funding at the National Institute of Justice: Opportunities for Novel Spectroscopic and Analytical Techniques Applied to Forensic Problems
Gregory Dutton
- 1:50 PM Utilization of Portable Gas-chromatographic Systems Coupled with CMV for On-site Detection of Ignitable Liquid Residues
Jose Almirall
- 2:10 PM On the Mass Spectral Interpretation of Cathinones and Fentanyl Analogs
Glen Jackson
- 2:30 PM Nondestructive Analysis of a Bloodstain by ATR FT-IR Spectroscopy for Forensic Purposes
Ewelina Mistek
- 2:50 PM On-scene Trace Identification of Materials of Grave Toxicity with Handheld Mass Spectrometry
Christopher Brown
- IR-08 **Recent Advances in Chemical and Material Detection Using Molecular Spectroscopy****
Chair: Mike George
- 1:30 PM Standoff Detection of Threat Chemical Traces on Surfaces by active Long Wave Infrared Backscatter Imaging Spectroscopy
Robert Furstenberg
- 1:50 PM Detection and Identification of Deposited Biological Hazards Using Infrared Spectroscopy
Kelly Curtis
- 2:10 PM An Infrared Spectroscopic Study of Hazardous Chemicals Deposited Using a Piezoelectric Printer
Linda Lee
- 2:30 PM Advances in Sorbent Materials for Detection and Protection Applications
Tyler Grissom
- 2:50 PM Frequency Comb Spectroscopy as a New Modality for Infrared Micro-spectroscopy
Henry Timmers
- LIBS-11 **2019: International Year of the Periodic Table at the Speed of Light (New Methodology)****
Chair: Sebastian Wachsmann-Hogiu
- 1:30 PM Elemental Concentrations Calibrations of Phosphate Slurries and Solid Pellets Using Laser Induced Breakdown Spectroscopy
Driss Lahlou Kitane
- 1:50 PM LIBS as a method to study and characterize biological materials
Sebastian Wachsmann-Hogiu
- 2:10 PM 2.5D LIBS Imaging Using Adaptive Optics
Pablo Sobron

- 2:30 PM Fast Compositional Tomography of Ore Samples by Laser Induced Breakdown Spectroscopy
Nicolas Montreuil
- 2:50 PM Molecules in Laser Induced Plasma: Plasma Characterization and Applications
Timur Labutin
- PAT-03 Industrial Applications of Vibrational Spectroscopy**
Chair: Mark Rickard, Xiaoyun Chen
- 1:30 PM Advanced Fiber Spectroscopy in 0.3-16 μ m Range for Biomedical & Process Control Applications
Viacheslav Artyushenko
- 1:50 PM Raman spectroscopic quantitative analysis of a water soluble polymer synthesis: From the lab to the plant
Peter Larkin
- 2:10 PM Detecting Organic Contaminants in Water via Mid-infrared Fiber-optic Evanescent Field Spectroscopy
Carina Dettenrieder
- 2:30 PM Novel Attenuated Total Reflection Sensor Concepts for Quantum Cascade Laser - Based Infrared Spectroscopy in Harsh Environments
Andrea Teuber
- 2:50 PM Fabrication and Analysis Tools for Real-time Environmental Monitoring by Surface-enhanced Raman Spectroscopy (SERS)
Jason Dwyer
- PMA-11 Spectroscopy for Pharmaceutical Applications**
Chair: Shengli Ma, Raphael Fish
- 1:30 PM Characterize Complex Drug Products Using Morphologically Directed Raman Spectroscopy (MDRS)
Changning Guo
- 1:50 PM Characterization of linker Bond in Pharmaceutical Molecules by Vibrational Spectroscopy
Shengli Ma
- 2:30 PM *Michelle Raikes*
- 2:50 PM Speaker Roundtable
Shengli Ma
- RAM-05 Portable Raman**
Chair: Neil Shand
- 1:30 PM Mobility Integration into Handheld Raman Devices
Keith Carron
- 1:50 PM Sense and Sensitivity: Compact Raman Without Compromise
David Creasey
- 2:10 PM Portable Raman Spectroscopy for Medical Applications
Fay Nicolson
- 2:30 PM Raman-on-chip for High-throughput, High-resolution Handheld Spectroscopy
Hilde Jans
- 2:50 PM Fiber-based Raman In-situ Chemical Sensing Using Modular and Monolithic Spatial Heterodyne Raman Spectrometers (SHRS)
J. Chance Carter
- SPEC-01 SAS Session Commemorating John Jackovitz**
Chair: Robert Lascola
- 1:30 PM How a Spectroscopy Legend Helped a Pittsburgh Start Up
Chuck Gardner
- 1:50 PM Deep Ultraviolet Standoff Photoacoustic Spectroscopy of Trace Explosives
Sandy Asher

- 2:10 PM Biosensing with Raman Spectroscopy - A Career Influenced by John F. Jackovitz
Bhavya Sharma
- 2:30 PM Innovative Vibrational and Rotational Spectroscopy for Pharmaceutical Industry - From Small Molecules to Biologics
Rina Dukor
- 2:50 PM Hyperspectral Raman Imaging Using a Monolithic Spatial Heterodyne Raman Spectrometer
S. Michael Angel

SPR-05 Multimodal and Multifunctional Plasmonics

Chair: Wei-Chuan Shih

- 1:30 PM Nanostructured Metasurfaces for Plasmon-enhanced Nonlinear Optical Spectroscopy
Andrea Tao
- 1:50 PM Plasmonic Structures and Applications Fabricated Using Collapsible Nano-Fingers
Boxiang Song
- 2:10 PM Plasmonic Bio-chip for RGB Cameras
Wei-Chuan Shih
- 2:30 PM Asymmetric Deposition of Platinum Atoms on Gold Nanorods Induced by a Substrate for Synthesis of Anisotropic Bimetallic Nanostructures
Mahmoud Abdelwahed
- 2:50 PM Utilization of Plasmonic Nanostructures for Highly Sensitive Vibrational Biospectroscopy
Jürgen Popp

3:10 pm – 3:50 pm Poster Viewing and Break

3:50 pm – 5:30 pm Afternoon Symposia

ATOM-06 Atmospheric Pressure Glow Discharge Spectroscopies III (Molecular)

Chair: Jacob Shelley, Steven Ray

- 3:50 PM Atmospheric Pressure Plasmas Coupled with Differential Mobility Spectrometry
Theresa Evans-Nguyen
- 4:10 PM Simple, Rapid Chemical Modification and Analysis of n-Alkanes with Flowing Atmospheric-pressure Afterglow (FAPA) Mass Spectrometry
Brian Molnar
- 4:30 PM Molecular Analysis with High Repetition-rate Laser-induced Micro Plasma in Air
Yi You
- 4:50 PM SAS Atomic Section Student Award Winner: An Exploratory Investigation of the Liquid Sampling – Atmospheric Pressure Glow Discharge for the Mapping of Molecular and Atomic Species of Biological Samples
Htoo Paing
- 5:10 PM Evaluating the Use of the LS-APGD Ionization Source for Protein Analysis
Edward Hoegg

AWD-09 AES Lifetime Achievement Award Session Honoring Hsueh-Chia Chang

Chair: Satyajyoti Senapati, Gongchen Sun

- 3:50 PM Isolation, Fractionation and Analysis of Exosomes
Hsueh-Chia Chang
- 5:10 PM Acoustic-electric Interactions at Micron and Nanometre Scales
Leslie Yeo
- 4:30 PM Nanochannel Electroporated Cell Transfection And Vesicle Secretion For Nucleic Acid Delivery - -cancer Therapy, Immune Disease Treatment, and Regenerative Medicine
James Lee

- CHEM-06** **Sample and Variable Selection: Memorial Session Honoring Frank Vogt**
Chair: Barry Lavine
- 3:50 PM A Novel Multivariate Curve Resolution-alternating Least Squares (MCR-ALS) Methodology for Application in Hyperspectral Raman Imaging Analysis
Joseph Smith
- 4:10 PM Variable Selection to Improve the Classification and Authentication of Edible Oils
Barry Lavine
- 4:30 PM Speciation of Dalbergia (Rosewood) via Hand-held Laser Induced Breakdown Spectroscopy (LIBS) and Chemometric Analysis
James Jordan
- 4:50 PM Assessing Hand-Held LIBS for Speciation of Rosewood with PLS-DA and KNN
Karl Booksh
- 5:10 PM Comparison of Spectroscopic Techniques Paired with Chemometrics for Determining the Peroxide Value of 19 Classes of Naturally Aged, Plant-based Edible Oils
Joshua Ottaway
- CTP-02** **Women in Analytical Chemistry**
Chair: Rina Dukor
- 3:50 PM Women in Analytical Chemistry - Panel Discussion
Bhavya Sharma
- LIBS-07** **Innovation in Instrumentation**
Chair: Francois Doucet
- 3:50 PM Design and Development of Industrial Instrumentation
Steve Buckley
- 4:10 PM Evaluation of Portable LIBS and Portable XRF in the Frame of Multi-elemental Analysis of Agricultural Soils and Plants
Bruno Bousquet
- 4:30 PM Application of Advanced Machine Learning Classification Techniques to Analyze Complex LIBS Spectra
Prasoon Diwakar
- 4:50 PM Plant Analysis by Laser-induced Breakdown Spectrometry (LIBS)
Aleksandr Zakuskin
- MASS-01** **MS Characterization of Proteins, Protein Complexes, and Therapeutic Proteins**
Chair: Joseph Loo
- 3:50 PM The Role of Denaturing and Native-MS in Biopharma: From Target Validation to mAbs, ACDs and Beyond
Iain Campuzano
- 4:10 PM Measuring Membrane Interactions by Mass Spectrometry of Intact Lipoprotein Complexes
Michael Marty
- 4:30 PM Native Mass Spectrometry and Surface Induced Dissociation for the Study of Membrane Proteins
Sophie Harvey
- 4:50 PM Probing Protein structure by Cyclic Ion mobility and IMSn: When Resolution Just isn't enough
Roy Martin
- 5:10 PM Native Mass Spectrometry for a Top-down View of Protein Structures
Joseph Loo
- PAT-04** **Online Analysis of Industrial Processes and Reactions**
Chair: Anna Sandlin, J.D. Tate
- 3:50 PM Shelterless Gas Chromatographs for On-line Analysis: Past, Present, and Future
Eric Schmidt
- 4:10 PM Implementing Process Optical Spectrometers
Edward Orr

- 4:30 PM Microspectrometer Chips for Integrated Applications
Nadia Pervez
- 4:50 PM Revolutionizing Process Monitoring in Mining Industry with Time-gated Raman Spectroscopy
Mari Tenhunen
- 5:10 PM Deep UV Raman & Fluorescence Spectroscopy for in Situ Process Analysis
William Hug
- PMA-04 **Advanced Spectroscopic Techniques in Pharma****
Chair: Sergey Arzhantsev
- 3:50 PM Raman Optical Activity in Pharma: Studying Pharmaceutical Peptides in Solution
Christian Johannessen
- 4:10 PM Enabling Faster Route Discovery and Process Optimization with Molecular Rotational Resonance Spectroscopy
Justin Neill
- 4:30 PM Protein Solutions: Routine Higher Order Structure Analysis by Raman and Scattering Techniques
Eunah Lee
- 4:50 PM Analysis of Biomolecules by Raman Spectroscopy
Shengli Ma
- 5:10 PM Real-time Monitoring of Polymorphic Transformations with Thz Spectroscopy
Mark Arnold
- PMA-06 **Counterfeits Food Products and Dietary Supplements****
Chair: Sulaf Assi
- 3:50 PM At-Line Optical Porosity Measurements of Pharmaceutical Solids by GASMAS spectroscopy
Jonas Johansson
- 4:10 PM Using Ion Chromatography to Judge Food Authenticity and Detect Adulteration
Jeff Rohrer
- 4:30 PM Identification of Counterfeit Medicines Using Near-infrared Imaging
Ian Robertson
- 4:50 PM PharmaChk: Testing the Quality of Medicines in the Field
Darash Desai
- 5:10 PM Speaker Roundtable
Jonas Johansson
- RAM-10 **Raman Imaging/Microscopy****
Chair: Katsumasa Fujita, Duncan Graham
- 3:50 PM Raman Imaging of the Immune Cell Response to Local Environmental Changes
Alison Hobro
- 4:10 PM Saturated Stimulated Raman Scattering Microscopy for Super-resolution Vibrational Imaging
Zhiwei Huang
- 4:30 PM Novel Applications of SERS Labels in Molecular Sensing and Imaging
Wei-Chuan Shih
- 4:50 PM Imaging Intracellular Drug Distribution in Prostate Cancer Cells Using Ratiometric Raman and Stimulated Raman Scattering Microscopy
William Tipping
- 5:10 PM Evaluation of Single-cell Type, Function, and Heterogeneity Through Label-free Spectroscopic and Morphological Metrics
Nicholas Smith

- RAM-19 Raman with Spatial Light Modulators**
Chair: Ioan Notingher
- 3:50 PM Integrated Holographic Optical Tweezers Raman (HOT-Raman) Imaging
Wei-Chuan Shih
- 4:10 PM Multi-beam Raman Microscopy Using Spatial Light Modulators
Zhiyu Liao
- 4:30 PM Compressive Raman Imaging via Digital Micromirror Devices
Hilton de Aguiar
- 4:50 PM Shaping Light Through a Single Multimode Fibre for Wide-field Raman Imaging
Mingzhou Chen
- 5:10 PM Holographic Plasmonic Tweezing for Dynamic Trapping and Manipulation
John McCauley

- SPR-04 Plasmon-enhanced Techniques**
Chair: Gregory Wallace
- 3:50 PM Hybrid Gold-conductive Metal Oxide Films for Attenuated Total Reflectance Surface Enhanced Infrared Absorption Spectroscopy
J Burgess
- 4:10 PM Single-molecule Spectrum and Polarization Reshaping by Plasmonic Nanoparticles
Julie Biteen
- 4:30 PM Single Nanoparticle SPRI for Ultrasensitive Biosensing with Magnetic Hydrogel Nanoparticles
Robert Corn
- 4:50 PM Plasmonic Nanoparticles for Enhanced Nonlinear Photoabsorption Cross-Sections
Andrea Tao
- 5:10 PM Rational Design and Synthesis of Tuneable Plasmonic Nanostructures for Sensitive and Direct DNA Mutation Detection by Surface Enhanced Raman Spectroscopy
Yuan Liu

THURSDAY, OCTOBER 17

7:45 am – 9:00 am Plenary Session

Chair: Mary Kate Donais

8:00 am Applied Spectroscopy William F. Meggers Award



Reflectance Spectra of Solids & Liquids - Easier to Obtain, Harder to Interpret: The Case for the Optical Constants

Tim J. Johnson, Pacific Northwest National Laboratory

8:30 AM Coblenz Society Craver Award ***Have Fun & Impact with in situ Spectroscopy in the Chemical Industry***



Company

Xiaoyun "Shawn" Chen, Dow Chemical

9:15 am – 10:55 am Morning Symposia

ATOM-07 Atomic Spectroscopy Techniques for Nano & Bioanalysis

Chair: Martin Resano, Jose Manuel Costa-Fernandez

9:15 AM AF4 Coupled to ICP-MS/MS and Molecular Detectors for Quantitative Assessment of Nanoparticle Populations Present in Bioconjugate Mixtures
Jose Manuel Costa-Fernandez

9:35 AM SAS Atomic Section Student Award Winner: Single-particle ICP-MS for the Characterization of Nanoparticles: On Recent Improvements in Data Acquisition, Processing, Sensitivity and Dynamic Range
Ingo Streng

- 9:55 AM New Developments in the Generic Quantification of Organic Compounds and Biomolecules Using Mass Spectrometry
Jorge Ruiz Encinar
- 10:15 AM Copper and Iron Tissue Analysis: Clinical Significance and Analytic Challenges
Sarah Erdahl
- 10:35 AM Dried Blood Spots for Elemental Analysis
Martin Resano
- AWD-04 William F. Meggers Award Symposium Honoring Tim Johnson**
Chair: Tim Johnson
- 9:15 AM Accurate Methods to Determine the Optical Constants n/k for Liquids
Tanya Myers
- 9:35 AM Using Reference Spectra in the Form of n/k Values to Enable Improved Opticaltrace Surface Detection: Examples from IARPA'S SILMARILS Program
Kristin Dewitt
- 9:55 AM Applications of Optical Constants (n and k) to Standoff Detection of Threat Chemicals
Robert Furstenberg
- 10:15 AM First Principles Calculation of Reflectance Spectra of Solid Materials from N/k Values
Bradley Henderson
- 10:35 AM Speaker Roundtable
Tanya Myers
- BIM-06 Machine and Deep Learning for Biomedical Diagnostics**
Chair: Thomas Bocklitz, Rohith Reddy
- 9:15 AM Toward a Thinking Microscope: Deep Learning-enabled Computational Microscopy and Sensing
Aydogan Ozcan
- 9:35 AM Classical Machine Learning and Deep Learning for Multimodal Imaging
Thomas Bocklitz
- 9:55 AM Your Deep Learning Toolbox: Selecting the Appropriate Architecture for Spectral Images
David Mayerich
- 10:15 AM Deep Representation and Transfer Learning for Infrared Spectral Imaging Data
Arne Raulf
- 10:35 AM A Deep Learning Framework for Image Details Beyond the Infrared Spectroscopic Imaging Diffraction Limit
Kianoush Falahkheirkhah
- CHEM-07 Chemotyping Complex Materials by Chemometrics**
Chair: Mengliang Zhang
- 9:15 AM Classification of Cultivation Locations of Black Pepper (*Piper Nigrum* L.) Using DART-MS and Chemometrics
Mengliang Zhang
- 9:35 AM Raman Mapping and Multivariate Image Analysis for Characterization of Transdermal Delivery Systems
Daniel Willett
- 9:55 AM Deconvolving Co-eluted Peaks in GC-MS Fuel Data via EWFA-MCR with Automated Library Matching
Jeffrey Cramer
- 10:15 AM High-coverage and Quantitative Metabolome Analysis for Fingerprinting Complex Biological Samples
Liang Li

- FORENS-04 Environmental Forensics**
Chair: Mark Cejas, Luis Rodriguez-Saona
- 9:15 AM Analysis of PCB and Dioxin/furan Data in Environmental Forensics: Experience and Application
Glenn Johnson
- 9:35 AM Forensic Problem-solving in the Subsurface with Multiple Lines of Evidence
Mark Cejas
- 9:55 AM The Application of Multi-proxy Statistical Techniques in Identifying the Sources, Fate and Transformation of Natural Organic Carbon in South Florida Wetlands
Alice Chao Ya
- 10:15 AM Development of an R-based Implementation of the Polytopic Vector Analysis Mixing Model
Nicholas Rose
- 10:35 AM Using Aqueous Geochemical Parameters and Isotopes to Investigate the Source of Surface Water Contamination
Aaron Peacock
- LIBS-10 Environmental Monitoring**
Chair: Cassiana Nomura
- 9:15 AM Laser-induced Breakdown Spectroscopy: An Interesting Tool for Monitoring Potentially Toxic Metal in Water
Cassiana Nomura
- 9:35 AM Effect of Powder Compact Parameters on LIBS Quantitative Analysis
Matthieu Baudelet
- 9:55 AM Solid Phase Extraction Combined with Laser-induced Breakdown Spectroscopy to Elemental Analysis
Ivanise Gaubeur
- 10:15 AM Monitoring the Uptake and Toxicity of Nanoparticles in Plants Using Laser-induced Breakdown Spectroscopy
Pavel Porizka
- 10:35 AM Analysis of Plant Leaves Using Laser Ablation: Optical Emission Spectrometry
Jhanis Gonzalez
- PAT-01 SAS PAT Technical Section: PAT in the Pharmaceutical Industries Session I**
Chair: Jim Rydzak
- 9:15 AM Interfacing PAT Sensors with Processing Equipment
Steve Hammond
- 9:35 AM Quantitative In-process Raman Measurements of Solids During Continuous or Batch Manufacturing Operations
Karen Esmonde-White
- 9:55 AM In-Process Control Assessment of Final Blend Potency Using Loss-in-Weight Feeders and Near Infrared Analysis
Caitlin Schram
- 10:15 AM Distillation Process Understanding from In-situ Headspace Vapor Condensate Monitoring with Infrared Spectroscopy and Computational Modeling
Charles Goss
- 10:35 AM Multi-spectroscopic Analysis of Crystallization Processes at Extreme Environmental Conditions
Patrick Krebs
- PMA-05 Atomic Spectroscopy Applications in Pharmaceuticals**
Chair: Sharla Wood
- 9:15 AM Analysis of Common Counter-ions in Pharmaceuticals by XRF
Sharla Wood
- 9:35 AM Ion Chromatography for Determining Metals in Pharmaceuticals
Jeff Rohrer

- 10:15 AM Determination of Total Vitamin B12 in Infant Formula by LC-ICP-MS
Lee Yu
- 10:35 AM Speaker Roundtable
Sharla Wood
- RAM-02 Raman Spectroscopic Sensing**
Chair: Torsten Frosch
- 9:15 AM Surface Enhanced Resonance Raman Spectro-electrochemistry for Target Specific Analysis
Inez Weidinger
- 9:35 AM New Developments in Raman Gas Sensing for Energy and Environmental Research
Torsten Frosch
- 9:55 AM Early Disease Detection by Raman Spectroscopy over Quantitative Polymerase Chain Reaction in Plant Disease Diagnostics
Dmitry Kurouski
- 10:15 AM Enhancing DUV Raman Sensing and Imaging with Surface Plasmons
Atsushi Taguchi
- 10:35 AM Deuterium Uptake as Raman-based Antibiotic Susceptibility Test in a Clinical Scenario
Christoph Haisch
- RAM-15 Spatially Offset Raman Spectroscopy (SORS)**
Chair: Pavel Matousek
- 9:15 AM Surface-enhanced Spatially Offset Raman Spectroscopy for in Vivo Neurochemical Detection
Bhavya Sharma
- 9:35 AM In Vivo Imaging of Cancer Using Surface Enhanced Spatially Offset Raman Spectroscopy (SESORS)
Fay Nicolson
- 9:55 AM Sensitivity of Transmission Raman Spectroscopy Signals to Temperature of Biological Tissue
Adrian Ghita
- 10:15 AM Spatially Offset and Transmission Raman Spectroscopy for Determination of Depth of Inclusion in Turbid Matrix
Sara Mosca
- 10:35 AM Offset Geometry for Deep Tissue Raman Imaging with OCT
Mingzhou Chen
- SPEC-06 SAB Special Session**
Chair: Sara Tufi, Alessandro De Giacomo
- 9:15 AM Local Thermodynamic Equilibrium in a Laser-induced Plasma Evidenced by Blackbody Radiation
Jörg Hermann
- 9:35 AM Investigation of the Atomization Mechanism of Gold Nanoparticles in Graphite Furnace Atomic Absorption Spectrometry
Kerstin Leopold
- 9:55 AM Quantification of Water Content by Laser Induced Breakdown Spectroscopy on Mars
William Rapin
- 10:15 AM Depth Profile Analyses with Sub 100-nm Depth Resolution of a Metal Thin Film by Femtosecond - Laser Ablation - Inductively Coupled Plasma - Time-of-flight Mass Spectrometry
Debora Käser
- 10:35 AM Editing *Spectrochimica Acta* Part B: Personal Reflections and Considerations on the Development of Analytical Spectroscopy
Nicolò Omenetto

SPEC-07	New Developments in Measurement Science <i>Chair: Garth Simpson</i>
9:15 AM	Spectroscopy, whales, lifespan, phospholipids and the cause and cure for cataracts <i>Douglas Borchman</i>
9:35 AM	The coffee ring effect for tap water fingerprinting <i>Rebecca Lahr</i>
9:55 AM	An Electroanalytical Technique to Monitor Oxide Reduction Processes for Nuclear Safeguards <i>Ammon Williams</i>
10:15 AM	Langmuir-Blodgett Films of Two-Dimensional Metal-Organic Frameworks <i>Fangyuan Tian</i>

11:00 am – 11:45 am **Poster Viewing**

1:30 pm – 3:10 pm **Afternoon Symposia**

ATOM-08	Atomic Spectroscopy Techniques for Clinical/Medical <i>Chair: C Derrick Quarles</i>
1:30 PM	Accurate Quantification of Carboplatin Adducts with Serum Albumin by Monolithic Chromatography Coupled to ICP-MS with Isotope Dilution Analysis <i>Christian Ward-Deitrich</i>
1:50 PM	Automated Sample Preparation Techniques for Clinical Analyses Using a Single Platform Sample Introduction System <i>C Derrick Quarles</i>
2:10 PM	Copper Isotopic Composition as an Indicator of Changes in Copper Processing in the Colon of Mice Due to Antibiotic Treatment <i>Kerri Miller</i>
2:30 PM	Gd-based Contrast Agents: A Clinically Significant Analytical Interference in ICP-MS Elemental Analysis <i>Patrick Day</i>
2:50 PM	Enriched Stable Isotope Tracers in Medical Applications <i>Johanna Irrgeher</i>
AWD-11	Clara Craver Award Symposium Honoring Shawn Chen <i>Chair: Xiaoyun Chen</i>
1:30 PM	Molecular Structures of Buried Interfaces Involving Polymers <i>Zhan Chen</i>
1:50 PM	Industrial Spectroscopist: The Joys and Challenges of Delivering Solutions <i>Katherine Bakeev</i>
2:10 PM	Theoretical Support to Industrial Spectroscopy Application <i>William Wang</i>
2:30 PM	Agricultural Spray Droplet Characterization Using Raman Chemical Imaging <i>Michael Bishop</i>
2:50 PM	Measuring the Infrared Absorption and Scattering Coefficients of Polymeric Foams <i>Mark Rickard</i>
BIM07	New Frontiers in Biomedical Analysis
1:30 PM	Dielectrophoretic Differentiation of <i>Klebsiella pneumoniae</i> Based on Antibiotic Resistance <i>Shannon Huey Hilton</i>
1:50 PM	Isolation and Fractionation of Extracellular Vesicles by Size & Immuno-based Asymmetric Nanopore Membrane Filtration <i>Ceming Wang</i>
2:10 PM	Noninvasive Manipulation of Cells and Chemicals within Live Cultures via Addressable Microfluidics <i>Anh Tong</i>

- 2:30 PM An Integrated Microfluidic Device with Nano-Magnetic Bead Capturing for Cancer-Derived Extracellular Vesicle Characterization
Chenguang Zhang
- CHEM-02 Exploiting Spatial and Spectral Information in Hyperspectral Images**
Chair: Thomas Bocklitz
- 1:30 PM Very Important Pixels in MCR Analysis of Hyperspectral Images
Cyril Ruckebusch
- 1:50 PM Can deep learning beat model-based pre-processing of infrared spectral data of cells and tissues?
Achim Kohler
- 2:10 PM Chemical Imaging Modalities Combined with Chemometrics for Characterization of Interfacial Water: Potential and Current Challenges
Junli Xu
- 2:30 PM A Comparison of ANNS, SVMs, and XGBoost in Challenging Classification Problems
Manuel Palacios
- 2:50 PM Investigations on the Data Analysis Pipeline Raman Spectroscopic Imaging
Thomas Bocklitz
- IR-01 Optical Photothermal Infrared Spectroscopy I**
Chair: Curtis Marcott, Andrea Centrone
- 1:30 PM Bone and Ligament Structure and Failure as Studied by Photothermal Infrared Microscopy
Mark Banaszak-Holl
- 1:50 PM Photothermal Infrared Spectroscopy: Growing Applications for Polymers and Materials Analysis
Dennis Walls
- 2:10 PM Biomedical Applications of Photothermal Spectroscopic Imaging
Rohith Reddy
- 2:30 PM Investigation of Breast Calcification Microstructure in Ductal Carcinoma in Situ Using Multi-modal Spectroscopy
Jayakrupakar Nallala
- 2:50 PM Recent Advances in Submicron Photothermal Infrared Spectroscopy and Imaging
Curtis Marcott
- LIBS-06 Forensics and Security**
Chair: Jose Almirall
- 1:30 PM Using LIBS for Elemental Signature Discovery in Forensic Applications
Tatiana Trejos
- 1:50 PM Improving the Forensic Relevance of LIBS by Quantifying Spectral Interferences
Matthieu Baudelet
- 2:10 PM Analysis of Nuclear Material with Heterogeneous Isotopic Composition by Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) and Laser Induced Breakdown Spectroscopy (LIBS) Tandem System
Jhanis Gonzalez
- 2:30 PM Forensic Application of Micro-XRF: Glass Analysis
Sergey Mamedov
- 2:50 PM Signal Processing of Handheld Libs-raman-xrf Multisensor Data for Soil Analysis
Richard Hark
- MASS05 Mass Spectrometry of In-tact Proteins and Protein Complexes**
Chair: Kermit Murray
- 1:30 PM Native ion-mobility mass spectrometry of Staphylococcus aureus α -hemolysin
Jesse Wilson

- 1:50 PM Direct Electrospray Photochemical Oxidation of Proteins
Kermit Murray
- 2:10 PM Structural analysis of isolated heme protein based on gas-phase resonance Raman spectroscopy: Identification of the oxidation state, spin state, and coordination
Hiroya Asami
- 2:30 PM Determining what really counts: Modeling and measuring nanoparticle number concentrations
Antonio Montoro Bustos
- PAT-02 SAS PAT Technical Section: PAT in the Biopharmaceutical Industries Session II**
Chair: Daniel Hill, Daniel Hill
- 1:30 PM Enabling Process Optimization, Scale-up and Technical Transfer Using Raman Spectroscopy in Production Bioreactors
Karin Balss
- 1:50 PM Streamlining CHO Cell Culture Process Development Using a Generic Model for Glucose Determination
Kurtis Denny
- 2:10 PM Use of Integrated Process Models Towards Data Driven Risk Assessments and Optimized Characterization
Christopher Taylor
- 2:30 PM A Hybrid Modeling Approach Using Monod Kinetics to Model Growth and Data Driven Methods for Modeling Protein Production and Product Quality Focusing on Analysis of Specific Consumption/secretion of Metabolites
Chris McCready
- 2:50 PM Fault Detection and Oligonucleotide Sequence Identification using an ATR-FTIR/Conductivity-based PAT Measurement System
Daniel Hill
- PMA-10 Enable Intensified Downstream Manufacturing by Advanced Online Sensor Technologies**
Chair: Richard Wu
- 1:30 PM Title TBD
Sean Gilliam
- 1:50 PM Variable Pathlength Spectrophotometry as a PAT Tool for Downstream Processes
Ramsey Shanbaky
- 2:10 PM Raman Spectroscopy for Bioprocesses: How Hardware, Sampling and Data Analysis Decisions Drive Success
Brian Marquardt
- 2:30 PM Turning off "Autopilot" on an Adaptive, Handheld Raman Spectrometer
Robert Brush
- 2:50 PM Raman Spectroscopy in Biosensing
Mehran Mojarrad
- RAM-04 Industrial Raman**
Chair: Karen Esmonde-White
- 1:30 PM Real-time Monitoring of Amino Acid Consumption in CHO Fed-batch Production Media by Raman Spectroscopy and Regression Models
Christopher Mahoney
- 1:50 PM Raman Spectroscopy: A Process Control Tool in Enzymatic Protein Hydrolysis
Ulrike Böcker
- 2:10 PM Identification and Verification of Dietary Supplement Raw Materials and Finished Goods Using Handheld Raman Spectroscopy
Mohamed Koroma

2:30 PM Raman Concatenation for Enhanced Process Control in Biomedical, Pharmaceutical & Petrochemical Applications

Scott Rudder

2:50 PM Industrial Applications of Raman Spectroscopy

William Wang

RAM-14 Transmission Raman Spectroscopy

Chair: Mark Mabry

1:30 PM Evaluation of a Low Cost Portable Transmission Raman System for Content Uniformity Analysis of Solid Pharmaceutical Dosage Forms

Jun Zhao

1:50 PM Comparison of Raman Imaging & Transmission Raman Spectroscopy Results on a Pharmaceutical Tablet

Tim Prusnick

2:10 PM Transmission Raman Spectroscopic Quantification of Active Pharmaceutical Ingredient in Coated Tablets of Hot-melt Extruded Amorphous Solid Dispersion

Yemin Liu

2:30 PM Drug Product Identification and Physical Stability Analysis by Transmission Raman Based Chemometrics

Ashish Punia

2:50 PM Quantification and Control of Amorphous Contents by Raman. Applications and Case Studies in Pharmaceutical Processing

Michelle Raikes

SPR-03 Plasmon and Imaging: Catalysis

Chair: Zachary Schultz

1:30 PM Tailoring Plasmons and Interfaces Toward Optimized Hot Electron Generation and Injection

Laura Fabris

1:50 PM Catalytic Nanoparticles as Labels for Biosensing

Xiaohu Xia

2:10 PM Quantifying Plasmon-generated Hot Carrier Energies

Katherine Willets

2:30 PM Imaging Plasmons with Electrons: Coupling Molecular Vibrations and Infrared Plasmons

Jon Camden

2:50 PM Hybrid Plasmonic/semiconductor Materials for CO₂ Reduction

Zachary Schultz

3:10 pm – 3:50 pm Poster Viewing and Break

3:50 pm – 5:30 pm Plenary Session: Innovation Award Symposium

Chair: Mary Kate Donais

3:50 PM Accelerated Restricted Boltzmann Machines

Peter Harrington

4:10 PM Molecular Basis for Chirality-regulated A β Self-assembly and Receptor Recognition Revealed by Ion Mobility-mass Spectrometry

Gongyu Li

4:30 PM Chemical Approaches to Improve Nanopore Single-Molecule Sensing

Jason Dwyer

4:50 PM Enhancing Enantioselective Absorption with Plasmonic and Dielectric Metasurfaces

John Abendroth

FRIDAY, OCTOBER 18

7:30 am – 8:00 am Continental Breakfast

8:00 am – 10:30 am Plenary Session: Innovation Award Winner, SciFri, and 2020 Preview

Chair: Garth Simpson

7:45 am Announcement of 2019 Innovation Award Winner

8:00 AM Phase Engineering for Targeted Super-Resolution Applications
Christy Landes

8:30 AM Multiplexing spatial and hyperspectral imaging with dynamically structured illumination
Randy Bartels

9:00 AM TBD

9:30 AM Preview of 2020

Linda Kidder Yarlott, 2020 General Chair
Mary Kate Donais, 2020 Program Chair

WORKSHOPS/SHORT COURSES

SUNDAY, OCTOBER 13

9 am – 12 pm A Practical Introduction to Infrared, Raman, and Near Infrared Spectroscopy - James A. de Haseth, University of Georgia (SAS)

9 am – 4 pm Basic Chemometrics - Barry Wise, Eigenvector

1 pm – 4 pm Searching Infrared and Raman Spectra - James A. de Haseth, University of Georgia (SAS)

MONDAY, OCTOBER 14

9 am – 12 pm Introduction to Hyperspectral/Multivariate Image Analysis - Robert T. Roginski, Eigenvector

9 am – 12 pm Introduction to Raman with Imaging Applications - David Tuschel, HORIBA Scientific (SAS)

1 pm – 4 pm Non-Linear Methods for Regression and Classification - Donal O'Sullivan, Eigenvector

1 pm – 4 pm Problems with FT-IR Spectra & How to Avoid Them - Ellen Miseo, TeakOrigin; Jenni Briggs, Pike Technologies; Gloria Story, Procter & Gamble (SAS)

TUESDAY, OCTOBER 15

9 am – 12 pm Laser Fundamentals for Spectroscopy - Robert Chimenti, RVC Photonics/Rowan University

9 am – 12 pm Electrokinetic Microfluidics: Theory and Hands-on Simulations - Cornelius (Neil) Ivory/Washington State University (AES)

1 pm – 4 pm Portable Raman: What It Takes to Create Small Systems & What They Can Do for You - Katherine Bakeev, B&W Tek; Adam Hopkins, Metrohm

1 pm – 4 pm Advance Applications of LAICPOES, LAICPMS and LIBS - Jhanis Gonzalez, Applied Spectra/Lawrence Berkeley National Laboratory

WEDNESDAY, OCTOBER 16

9 am – 4 pm Process Analytical Technology: Out of the Lab and into the Line - Jim Rydzak, Specere Consulting (SAS)