TECHNICAL PROGRAM – SUNDAY AND MONDAY

5:00 PM FACSS LIFETIME SERVICE AWARD, PRESENTED TO JEANETTE GRASSELLI BROWN
Accepted by Peter Griffiths
"The Early Days of FACSS:
Can we learn today from past experiences?"
and
SUNDAY POSTER SESSION
5:30 – 7:00 PM, Room 315-318

Your poster should be put up by 5:00 PM Sunday and removed after 7:00 PM

5:00 (1) **Historical Review of Standard Reference Materials for Analytical Spectrophotometry – A Tribute to Dr. Radu Mavrodineanu**; Jerry Messman, *Stranaska LLC*

5:00 (2) **Celebrating 30 Years Since the Discoveries of VCD and ROA**; Rina Dukor; Laurence Nafie, *BioTools, Inc*

5:00 (3) **Milestones in the History and Evolution of the Raman Effect**; Michel Delhaye, *U Lille (retired)*; Wolfgang Kiefer, *U Wurzburg*; Derek Long, *U Bradford*; Edouard DaSilva, *Jobin Yvon*; Jacques Barbillat, *U Lille*; Paul Dhamelincourt, *U Lille*

5:00 (4) **Foibles to Fibers: A Retrospective Pictorial Look of How We Got From Menlo Park the Smart Sensors**; James Jordan, *Arizona State University*

5:00 (5) **FT-Raman: Then and Now**; Bruce Chase

5:00 (6) **The Renaissance of Step-Scan FT-IR;**.Richard Palmer, *Duke University*

5:00 (7) **The Evolution of 2-D IR Spectroscopy**; Curt Marcott & Isao Noda, *Procter & Gamble*

5:00 (8) **History and Development of Analytical Chemical Imaging;** L. Kidder; N. Lewis; H. Haber, Spectral Dimensions

Monday Morning, Room 113
MULTIVARIATE CURVE RESOLUTION: THE SLEEPING GIANT OF CHEMOMETRICS
Presider: David Haaland, *Sandia National Labs*

8:30 (10) **New Challenges and Proposals for Multivariate Curve Resolution**; Roma Tauler, *University of Barcelona*; Anna de Juan, *University of Barcelona*

9:10 (11) **Advantages of Soft vs. Hard Constraints in Self-Modeling Curve Resolution Problems – Alternating Least-Squares with Penalty Functions (P-ALS)**; Paul Gemperline, *East Carolina University*; Eric Cash, *East Carolina University*

9:50 **Coffee Break**

10:30 (12) **Local Functional Constraints in Multivariate Curve Resolution**; Jeremy Shaver, *Eigenvector Research Inc.*; Neal Gallagher, *Eigenvector Research Inc.*; Rasmus Bro, *Royal Veterinary and Agricultu*

11:10 (13) **Computing Rigorous Solutions to Equality and Inequality Constrained Least Squares Problems During Multivariate Curve Resolution**; Mark Van Benthem;,Michael Keenan; David Haaland, *Sandia National Lab*

Monday Morning, Room 204
NEW APPROACHES TO TEACHING ANALYTICAL CHEMISTRY – MATERIALS CHEMISTRY
Presider: Ingrid Fritsch, *University of Arkansas*

8:30 (14) **New Approaches to Teaching Analytical Chemistry: From High School to Graduate School**; Thomas Beebe, Jr., *University of Delaware*

8:50 (15) **Thin Film Studies for Environmental and Medical Applications**; Maria Hepel, *SUNY Potsdam*

9:10 (16) **Problem-driven Demonstrations of Materials Characterization Techniques for Students in an Instrumental Analysis Laboratory Course**; Ingrid Fritsch, *University of Arkansas*; John Shultz, *University of Arkansas*

9:30 (17) **Scaling Up: Using Optical Diffraction to Explain X-ray Diffraction**; Anne-Marie Nickel, *Milwaukee School of Engineerin*; George Lisensky, *Beloit College*; Karen Nordell, *Lawrence University*; Arthur Ellis, *University of Wisconsin-Madison*

9:50 **Coffee Break**

10:30 (18) **Western's Integrated Laboratory Network: Laboratory Science Anytime and Anyplace**; Devon Cancilla, *Western Washington University*

10:50 (19) **Exploring Materials Science with LEGO Bricks**; Dean Campbell, *Bradley University*

11:10 **Discussion**, Ingrid Fritsch

Monday Morning, Room 213
PROCESS ANALTYICAL: ISA ANALYTICAL DIVISION
Presider: Gary Brewer, *ABB*

8:30 (20) **Application of Filter Photometers in the Production of Ethylene and Propylene**; Gary Brewer, *ABB*

9:10 (21) **Trace Total Sulfur Measurement with a Flame Photometric Detector**; Kenneth Melda, *ABB Inc.*; Jerry Clemons, *ABB Inc.*

9:50 **Coffee Break**

10:30 (22) **Stack HF and NH3 Monitoring with a Portable TDL Analyzer**; Hamish Adam, *Boreal Laser*

11:10 (23) **Why Are There So Many Types of Ph Electrodes?**; Kenneth Queeney, *Mettler-Toledo Ingold, Inc.*

Monday Morning, Room 216
FORENSIC MASS SPECTROMETRY
Presider: Bruce McCord, *Ohio University*

8:30 (24) **Advanced Nuclear Forensic Technologies For Uranium and Plutonium Sampling, Separation, and Analysis**; Douglas C. Duckworth, *ORNL*; Sea H. Park, *ORNL*; Debra T. Bostick, *ORNL*; Paula Cable-Dunlap, *SRTC*

8:50 (25) **Laboratory and Field Experiments used to Identify Canis Lupus Var. Familiaris Active Odor Signature Chemicals from Drugs, Explosives and Humans**; Kenneth Furton, *Florida International Universi*; Norma Lorenzo, *Florida International Universi*; Ross Harper, *Florida International Universi*; Ya-Li Hsu, *Florida International Universi*; Samantha Tolliver, *Florida International Universi*; Allison Curran, *Florida International Universi*; Jose Almirall, *Florida International University*

9:10 (26) **New Developments in SPME: on-Fibre Derivatization Applied to the Recovery of Ammonium Nitrate-Based Explosives and Amphetamine Drug traces.**; Paul Kirkbride, *Forensic Science, South Austra*; Paul Pigou, *Forensic Science, South Austra*; Hayley Brown, *Flinders University*; Stewart Walker, *Flinders University*

9:30 (27) **Electrospray Ionization Mass Spectrometry of Organic Explosives**; John Mathis, *Ohio University*; Olivier Collin, *Ohio University*; Bruce McCord, *Ohio University*

TECHNICAL PROGRAM – MONDAY

9:50 **Coffee Break**

10:30 (28) **Thermal Desorption GC-MS Analysis of Organic Explosives**; Michael Sigman, *University of Central Florida*; Ralph Ilgner, *Oak Ridge National Laboratory*

10:50 (29) **Relative Discriminating Power of Visible, UV/Visible, and UV/Fluoresence Microspectrophotometry for Forensic Analysis of Dyed Textile Fibers**; Stephen L. Morgan, *University of South Carolina;* Christopher R. Mubarak; James E. Hendrix; Edward G. Bartick, *FBI Laboratory*

11:10 (30) **Analytical Technologies and Applications at the Forensic Science Center at LLNL**; Greg Klunder, *Lawrence Livermore Natl. Lab*

11:30 (31) **Comparison of ICP-AES and ICP-MS Methods for Elemental Analysis of Bullet Lead Alloys**; Robert Koons; JoAnn Buscaglia, *FBI Laboratory*

Monday Morning, Room 220
BIOMOLECULAR INTERACTIONS I
Presider: Ulli Krull, *University of Toronto*

8:30 (32) **Application of Proteomics in Drug Discovery**; Daniel Figeys, *MDS Proteomics*

9:10 (33) **Global and Selective Mass Spectrometry-Based Analysis of Proteins**; K.W. Michael Siu, *York University*

9:30 (34) **Limited Proteolysis of Isotope-Labelled Proteins Combined with Quantitative Mass Spectrometry for Studying Protein Interactions**; Liang Li, *1*; Chris McDonald, *University of Alberta*

9:50 **Coffee Break**

10:30 (35) **NMR Approaches to the Determination of Drug-membrane Interactions**; R. Scott Prosser, *University of Toronto*; Bin Lu, *University of Toronto*

10:50 (36) **Cancer Cell Proteomics using Molecular Aptamers**; Weihong Tan, *University of Florida*

11:10 (37) **DNA Aptamers and DNA Enzymes with Fluorescence-Signaling Properties**; Yingfu Li, *McMaster University*; Razvan Nutiu, *McMaster University*; Shirley Mei, *McMaster University*

11:50 (38) **Molecularly Imprinted Polymers - Potential and Challenges in Analytical Chemistry**; Boris Mizaikoff, *Georgia Institute of Technology*

Monday Morning, Room 221
APPLICATION OF RAMAN MICROSCOPY
Presider: Andrew Whitley, *Jobin Yvon*

8:30 (39) **Use of Hydroxyproline and Proline Bands for Quantification of Type I Collagen in Raman Microspectroscopy of Bone Tissue**; Nicole J. Crane, *University of Michigan*; Michael D. Morris, *University of Michigan*

8:50 (40) **Protein Secondary Structure Analysis with FT-IR, CD, and Raman Spectroscopy**; Richard Larsen, *Jasco Inc*; Amanda Jenkins, *Jasco Inc.*; Tim Williams, *Jasco Corp.*; Kenichi Akao, *Jasco Corp*

9:10 (41) **3D Characterization of Paintable Displays Using Confocal Raman Spectroscopy**; Arjan Mank, *Philips Electronics*; Inge Vorstenbosch, *Philips Electronics*

9:30 (42) **Use of Raman Microscopy to Study Thin Film Inhibition in Hydrosilation Reactions**; Elmer Lipp, ; Mary Kay Tomalia, *Dow Corning Corp.*

9:50 **Coffee Break**

10:30 (43) **Forensic Raman Microscopy of Fibers: Evaluation of Mounting Media**; Edward G. Bartick, *FBI Laboratory*; William Pearman, *University of South Carolina*; James E. Hindrix, *University of South Carolina*; Stephen L. Morgan, *University of South Carolina*; S. Michael Angel, *University of South Carolina*

10:50 (44) **Genetic Defects of Bone Tissue Studied by Raman Microscopy**; Tsoching Chen, *University of Michigan*; Michael Morris, *University of Michigan*; Kenneth Kozloff, *University of Michigan*; Steven Goldstein, *University of Michigan*

11:10 (45) **Chemical Imaging of Food Systems**; Chad Leverette, *Cargill, Incorporated*; Douglas Elmore, *Cargill, Incorporated*; Sean Smith, *Cargill, Incorporated*; Allen Muroski, *Cargill, Incorporated*; Brian Anderson, *Cargill, Incorporated*; Gene Kaercher, *Cargill, Incorporated*; Abigail Lape, *Cargill, Incorporated*; John McDonald, *Cargill, Incorporated*

11:30 (46) **Rapid quantification of carotenoids and fat in Atlantic salmon (Salmo Salar) by Raman spectroscopy and chemometrics**; Jens Petter Wold, *MATFORSK – Norwegian Food Rese*; Brian Marquardt, *CPAC – Center for Process Anal*; Dave Robb, *EWOS Innovation*

Monday Morning, Room 222
RAMAN SPECTROSCOPY: BIOMEDICAL AND BIOCHEMICAL RAMAN SPECTROSCOPY
Presider: Shuliang Zhang, *Unilever Research and Development*

8:30 (47) **In vivo Raman spectroscopy**; Gerwin Puppels; Peter Caspers; Tom Bakker Schut, ; Rolf Wolthuis, ; Gerald Lucassen, *Philips Research*

8:50 (48) **Spectral Diagnosis and Analysis of Disease with Raman Spectroscopy**; Michael S. Feld, *G.R. Harrison Spectroscopy Laboratory*

9:10 (49) **Raman Spectroscopy For in vivo Skin Tissue Characterization and Evaluation**; Haishan Zeng; Zhiwei Huang, Abdulmajeed Ajlan; David McLean; Harvey Lui

9:30 (50) **Raman Detection of Carotenoid Antioxidants in Human Tissue**; Werner Gellermann, *Department of Physics Universiy*

9:50 **Coffee Break**

10:30 (51) **Raman Microspectroscopy and Imaging of Skeletal and Connective Tissue**; Michael D. Morris, *University of Michigan*

10:50 (52) **IR and Raman Microscopy of Skin and Bone**; Richard Mendelsohn, *Rutgers University*

11:10 (53) **Differentiating the Raman SpectraTumorigenic and Non-tumorigenic Cells**; Jon Schoonover, Rob Marx, Kristin Omberg; James Freyer, *Los Alamos National Labs*

Monday Morning, Room 223
REFLECTANCE SAMPLING TECHNIQUES FOR INFRARED SPECTROMETRY
Presider: John Hellgeth, *Hewlett Packard*

8:30 (55) **Diamond Internal Reflection Infrared Spectroscopy - The Current State of Affairs**; David Schiering, *SENSIR Technologies*

TECHNICAL PROGRAM - MONDAY

8:50 (56) **Micro ATR-FTIR Spectroscopy in Combination with Micro Raman Spectroscopy**; Fran Adar, *Jobin Yvon, Inc.*; Gwen LeBourdon, *Jobin Yvon, SA*; John Reffner, *SensIR*; Andrew Whitley, *Jobin Yvon, Inc.*

9:10 (57) **Infrared Imaging with a Diamond ATR-IR Accessory**; Sergei Kazarian; Andrew Chan, *Imperial College London*

9:30 (58) **Exchange Rates of Surfactant at the Solid-Liquid Interface Obtained by ATR-FTIR**; Spencer Clark, *Virginia Tech*; William Ducker, *Virginia Tech*

9:50 (59) **Evaluation of Dermal Pesticide Absorption Processes Using ATR-FTIR**; Angela Carden; Michael G. Yost; Richard A. Fenske, *University of Washington*

10:10 **Coffee Break**

10:30 (60) **Advanced ATR Correction Algorithm for Infrared Spectroscopy**; Koichi Nishikida, *Thermo Electron Corporation*; Kenneth Kempfert, *Thermo Electron Corporation*

10:50 (61) **Characterization of Ti Composite Pigments by Raman Microscopy and Micro ATR FT IR**; Laurie Smith, Gene Hall, *Rutgers University*

11:10 (62) **Determination of Transmission and Reflectance Characteristics of Biological Microorganisms Distributed on Porous Matrices**; Maria V. Schiza, *University of South Carolina*; Michael L. Myrick, *University of South Carolina*

11:30 (63) **Infrared Reflection Absorption Spectroscopy (IRRAS) of â-Amyloid Langmuir and Langmuir-Blodgett films**; Roger M. Leblanc, *University of Miami*; Jhony Orbulescu, *University of Miami*; Michelle Patrick, *University of Miami*; Changqing Li, *University of Miami*

11:50 (64) **Investigation of the Molecular Composition and Orientation of the Si/SiOx/TiO2 Interfaces Using Reflection-Absorption Infrared and X-ray Photoelectron Spectroscopies**; Vasilis Gregoriou; Georgia Kandilioti; Aggeliki Siokou; Syiridon Ntais, *SORTH-ICEHT*

Monday Morning, Room 301
CURRENT PROGRESS IN SEPARATIONS OF CARBON NANOTUBES I
Presider: Wei Zhao, *University of Arkansas*

8:30 (65) **Chemical Studies of Single-Walled Carbon Nanotubes**; Robert Haddon, *University of California, Riverside*

8:50 (66) **Geometry-Based Separations of Carbon Nanotubes Using Capillary Electrophoresis**; Stephen Doorn, *Los Alamos National Lab*; Hui Hu, *University of California, Rive*; Mark Hamon, *University of California, Rive*; Robert Haddon, *University of California, Rive*; John Selegue, *University of Kentucky*; Michael Strano, *Rice University*; Michael O'Connell, *Rice University*; Erik Haroz, *Rice University*; Robert Hauge, *Rice University*; Richard Smalley; *Rice University*

9:10 (67) **Dielectrophoretic and Electrophoretic Separation of Carbon Nanotubes**; Pehr Pehrsson, *Naval Research Laboratory*; Jeffrey Baldwin, *Naval Research Laboratory*

9:30 (68) **BULK Separation of Metallic from Semiconducting Single Wall Carbon Nanotubes**; Fotios Papadimitrakopoulos, *University of Connecticut*; Debjit Chattopadhyay, *University of Connecticut*; Izabela Galeska, *University of Connecticut*; Sang Nyon Kim, *University of Connecticut*

9:50 **Coffee Break**

10:30 (69) **Analytic Emission Assay of Single-Wall Carbon Nanotubes - Solutions and Dispersions**; Dirk Guldi, *University of Notre Dame*; Michael Holzinger, *Universität Erlangen-Nürnberg*; Andreas Hirsch, *Universität Erlangen-Nürnberg*; Vasilios Georgakilas, *Università degli Studi di Trie*; Maurizio Prato, *Università degli Studi di Trie*

10:50 (70) **Solution Chemistry and Chemical Alignment of Single Walled Carbon Nanotubes**; Zhongfan Liu; Yanlian Yang; Bin Wu, ; Peng Diao; Jin Zhang, *Peking University*

11:10 (71) **Controlled Assembly of Carbon Nanotubes in Aqueous Solution with Designed Amphiphilic Peptides**; Gregg R. Dieckmann, ; Alfonso Ortiz-Acevedo; Alan B. Dalton; Vasiliki Zorbas; Ray H. Baughman, ; Rockford K. Draper; Inga H. Musselman

11:30 (72) **DNA-assisted dispersion and separation of carbon nanotubes**; Ming Zheng, *DuPont CR & D*; Anand Jagota, *DuPont CR & D*; Bruce Diner, *DuPont CR & D*; Robert Mclean, *DuPont CR & D*; Bibiana Onoa, *DuPont CR & D*; Ellen Semke, *DuPont CR & D*; Dennis Walls, *DuPont CR & D*

Monday Morning, Room 304
ION-MOLECULE CHEMISTRY, REACTION CELLS AND COLLISION CELLS FOR ICP-MS
Presider: Dmitry Bandura, *MDS Sciex*

8:30 (73) **Ion-Molecule Kinetics: Theoretical and Practical Considerations**; Greg Koyanagi, *York University*; Diethard Bohme, *York University*

9:10 (74) **Successes of Ion-Molecule Chemistry in ICP-MS**; Gregory Eiden; Charles Barinaga; David Koppenaal, *Pacific Northwest National Lab*

9:50 **Coffee Break**

10:30 (75) **Reaction Cell ICP-MS and Laser Ablation Sampling: Worth a While or Waste of Time?**; Bodo Hattendorf, *ETH Zürich*; Detlef Günther, *ETH Zürich*

11:10 (76) **Measurement of Sulphur and Chlorine by Collision Cell, Multi-Collector ICPMS**; Zenon Palacz, *GV Instruments*

11:30 (76b) **Chemical Resolution of Interferences Typical for Environmental Samples via Ion-Molecule Reactions with Ethylene**; Dmitry R. Bandura, *PerkinElmerSCIEX*

Monday Morning, Room 305
LASER-BASED METHODS IN ATOMIC SPECTROSCOPY I
Presider: Ben Smith, *University of Florida*

8:30 (77) **Laser-Induced Breakdown Spectroscopy of Airborne Bioaerosol Particles**; John Hybl, *MIT Lincoln Laboratory*; Shaun Berry, *MIT Lincoln Laboratory*; Xuan Le, *MIT Lincoln Laboratory*; Eric Lynch, *MIT Lincoln Laboratory*

9:10 (78) **Plasma-Particle Interactions in LIBS-Based Aerosol Anlaysis**; David Hahn, *University of Florida*; Jorge Carranza, *Polytechnic University of Puer*4

9:50 **Coffee Break**

10:30 (79) **Using Self-Reversed Spectral Lines for Diagnostics of Laser Induced Plasma**; Igor Gornushkin, *University of Florida*; Nico Omenetto, *University of Florida*; Ben Smith, *University of Florida*; James Winefordner, *University of Florida*

10:50 (80) **Laser-Induced Breakdown Spectroscopy with a Microchip Laser**; Ben Smith; Igor Gornushkin, ; James Winefordner, *University of Florida*

11:10 (81) **Optimization of Ablation Parameters for the Analysis of Nickel-based Alloys by Laser Induced Breakdown Spectroscopy**; Suh-Jen Jane Tsai, *Department of Applied Chemistry*; Shi-Yang Chen, *Department of Applied Chemistyr*; Pai-Chung Tseng, *Department of Mechanical Engineering*

11:30 (82) **Quantitative Analysis of Carbon in the Low Carbon Steel Using Laser-Induced Breakdown Spectroscopy**; Yukio Usui; Shin Ishikawa; Akira Yamamoto; Hisao Yasuhara, *JFE Steel Corporation*

Monday Morning, Room 317
FLUORESCENCE: SENSOR & INSTRUMENT DEVELOPMENT
Presider: Sharon Neal, *University of Delaware*

8:30 (83) **Metal Substrate-Based Fluorescent Biosensing**; Jian Wang, *Department of Chemistry, Boston*; Joel Rivera-Gandia, *Department of Chemistry*; Rosina Georgiadis, *Department of Chemistry, Boston*

8:50 (84) **Chemometric Approaches to Quantifying Single-Molecule Surface Diffusion with the Single Event Duration Histogram**; Michael Culbertson, *Wheaton College*; Daniel Burden, *Wheaton College, Biomolecular*

9:10 (85) **Two-Color Time-Resolved Near-IR Fluorescence Microscope for Reading Fluorescence from Micro-electrophoresis Devi ces**; Li Zhu, *Louisiana State University*

9:30 (86) **Portable, Battery-Operated Hg Monitor**; Vassili Karanassios, *University of Waterloo*; William Vander Wilp, *University of Waterloo*

9:50 **Coffee Break**

10:30 (87) **Design and Performance Characteristics of a New Hyperspectral Microarray Scanner***; Michael B. Sinclair, *Sandia National Laboratories*; Jerilyn A. Timlin, *Sandia National Laboratories*; David M. Haaland, *Sandia National Laboratories*

10:50 (88) **Development of Fluorescence Standards for Biological Assays Using Modern Fluorometers and Microarray Readers**; Paul C DeRose, *National Institute of Standard*; Douglas H Blackburn; Gary W Kramer

11:10 (89) **Fiber Optic Chemical Sensing Excitation Emission Matrix Fluorometry**; James Jordan, *Arizona State University*; Karl Booksh, *Arizona State University*; Yoon-Chang Kim, *Arizona State University*

11:30 (90) **Characterizing Diffusion on Biomimetic Surfaces with Single-Molecule Fluorescence Microscopy and Single-Event Duration Histograms**; Daniel Burden, *Wheaton College and Biomolecul*; Michael Culbertson, *Wheaton College*; John Elliott, *National Institute of Standard*; John Woodword, *National Institute of Standard*; Dee Ann Stults, *Wheaton College*; Steven Poppen, *Wheaton College*; Emily Rupp, *Wheaton College*

Monday Morning, Room 318
SURFACE ANALYTICAL TECHNIQUES
Presider: Shane Street, *University of Alabama*

8:30 (91) **Quantitative Modeling of Intrinsically Chiral Metal Surfaces and Amino-acid Templated Metal Surfaces**; David Sholl, *Carnegie Mellon University*; Rees Rankin, *Carnegie Mellon University*

9:10 (92) **Enantioselective Chemisorption on a Chirally Patterned Surface in Ultrahigh Vacuum**; Wilfred Tysoe, *University of Wisconsin-Milwaukee*; Dario Stacchiola, *University of Wisconsin-Milwaukee*; Luke Burkholder, *University of Wisconsin-Milwaukee*; Giorgio Zgrablich, *Universidad Nacional de San Lu*

9:50 **Coffee Break**

10:30 (93) **Adsorption of chiral modifiers on catalytic surfaces**; Francisco Zaera; Jun Kubota; Zhen Ma, *University of California - Riverside*

11:10 (94) **Reactivity and Longevity Studies on Iron-Based Bimetallic Catalysts During Organohalide Remediation**; Howard Fairbrother; Lynn Roberts; Stephen Bransfield; Adam Grenier; Molly McGuire; David Cwiertney, *Johns Hopkins University*

11:30 (95) **Surface Science Study of the Ethching of Alumina by 2,4 Pentanedione**; Shane Street; Brent Helms; James Burgess, *University of Alabama*

11:50 (96) **Synthesis, Characterization and Photoactivity of Mesoporous silica supported Titanium dioxide**; William Adams, *Department of Chemistry*, Martin Bakker, *Department of Chemistry*, Hye-Won Oh, *Department of Chemistry*; Transito Macias, *Dave C. Swalm School of Chemic*; I. Atly Jefcoat, *Dave C. Swalm School of Chemic*

Monday Afternoon, Room 113
CHEMOMETRIC METHODS FOR HYPERSPECTRAL IMAGE ANALYSIS
Presider: David Haaland, *Sandia National Labs*

1:30 (97) **Digital Image Processing of Hyperspectral Data**; Chris W. Brown, *University of Rhode Island*

2:10 (98) **Discriminant MCR Image Analysis: A New Image Feature Clustering Algorithm Utilizing Both Spatial and Spectral Information**; Thomas Hancewicz, *Unilever R&D., Ed*; Ji-hong Wang, *JHW Consulting, Cardinal*

2:50 **Coffee Break**

3:30 (99) **Some New Twists on the Multivariate Analysis of Spectral Images**; Michael Keenan, *Sandia National Laboratories*; Mark Van Benthem, *Sandia National Laboratories*; Paul Kotula, *Sandia National Laboratories*

4:10 (100) **Using PCA to Interpret FT-IR Images**; Richard Spragg; Robert Hoult; *PerkinElmer LAS, Chalfont Road, Seer Green, Bucks*

4:30 (101) **Multivariate Curve Resolution for the Analysis of Hyperspectral Images**; David Haaland, *Sandia National Laboratories*; Jerilyn Timlin, *Sandia National Laboratories*; Michael Keenan, *Sandia National Laboratories*; Mark Van Benthem, *Sandia National Laboratories*; Michael Sinclair, *Sandia National Laboratories*; Juanita Martinez, *University of New Mexico*; Margaret Werner-Washburne, *University of New Mexico*

TECHNICAL PROGRAM - MONDAY

Monday Afternoon, Room 213
APPLICATIONS OF PROCESS ANALYTICAL CHEMISTRY
Presider: David Littlejohn, *University of Strathclyde*

1:30 (102) **Development of a Phase Diagram to Control Composite Manufacturing using Raman Spectroscopy**; Jessica Carignan, *Real-Time Analyzers*; Victor Khitrov, *Real-Time Analyzers*; Stuart Farquharson, *Real-Time Analyzers*; Antonio Senador, *University of Connecticut, Ins*; Montgomery Shaw, *University of Connecticut, Ins*

1:50 (103) **Monitoring All Reaction Chemistry Around the Clock**; Jeffrey W. Sherman, Ph.D.; Norman E. Van Order, Jr., Ph.D., Veronica A. Bracken, Ph.D.; *Mettler-Toledo AutoChem*

2:10 (104) **Detection of Selected Chlorinated Hydrocarbons Using a Resonance-Enhanced Multiphoton Ionization (REMPI) Probe**; Kui Chen, ; Mike Angel; *University of South Carolina*

2:30 (105) **Applications of In-Situ Mid-infrared Spectroscopy to Process Research**; Wes Walker, *Mettler Toledo AutoChem*

2:50 **Coffee Break**

3:30 (106) **Supramolecule and Polymer Identifications with the Use of Mass Spectrometry**; Badia Amekraz, *CEA*; Gabriel Plancque, *CEA*; Pascal Reiller, *CEA*; Christophe Moulin, *CEA*

3:50 (107) **Colorimetric Determination of Arsenic with 0.5 ug/L Detection in 14 Minutes.**; Ivars Jaunakais, *Industrial Test Systems, Inc.*; Corlyss Lewis, *Industrial Test Systems, Inc.*; Howard Ray, *Industrial Test Systems, Inc.*; Dick Wood, *Industrial Test Systems, Inc.*

Monday Afternoon, room 216
MINIATURIZATION OF ANALYZERS
Presider: Gary Brewer, *ABB*

1:30 (108) **Optical, Tunable Filter-Based Micro-Instrumentation for Industrial Process Control**; Petros Kotidis; Richard Crocrombe; Walid Atia; *AXSUN Technologies*

1:50 (109) **Metal Halide Salts Doped into the Original Silicone Cladding of an Optical Fiber for optical Humidity Sensing**; Timothy L Danielson, *Indiana University*; Gary M Hieftje, *Indiana University*

2:10 (110) **Portable, Palm-Size Data Acquisition**; Vassili Karanassios, *University of Waterloo*; Agnes Kolkiewicz, *University of Waterloo*

2:30 (111) **High Sensitive Near Infrared Spectroscopy based on Absorption-Sensitive Surface Plasmon Resonance**; Akifumi Ikehata, *Kwansei Gakuin University*; Xiaoling Li, *Kwansei Gakuin University*; Tamitake Itoh, *Kwansei Gakuin University*; Jian-Hui Jiang, *Hunan University*; Yukihiro Ozaki, *Kwansei Gakuin University*

2:50 **Coffee Break**

3:30 (112) **Fiber-Optic Based Surface Plasmon Resonance Sensor for In-Vivo Biochemical Monitoring: Detection of Myocardial Infarction**; Jean-Francois Masson; Karl Booksh; Stephen Beaudoin; *Arizona State University*

3:50 (113) **Surface Plasmon Resonance Spectroscopy based on Probe Geometry**; Yoon-Chang Kim, *Dept of Chem & Biochem, ASU*; Jean-Francois Masson, *Dept of Chem & Biochem, ASU*; Karl S. Booksh, *Dept of Chem & Biochem, ASU*

4:10 (113b) **Recent Applications of Raman Spectroscopy for On line Monitoring of Polymerisation Reactions**; Sophie Morel, *Jobin Yvon SAS*; Ingo Reese, *Jobin Yvon GmbH*; Ruth Geiger, *Jobin Yvon GmbH*; Fran Adar, *Jobin Yvon Inc*

4:30 (113c) **Chemometrics for On-line Process Analytics COPA - A CPAC Industry Initiative;** David Marrow, *ExxonMobil*

Monday Afternoon, Room 220
BIOMOLECULAR INTERACTIONS II
Presider: Ulli Krull, *University of Toronto*

1:30 (114) **Protein and Peptide Microarrays for SPR Imaging Measurements of Bioaffinity Interactions**; Hye Jin Lee, *University of Wisconsin-Madison*; Greta Wegner, *University of Wisconsin-Madison*; Robert Corn, *University of Wisconsin-Madison*

1:50 (115) **Design of DNA Probe Selectivity for Biosensors and Biochips by Control of Nearest-Neighbor Intermolecular Interactions**; Ulrich Krull, *University of Toronto at Mississauga*; Paul Piunno; Christopher Kotoris; James Watterson; *FONA Technologies, Inc.*

2:10 (116) **DNA Probe/Target Interactions at Base Pair Resolution by Single Molecule Force Spectroscopy**; M. Cynthia Goh, *University of Toronto*; Bernie Sattin, *University of Toronto*

2:30 (117) **G-quartet Stationary Phases for Proteins**; Linda B. McGown, *Duke University*; Lawrence W. Dick, *Duke University*; Trang U. Vo, *Duke University*; Adam C. Connor, *Duke University*; Melanie A. Rehder-Silinski, *Duke University*

2:50 **Coffee Break**

3:30 (118) **Luminescent Quantum Dot Reagents for Bioassays**; Ellen Goldma; George Anderson, Aaron Clapp; Igor Medintz; Hedi Mattoussi; J. Matthew Mauro; *Naval Research Laboratory*

3:50 (119) **Utilization of Surface Enhanced Fluorescence for Direct Detection of Organophosphate Chemical Warfare Agents and Neurotoxic Pesticides**; Alex Simonian, *Auburn University*; Theresa Good, *University of Maryland Baltimo*; Steven Wang, *Texas A&M University*; James Wild, *Texas A&M University*

4:10 (120) **Aparent Electrophoretic Mobilities of Individual Organelles**; Edgar Arriaga; Hossein Ahmadzadeh; Guohua Xiong; Kathryn Fuller; *University of Minnesota*

Monday Afternoon, Room 222
RAMAN CHEMICAL IMAGING
Presider: Matt Nelson, *ChemImage*

1:30 (127) **Raman imaging in addressing the questions of very ancient life on Earth and elsewhere in the Solar System**; Thomas J. Wdowiak, *University of Alabama at Birmingham*

2:10 (128) **Analysis of alpha-Radiation Damage in Polytetrafluoroethylene**; David Pugmire; Rollin Lakis; Jon Bridgewater; Chris Wetteland;; *Los Alamos National Laboratory*

2:30 (129) **Raman Chemical Imaging of Tissues and Single Cells**; John Maier, *ChemImage Corp.*; Shona Stewart, *ChemImage Corp.*; Matthew Nelson, *ChemImage Corp.*; Joseph Demuth, *ChemImage Corp.*; Jeffrey Cohen, *Allegheny General Hospital*; Patrick Treado, *ChemImage Corp*

2:50 **Coffee Break**

3:30 (130) **Imaging Techniques in the Pharmaceutical Industry**; Rachel Brody, *University of Greenwich/Pfizer*; Don Clark, *Pfizer Global R&D*

4:10 (131) **New Directions in Raman Imaging: New SEM-Raman Interface for Material Analysis**; Richard Bormett, *Renishaw Inc.*; Ken Williams, *Renishaw plc*; Robert Bennett, *Renshaw plc*; Alan Brooker, *Renishaw plc*

4:30 (132) **Raman Imaging as a Tool for the Characterization of Aqueous Suspension Formulations of Nasal Sprays**; William Doub, *US FDA/CDER/OPS/OTR/DPA*; Wallace Adams, *US FDA/OPS-IO*; John Spencer, *US FDA/CDER/OPS/OTR/DPA*; Lucinda Buhse, *US FDA/CDER/OPS/OTR/DPA*; Patrick Treado, *ChemImage, Inc.*; Matthew Nelson, *ChemImage, Inc.*

Monday Afternoon, Room 223
MEGGERS AWARD TO IRA LEVIN, SCOTT W. HUFFMAN AND ROHIT BHARGAVA
Presider: Peter Griffiths, *University of Idaho*

1:30 (133) **Biomedical Applications of Infrared and Visible Reflectance Spectroscopic Imaging: From Bench to Bedside**; Ira W. Levin; Scott W. Huffman; Rohit Bhargava; Daniel C. Fernandez, Karel Zuzak; *National Institutes of Health*

2:10 (134) **Infrared Focal Plane Arrays; They Are Not Just for Imaging,** Bruce Chase, *E. I. Du Pont de Nemours & Co., Inc.*

2:50 **Coffee Break**

3:30 (135) **Real Time Studies of Molecular Assembly in Thin Films Using a Planar Array IR (PA-IR) Spectrograph**; John Rabolt, *Delaware Biotechnology Institu*; Julia Liu, *University of Delaware*; Christian Pellerin, *University of Delaware*; Chris Snively, *University of Delaware*; Bruce Chase, *DuPont CR&D*

4:10 (136) **Industrial Applications of Near-Infrared Spectral Imaging**; Curtis Marcott, *The Procter & Gamble Company*; Anthony E. Dowrey, *The Procter & Gamble Company*; Gloria M. Story, *The Procter & Gamble Company*

4:50 (137) **What Can We Learn About Polymer Dissolution From FT-IR Imaging?;** Jack Koenig, *Case Western Reserve University*

Monday Afternoon, Room 301
CURRENT PROGRESS IN SEPARATIONS OF CARBON NANOTUBES (II)
Presider: Stephen Doorn

1:30 (138) **Separation and Characterization of Carbon Nanotubes and Nano-onions by Using Flow Field-Flow Fractionation**; John Selegue, *University of Kentucky*; Bailin Chen, *University of Kentucky*; Huijian Jiang, *University of Kentucky*

1:50 (139) **Separation of Metallic From Semiconducting**; Frank Hennrich, *Institut für Nanotechnologie*; Ralph Krupke, *Institut für Nanotechnologie*; Manfred Kappes, *Institut für Physikalische Che*; Hilbert von Löhneysen, *Physikalisches Institute*

2:10 (140) **Chemical Functionalization Strategies for Carbon Nanotubes**; Stanislaus S. Wong, *Department of Chemistry; SUNY*; Sarbajit Banerjee, *Department of Chemistry, SUNY*; Michael G.C. Kahn, *Department of Chemistry, SUNY*

2:50 **Coffee Break**

2:30 (141) **Separation of Carbon Nanotubes by Selective Chemical Functionalization**; Michael Strano, *Univeristy of Illinois - Urban*

3:30 (142) **Noncovalent Engineering of Carbon Nanotube Surfaces**; Jian Chen, *Zyvex Corporation*; Haiying Liu, *Department of Chemistry, Michigan Techn*; Rajagopal Ramasubramaniam, *Zyvex Corporation*

3:50 (143) **Gel Electrophoretic Separations of SWNTs**; Michael O'Connell, *Los Alamos National Lab*

4:10 (144) **Sonication and pH Effects on Micelle-Encased Hipco Carbon Nanotubes**; Wei Zhao; Brian Benedict, *University of Arkansas*

Monday Afternoon, Room 302
ELECTROTHERMAL VAPORIZATION SAMPLE INTRODUCTION TECHNIQUES
Presider: Greet de Loos, *Delft University of Technology*

1:30 (145) **ETV-ICP-MS: Can It Be More Useful Than We Thought?**; James Holcombe, *Univ. of Texas at Austin*; William Balsenek, ; John Venable, ; Gulay Ertas, *METU; Turkey*

2:10 (146) **Progress in ETV/ICP-OES and MS for the Direct Analysis of Ceramic Powders**; Jose A.C. Broekaert, *University of Hamburg, Institute*

2:50 **Coffee Break**

3:30 (147) **Elemental Analysis of Airborne Micro- and Nano-Particles by In-Torch Vaporization-Inductively Coupled Plasma-Atomic Emission Spectrometry**; Vassili Karanassios, *University of Waterloo*; Greg Sprah, *University of Waterloo*

3:50 (148) **Influence of the Carrier Gas Flow in Electrothermal Vaporization Sample Introduction for Plasma Source Spectrometry**; Greet de Loos, *Delft University of Technology*; Tibor Kantor, *L. Eotvos University Budapest*

4:10 (149) **Investigation and Optimization of a New Electrothermal Vaporization Unit with Analyte Vapor Condensation in An Axially Focusing Upstream Convection Zone*)**; Alexander Trenin, *I. Physikalisches Institut, Ju*; Gerd Hermann, *I. Physikalisches Institut, Ju*; Marat Gafurov, *I. Physikalisches Institut, Ju*; Rudolf Matz, *I. Physikalisches Institut*

Monday Afternoon, Room 304
ICP MS: NEW DEVELOPMENTS AND APPLICATIONS
Presider: Dmitry Bandura, *MDS SCIEX*

1:30 (150) **A New Approach to Sampling Ions from the ICP for Mass Spectrometry**; Don Douglas; Chuanfan Ding; Samir Al Moussalami, *University of British Columbia*

2:10 (151) **New Directions in ICP-MS**; R. S. Houk; David Aeschliman; Fumin Li; Bo Zhang; Dan Armstrong; Elizabeth McKinney; Mark Gordon, *Ames Lab USDOE, Department of Chemistry, Iowa State*

2:50 **Coffee Break**

3:30 (152) **Laser Ablation ICP-MS of Blot-Membranes - a New Tool for the Analysis of Proteines**; Norbert Jakubowski, *Institute for Spectrochemistry*; Ingo Feldmann, *Institute for Spectrochemistry*; Wolf Lehmann, *Central Spectroscopy*

3:50 (153) **Advancing Laser Ablation using High Sensitivity ICP-MS**; Shane Elliott, *Varian Analytical, Melbourne*; Stephen Anderson, *Varian Analytical, Melbourne*; Michael Plantz, *Varian Inc*

4:10 (154) **A Study of Ion Loss Mechanisms in the First Vacuum Stage of An Inductively Coupled Plasma Mass Spectrometer**; Paul Farnsworth, *Brigham Young University*; Jeffrey Macedone, *Brigham Young University*; Andrew Mills, *Brigham Young University*

4:30 (155) **ICP-MS Based Immunoassays: From Elements to Macromolecules**; Xinrong Zhang, *Department of Chemistry, Tsing*; Chao Zhang, *Department of Chemistry, Tsing*

Monday Afternoon, Room 305
LASER-BASED METHODS IN ATOMIC SPECTROSCOPY II
Presider: Nicolo Omenetto, *University of Florida*

1:30 (156) **Introductory Overview of Laser Atomic Spectroscopy with Emphasis on Analytical Applications**; Nicolo' Omenetto, *University of Florida*

1:50 (157) **Trace, Isotopic Analysis in the Atom Counting Limit Using Resonant Ionization Mass Spectrometry.?**; Michael Pellin, *Argonne National Laboratory*

2:30 (158) **High Resolution Resonance Ionization Mass Spectrometry**; Bruce Bushaw, *Pacific Northwest National Lab*

2:50 **Coffee Break**

3:30 (159) **Cavity-Enhanced Laser Spectroscopy: A Demonstrated Path to Ultrahigh Detection Sensitivities**; Jun Ye, *JILA, NIST and Univ. of Colorado*

4:10 (160) **Microchip Lasers and Applications in Fieldable Instruments**; John J. Zayhowski, *MIT Lincoln Laboratory*; John D. Hybl, *MIT Lincoln Laboratory*

4:50 (161) **Spectrally-Selective Photon Detection by Coherent Excitation of Cesium Vapor**; Tiffany Correll; Benjamin Smith; Nicolo Omenetto; James Winefordner, *University of Florida*

Monday Afternoon, Room 317
MASS SPECTROMETRY'S ROLE IN PHARMACEUTICAL DRUG DEVELOPMENT
Presider: Joseph McClellan, *Wyeth Pharmaceutical*

1:30 (162) **Integrated Strategies for Drug Development Using Mass Spectrometry**; Mike Lee, *Milestone Development Services*

2:10 (163) **LC/MS Applications for Screening: A Highlight Tour**; Todd Gillespie, *Lilly Research Laboratories*; Kenneth Cassidy, *Lilly Research Laboratories*; Brad Ackermann, *Lilly Research Laboratories*

2:50 **Coffee Break**

3:30 (164) **Leveraging the Use of Modern Mass Spectrometry Instrumentation in Drug Developmment**; Brent Kleintop, *Bristol-Myers Squibb*; Haiying Zhang, *Bristol-Myers Squibb*; Rich Gedamke, *Bristol-Myers Squibb*; Ken Ray, *Bristol-Myers Squibb*; Nona Khaselev, *Bristol-Myers Squibb*; Gerald DiDonato, *Bristol-Myers Squibb*

4:10 (165) **High Throughput Compound Screening and Characterization Employing Microfluidic LC**; Gene Dantsker, *Nanostream Inc.*

Monday Afternoon, Room 318
SEPARATION SCIENCE: BIOMEDICAL AND PHARMACEUTICAL SEPARATION APPLICATIONS
Presider: Mary Ellen McNally, *Dupont*

1:30 (166) **Application of CLND Detection to Cleaning Validation Studies in the Pharmaceutical Industry**; John Guzowski, *BMS*; Leon Liang, *BMS*; Frank Tomasella, *BMS*

1:50 (167) **Determination of S and Se Containing Amino Acids in Biological Tissue Using Extraction with Modified Supercritical Fluid**; Luis Rodriguez, ; James Harnly, *U.S. Department of Agriculture*

2:10 (168) **Hypernated Liquid Chromatography: A Significant Improvement to Extractables Evaluation Programs for Pharmaceutical Containers**; David Albert, *NAMSA*

2:50 **Coffee Break**

3:30 (170) **Unlocking the Secrets to Validation of TLC Methods**; Pamela Gorman, *Pfizer*;

3:50 (171) **Development of Splitless GC Methodology for Acetic Acid, Dimethylformamide, Pyridine and Other Polar Solvents Used in Manufacture of Bulk Pharmaceuticals**; David McCollum, *Pfizer*; Steven MacLeod, *Pfizer*

4:10 (173) **Multiplexed Detection for Microchannel Electrophoresis with A Charge Coupled Device**; Jennifer McReynolds, *University of Illinois at Chic*; Scott Shippy, *University of Illinois at Chicigo*

Tuesday Morning, Room 113
MULTIVARIATE APPROACHES IN CHROMATOGRAPHIC APPLICATIONS
Presider: Scott Ramos, *Infometrix*

8:30 (174) **Feature Selection and Discrimination for Chromatographic and Spectroscopic Applications of Pattern Recognition**; Stephen L. Morgan, *University of South Carolina*

9:10 (175) **Principal Components Analysis and Linear Discriminant Analysis**; Mary Mulholland, *UTS*; Ashwini Kher, *UTS*

9:50 **Coffee Break**

10:30 (176) **Application of HPLC-Coulometric Array Redox Profiling to Metabonomic Studies**; Paul Gamache, *ESA, Inc.;* Ian Acworth, *ESA, Inc. & Massachusetts College of Pharmacy;* John Waraska, *ESA, Inc.*; Timothy Maher, *Massachusetts College of Pharmacy*

11:10 (177) **Determination of the Number and Position of Components in On-flow LC-NMR of Mixtures: a Comparison with HPLC-DAD**; Richard Brereton, ; Mohammad Wasim; Hassan Sukri, *University of Bristol*

Tuesday Morning, Room 114
RSC SESSION: DEVELOPMENTS IN CHEMOMETRICS FOR PROCESS ANALYSIS AND CONTROL
Presider: David Littlejohn, *University of Strathclyde*

8:30 (178) **Mathematical Modeling of Batch Reactions and Processes with in-situ Spectroscopic and Calorimetric Measurements**; Paul Gemperline, *East Carolina University*; Samir Alam, *Oklahoma State University*; R. Russell Rhinehart, *Oklahoma state University*; Graeme Puxty, *Newcastle University, NSW, Aus*; Marcel Maeder, *Newcastle University, NSW, Aus.*

9:10 (179) **Application of Process Chemometrics to the Monitoring of Industrial Processes**; Anthony Walmsley, *University of Hull*
9:30 (180) **Multivariate Curve Resolution of Spectroscopic Data From a Hydrogenation Reaction**; Colin McGill, *Avecia Ltd.*; Ewan Polwart, *Avecia Ltd.*; Ian Wells, *Avecia Ltd.*
9:50 **Coffee Break**
10:30 (181) **Control Relevant Measurements and Chemometrics**; Barry Wise, *Eigenvector Research Inc.*
11:10 (182) **Multivariate Statisical Process Performance Monitoring: Its Impact on Variability Reduction**; Elaine Martin, *University of Newcastle*; Julian Morris, *University of Newcastle*
11:30 (183) **Increasing Process Understanding and Robustness Using Process Data and MSPC**; Richard Escott, *GlaxoSmithKline*; Christian Airiau, *GlaxoSmithKline*

Tuesday Morning, Room 204
NEW APPROACHES TO TEACHING MASS SPECTROMETRY
Presider: Cameron Dorey, *University of Central Arkansas*

8:30 (185) **Illustrating Mass Spectrometer Function in an Undergraduate Instrumenation Course using Computer Simulations**; William Taylor, *University of Central Arkansas*
9:10 (186) **Mass Spectroscopy Experience for Everyone Using Case Studies and a Virtual Laboratory**; Joseph Grabowski, *University of Pittsburgh*; Mark Bier, *Carnegie Mellon University*
9:50 **Coffee Break**
10:30 (187) **Integrating Ion Trap Mass Spectrometry in the Undergraduate Chemistry Curriculum**; Anna Cavinato, Ron Kelley, *Eastern Oregon Univeristy*
11:10 (188) **Bringing Proteomics into Chemical Education: An Approach to Teaching Peptide Mass Fingerprinting**; Jackson Lay; Rohana Liyanage; Maggie Brown, *University of Arkansas*

Tuesday Morning, Room 216
NEW DEVELOPMENTS IN FORENSIC SCIENCE RESEARCH
Presider: Bruce McCord, *Ohio University*

8:30 (189) **Determination of Heroin Metabolites in Human Urine Using Capillary Electrophoresis with Laser-Induced Fluorescence Detection**; Ahmed Alnajjar, *Ohio University*; Bruce McCord, *Ohio University*
8:50 (190) **Identification of Dyes Extracted from Textile Fibers by High Performance Liquid Chromatography-Mass Spectrometry (HPLC-MS)**; Min Huang, *University of Central Florida*; Michael Sigman, *University of Central Florida*
9:10 (191) **Fast Gas Chromatographic Analysis of Benzodiazepines from Blood and Urine Samples**; Alexander Nieuwland, *University of South Carolina*; Stephen Morgan, *University of South Carolina*; David Eagerton, *South Carolina Law Enforcement Division*; Steven Dubose, *Arizona Chemical Co.*
9:30 (192) **Improving the Detection and Sampling of Ignitable Liquid Residues and Explosive Compounds**; Jeannette Perr; Ken Furton; José Almirall, *Florida International University*
9:50 **Coffee Break**
10:30 (193) **The Detection of Inorganic Ions in Smokeless and Muzzleloading Powder Residue**; Kristy Hopper, *Ohio University*; Bruce McCord, *Ohio University*
10:50 (194) **Laboratory and Field Experiments Used to Identify the Uniqueness of Human Scent Identified by Canines, SPME/GC/MS and SPME/LC/MS**; Allison Curran, *International Forensic Researc*; Kenneth Furton, *International Forensic R*esearch
11:10 (195) **Identification of Canis Familiaris Active Odor Signature Chemicals in Human Remains.**; Samantha Tolliver;Michael Chow, ; Kenneth Furton, *Florida International University*
11:30 (196) **Micellar Electrokinetic Chromatographic Screening Method for Common Sexual Assault Drugs**; Sandra Bishop, *Ohio U*; Maggie Lerch, *Ohio U*; Bruce McCord, *Ohio University*

Tuesday Morning, Room 220
LAB-ON-A-CHIP SYSTEMS IN BIOANALYTICAL CHEMISTRY
Presiding: Adam Woolley, *Brigham Young University*

8:30 (197) **Polyacrylamide Hydrogel for Protein Analysis**; Gloria Thomas, *National Institute of Standard*; Laurie Locascio, *NIST*; Michael Tarlov, *NIST*
8:50 (198) **Single Cell Enzyme Activity Studies Using Microfluidic Devices**; Christopher Culbertson, *Kansas State University*; Luke T. Tolley, *Oak Ridge National Laboratory;* J. Michael Ramsey, *Oak Ridge National Laboratory;* Steven R. Gonda, *NASA-Johnson Space Center*
9:10 (199) **Enhancing Electrochemical Detection for Microchip Electrophoresis**; Charles Henry; Yan Liu; Jon Vickers, *Colorado State University*
9:30 (200) **Microfluidic Routes to the Controlled Production of Small Molecules and Nanoparticles**; Andrew de Mello, *Imperial College*
9:50 **Coffee Break**
10:30 (201) **New Materials and Modules for Lab-on-a-Chip Analysis**; Adam Woolley; Ryan Kelly; Tao Pan; Jason Munyan; Bridget Lewis, *Brigham Young Univ.*
10:50 (202) **Behavior of Fast Flows in Complex Microfluidic Systems**; Daniel T Chiu, *University of Washington*
11:10 (203) **Personal Microfluidics: Portable, Affordable, Programmable Microfluidic Systems for Bioanalysis**; shuichi takayama, *University of Michigan*

Tuesday Morning, Room 221
ANACHEM AWARD: MASS SPECTROMETRY FOR HOMELAND DEFENSE AND DISEASE DIAGNOSIS AWARDED TO CATHERINE FENSELAU
Presider: Robert Cotter, *The Johns Hopkins University*

8:30 (204) **Some Thoughts on Rapid Characterization of Microorganisms by MALDI Mass Spectrometry**; Catherine Fenselau, *University of Maryland*
8:50 (205) **Detection of Malaria in Blood by Laser Desorption Mass Spectrometry**; Plamen Demirev, *Johns Hopkins University*
9:30 (206) **Small, Acid-Soluble Proteins as Biomarkers in Mass Spectrometry Analysis of Bacillus Spores.**; Yetrib Hathout, *Department of Chemistry;* Barbara Setlow, *Department of Biochemistry;* Rosa-Martha Cabrera-Martinez, *Department of Biochemistry,* Catherine Fenselau, *Department of Chemistry;* Peter Setlow, *Department of Biochemistry*

9:50 **Coffee Break**
10:30 (207) **Advanced Methods for the Rapid Analysis of Microorganisms by MALDI-TOFMS and Proteomics**; Bettina Warscheid,*University of Maryland*
11:10 (208) **Miniaturized Time-of-Flight Mass Spectrometers for Biological Research and Bioagent Detection**; Robert Cotter, *Johns Hopkins School of Medicine*; Ben Gardner, *Johns Hopkins School of Medicine*

Tuesday Morning, Room 222
RAMAN SPECTROSCOPY IN PHARMACEUTICAL RESEARCH AND DEVELOPMENT
Presider: Don Pivonka, *Astra Zenecca*

8:30 (209) **The Role of Raman Microscopy in Polymorph Screening**; Clare Anderton, *GlaxoSmithKline*; David Lee, *GlaxoSmithKline*
9:10 (210) **Extending the Boundaries of Raman Spectroscopy in Pharmaceutical Development**; Don Clark, *Pfizer Global R&D*
9:50 **Coffee break**
10:30 (211) **Multidimensional Raman Mapping of Tablets**; Michael Longmire, *SSCI Incorporated*; David Bugay, *SSCI Incorporated*
11:10 (212) **Raman Spectroscopy in Drug Discovery**; Don Pivonka, *AstraZeneca*

Tuesday Morning, Room 223
CHIRAL CHROMATOGRAPHY AND DETECTORS I
Presider: Rekha Shah, *Johnson and Johnson*

8:30 (213) **Chiral Separations by Capillary Electrophoresis**; A. M. Stalcup, *University of Cincinnati*; C. E. Evans, *University of Cincinnati*
9:10 (214) **Strategies for Assessing Chiral Chromatographic Selectivity in Early Pharmaceutical Development**; George Reid, *Pfizer*; Daniel Brannegan, *Pfizer*
9:50 **Coffee Break**
10:30 (215) **A Comparative Study of Chiral Molecules Using Vibrational Circular Dichroism (VCD) and Polarimetry**; Douglas Minick, *GlaxoSmithKline*; Randy Rutkowske, *GlaxoSmithKline*
10:50 (216) **Chiral Issues in Early Drug Development**; Daksha Desai-Krieger, *J&JPRD, L.L.C.*; Rekha Shah, *J&JPRD, L.L.C.*

Tuesday Morning, Room 301
PRECONCENTRATION FOR ATOMIC SPECTROMETRY BY SOLID-PHASE EXTRACTION AND CHEMICAL VAPOR GENERATION I
Presider: Julian Tyson, *University of Massachusetts*

8:30 (218) **Sorption Preconcentration for Trace Elements Determination by Atomic Spectrometric Techniques**; Yuri Zolotov, *Lomonosov Moscow University*; Grigory Tsysin, *Lomonosov Moscow University*
9:10 (219) **Preconcentration of Trace Metal Ions by Solid Phase Extraction with Polymeric Resins for Flame Atomic Absorption Spectrometry**; Latif Elçý, *Pamukkale University*; Mustafa Soylak, *Erciyes University*; Mehmet Doðan, *Hacettepe University*
9:50 **Coffee Break**
10:30 (220) **Immobilized, Short Chain Biopolymer Metal Chelators**; James Holcombe, *University of Texas at Austin*; Ashley Johnson; Lisa Malachowski, ; Jacqueline Stair
11:10 (221) **Flow Injection and Sequential Injection: The Optimal Solutions for Executing Appropriate On-Line Separation and Preconcentration Schemes for ETAAS/ICPMS**; Elo H. Hansen, *Technical Univ. of Denmark*

Tuesday Morning, Room 302
NANOPARTICLES/NANOSTRUCTURES I
Presider: John Green, *University of Alberta*

8:30 (222) **Imaging at the Single Molecule Scale with Carbon Nanotubes**; Jason Hafner, *Rice University*
9:10 (223) **Aligned Carbon Nanotubes and Potential Applications**; Z. F. Ren, *Boston College*
9:50 **Coffee Break**
10:30 (224) **Fabrication of Carbon Micro- and Nanostructures by Electrochemical Etching**; Mark McDermott, *University of Alberta*; Solomon Ssenyange, *University of Alberta*; Aaron Skelhorne, *University of Alberta*; Dwayne Shewchuk, *University of Alberta*
10:50 (225) **Gaining Control in the Synthesis of Single Walled Carbon Nanotubes**; Jie Liu, *Duke University*
11:10 (225b) **Can Semiconductor Nanocrystals Emit Light?**; Zhifeng Ding,
11:30 (226) **Developments of AFM for Enhanced Chemical and Biological Discrimination**; John-Bruce Green, *University of Alberta*; Amanda Musgrove, *University of Alberta*; Sandra Chan, *University of Alberta*; Ademola Idowu, *University of Alberta*

Tuesday Morning, Room 304
COLLISION/REACTION CELLS VS. HIGH CELLS VS. HIGH RESOLUTION SECTOR FIELD ICP-MS: A CRITICAL EVALUATION 1. PERSPECTIVES AND FUNDAMENTALS
Presider: I.B. Brenner, *Ben Gurion University of the Negev*

8:30 (227) **A Comparison of High Resolution and Collision Cells for Removing Interferences From Polyatomic Ions in Clinical Analysis By ICP-MS**; R. S. Houk; Jill Ferguson; David Nixon; Mary Burritt; Steven Eckdahl; John Butz, *Ames Lab, Iowa State University*
9:10 (228) **Chemical Resolution of Isobaric Atomic Interferences by ICP-DRC-MS**; Dmitry R. Bandura, *PerkinElmerSCIEX*; Albert E. Litherland, *IsoTrace Laboratory, Universit*; Vladimir I. Baranov, *PerkinElmerSCIEX*; Scott D. Tanner, *PerkinElmerSCIEX*
9:50 **Coffee Break**
10:30 (229) **A Critical Comparison of High Mass Versus Chemical Resolution**; Norbert Jakubowski, *Institute for Spectrochemistry*; Michael Edler, *Institute for Spectrochemistry*; Ingo Feldmann, *Institute for Spectrochemistry*
11:10 (230) **Point-Counter Point. High Resolution Magnetic Sector vs Collision-Reaction Cells in ICP-MS**; John Olesik, *Ohio State University*

TECHNICAL PROGRAM - TUESDAY

Tuesday Morning, Room 305
ATOMIC SPECTROSCOPY IN THE CLINICAL FIELD
Presider: Patrick J. Parsons, *Wadsworth Center*

8:30 (231) **Maintenance Issues and Performance Diagnostics for the Elan DRC Plus ICP-MS.**; David Nixon, *Mayo Clinic*; Steven Eckdahl, *Mayo Clinic*; Gary Austin, *Mayo Clinic*; John Butz, *Mayo Clinic*; Mary Burritt, *Mayo Clinic*; Kenneth Neubauer, *PerkinElmer*; Ruth Wolf, *PerkinElmer*

8:50 (232) **Biomonitoring of Toxic Metals at CDC: Analytical Methods and Exposure Results**; Kathleen Caldwell, *CDC*; Robert Jones, *CDC*; Jeff Jarrett, *CDC*; Ge Xiao, *CDC*; Olga Piraner, *CDC*; Carl Verdon, *CDC*

9:10 (233) **Challenges Associated with the Determination of Non-Dietary Arsenic in Urine by Inductively Coupled Plasma Mass Spectrometry (ICP-MS).**; Ela Bakowska, *National Medical Services*; Manoch Muantongchin, *National Medical Services*; Judy Vinosky, *National Medical Services*

9:30 (234) **Validation of in vivo Bone Lead Measurements Obtained via 109Cd K-Shell X-Ray Fluorescence: Comparison with Electrothermal Atomic Absorption Spectrometry.**; Patrick J. Parsons, *New York State Dept of Health*; Ciaran Geraghty, *New York State Dept of Health*; Frank Blaisdell S., *New York State Dept of Health*; Andrew C. Todd, *Mt. Sinai School of Medicine*

9:50 **Coffee Break**

10:30 (235) **Investigation of Interference Effects in the Determination of Trace Elements in Serum by ICP-MS**; David Littlejohn, *University of Strathclyde*; P Ann Robin, *University of Strathclyde*; David Lyon, *Royal Infirmary, Glasgow*; Lu Yang, *National Research Council Cana*; Ralph Sturgeon, *National Research Council Canada*

10:50 (236) **Arsenic: Total and Speciated Analysis by HPLC-ICP-DRC-MS**; Kathleen Caldwell, *CDC*; Carl Verdon, *CDC*; Jeff Jarrett, *CDC*; Robert Jones, *CDC*

11:10 (237) **Improvements in Sample Introduction and Preparation Techniques for the Determination of Blood/Urine Mercury by ICP-MS: Comparison With a FI-CVAAS Method.**; Christopher D. Palmer, *Wadsworth Center*; Miles E. Lewis, *Wadsworth Center*; Fernando Barbosa Jr., *Universidade de Sao Paulo*; Francisco J. Krug, *Universidade de Sao Paulo*; Patrick J. Parsons, *Wadsworth Center*

11:30 (238) **Ten-year Performance Trends for Trace Metal Determination in Blood**; Jean-Philippe Weber, *Institut national de santé pub*; Alain LeBlanc, *Institut national de santé pub*.

Tuesday Morning, Room 315
INFRARED IMAGING I
Presider: Andre Sommer, *Miami University, Ohio*
Organized by the Coblentz Society

8:30 (239) **Imaging Methods Applied to Polymer Blends**; Peter Wilhelm; Andreas Gupper, ; Mario Schmied, ; Gerald Kothleitner, *Graz University of Technology*

8:50 (240) **Infrared Imaging of Self-Assembled Monolayers on Dielectric Substrates**; Douglas Elmore, *Cargill*; Chad Leverette, *Cargill*; Sean Smith, *Cargill*; Bruce Chase, *DuPont*; Yujuan Liu, *University of Delaware*; John Rabolt, *University of Delaware*

9:10 (241) **Molecular/Mechanical Imaging at the Material/Tissue Interface**; Yong Wang, *University of Missouri School*; Paulette Spencer, *University of Missouri School*; J. Lawrence Katz, *University of Missouri School*

9:30 (242) **Comprehensive Materials Characterization Using Elemental and Molecular Spectroscopic Imaging**; George Havrilla; Thomasin Miller, *Los Alamos National Lab*

9:50 **Coffee Break**

10:30 (243) **A Near-Infrared Chemical Imaging Approach to Measuring the Metrics of Pharmaceutical Blending**; E. Neil Lewis; Linda Kidder, ; Kenneth Haber, Eunah Lee, *Spectral Dimensions, Inc.*

10:50 (244) **Infrared Imaging: How far has it come and what can we do with it now?**; Norman Wright, *Digilab*

11:10 (245) **Immersion and ATR Infrared Imaging**; Andre' Sommer; Luis Lavalle-Castellanos, *Miami University*; Jessica Dellomo, *Miami University*

11:30 (245a) **Utility of Short Step (1 ? m) Functional Group Mapping with Synchrotron Infrared Microspectroscopy;** David L. Wetzel, Microbeam Molecular Spectroscopy Laboratory, Kansas State University

Tuesday Morning, Room 317
FLUORESCENCE METHODS I: ENVIRONMENTAL & TOXICOLOGICAL APPLICATIONS
Presider: Gary Rayson; *New Mexico State University*

8:30 (246) **Investigations of Passive Uranyl Ion Binding to Datura innoxia Cell Walls**; Debbie D. Martinez, *New Mexico State University*; Charlotte Sisk, *New Mexico State University*; Gary D. Rayson, *New Mexico State University*

8:50 (247) **Molecular Fluorescence Spectroscopy: Identification of Plants from Extract Solutions**; Gary Rayson; Timothy Danielson, *New Mexico State University*; Dean Anderson, *USDA*; Rick Estell, *USDA*; Eric Fredrickson, *USDA*; Kris Havstad, *USDA*

9:10 (248) **Natural Water Characterization By Multidimensional Fluorescence Lifetime Spectroscopy**; Kerin Clow, *Tufts University*; Gregory Hall, *U.S. Coast Guard, Tufts Univer*; Jonathan Kenny, *Tufts University*

9:30 (249) **Analysis with trilinear fluorescence**; Bjorn Sjogreen, *Royal Institute of Technology*; Mikael Kubista, *Chalmers University*; Amin Forootan, *MultiD Analyses AB*

9:50 **Coffee Break**

10:30 (250) **Photokinetic Analysis of Rank-deficient Fluorescence Decay Matrices using the Maximum Entropy Method linked to Principal Components Analysis**; Sharon Neal, *Univ of Delaware*; Brad Rowe, *Univ of Delaware*

10:50 (251) **Multidimensional Fluorescence Study of Lipid Aggregates using Novel Flavone Probes**; Brad Rowe, *University of Delaware*; Sharon Neal, *University of Delaware*

11:10 (252) **Optical Mapping Applications in Pathogen Discrimination**; Matthew Ferris, *Los Alamos National Laboratory*; Babetta Marrone, *Los Alamos National Laboratory*; James Jett, *Los Alamos National Laboratory*; Thomas Yoshida, *Los Alamos National Laboratory*; Richard Keller, *Los Alamos National Laboratory*

11:30 (253) **Probing the Interaction of PAH-Derivatives With Antibodies and enzyme Receptors Using Fluorescence Line-Narrowing Spectroscopy**; Arjen Bader; Maarten van Dongen, Ryszard Jankowiak, Cees Gooijer, *Vrije University*; Freek Ariese, *Ames Lab, Iowa State*

Tuesday Morning, Room 318
SEPARATIONS SCIENCE: FASTER CHROMATOGRAPHIC METHOD DEVELOPMENT: TOOLS AND RESULTS
Presider: Mary Ellen McNally, *Dupont*

8:30 (254) **An Automated Approach to the Optimization of HPLC Separations with Special Reference to Mass- and UV-Directed Autopurification**; Thomas Wheat, *Waters*; Jo-Ann Jablonski, *Waters*; Charles H. Phoebe, Jr., *Waters*

9:10 (255) **Using On-Line Knowledge and Software to Automate HPLC Method Development**; Jeffrey DeCicco, *Intelligent Laboratory Solutio*; Douglas Myers, *Intelligent Laboratory Solution*

10:30 (256) **Application of Computer Simulation Software for Development and Optimization of HPLC Analyses for Crop Protection-Based Process Samples and Actives**; David Brennan, *DuPont Crop Protection*

11:10 (257) **The Use of Adsorption Data to Predict Chromatographic Retention**; David Johnson, *Swedish Match Corporation*

11:50 (258) **Use of Response Surface Methodology As Part of an Optimization Strategy for Selection of Mobile Phase Solvents in Chiral HPLC**; William Champion, *Rhodia Pharma Solutions*

12:00 – 2:00 PM, Exhibit Hall C
TUESDAY MIDDAY POSTER SESSION

Your poster should be put up between 10:00 AM and noon on Tuesday and removed between 5:00 – 6:00 PM. Please leave your poster in place for the entire time. Check below for presentation time.

1:15 (3) **Milestones in the History and Evolution of the Raman Effect**; Michel Delhaye, *U Lille (retired)*; Wolfgang Kiefer, *U Wurzburg*; Derek Long, *U Bradford*; Edouard DaSilva, *Jobin Yvon*; Jacques Barbillat, *U Lille*; Paul Dhamelincourt, *U Lille*

12:15 (259) **Kinetics of Catalytic Isomerization of Quadricyclane to Norbornadiene Using Near Infrared Absorption Spectroscopy**; Hsiu-Fang Fan, *Department of Chemistry, Natio*; Thou-Long Chin, *Department of Chemistry*; King-Chuen Lin, *Department of Chemistry*

1:15 (260) **Application of Photothermal Lensing to the Investigation of Surface-Absorbed Transparent Solids**; Dmitry Nedosekin, *Chemistry Department, M.V. Lom*; Mikhail Kononets, *Chemistry Department, M.V. Lom*; Mikhail Proskurnin, *Chemistry Department, M.V.*

12:15 (261) **Investigation of the Flat Glass and Quartz Modified Surface by Thermal Lensing**; Dmitry Nedosekin, *Chemistry Department, M.V. Lom*; Mikhail Kononets, *Chemistry Department, M.V. Lom*; Mikhail Proskurnin, *Chemistry Department, M.V.*

1:15 (262) **Kinetic Determination of Organo-Sulphur Ligands by Inhibition: Trace Determination of Cysteine and Maleonitriledithiolate (MNDT)**; Dr. Surendra Prasad, *The University of the South Pa*;

12:15 (263) **Characterization of Resorcinol-Formaldehyde Organic Aerogel**; Farnoosh Mehrabi, *Amirkabir University*; A. Saadat, *Amirkabir University*

1:15 (264) **Combination of Nanosecond and Femtosecond Pulses in Laser-Induced Breakdown Spectroscopy of Aqueous Solutions**; Jonathan Scaffidi, *University of South Carolina*; Bill Pearman, *University of South Carolina*; Jack Pender, *University of South Carolina*; J. Chance Carter, *Lawrence Livermore National La*; Bill W. Colston Jr., *Lawrence Livermore National La*; Scott Goode, *University of South Carolina*; S. Michael Angel, *University of South Carolina*

12:15 (265) **Determination of U-236 by ICP-MS in Environmental Samples**; Sabine Becker, *Research Center Juelich*

1:15 (266) **Determination of 129I/127I Isotope Ratio by ICP-MS with Collision Cell in Environmental Samples**; J.Sabine Becker, *ZCH*

12:15 (267) **The Enhanced Parallel Path Pneumatic Nebulization Method ? A New Concept in Nebulization.**; John Burgener, *Burgener Research Inc.*

1:15 (268) **Determination of Trace Elements In Precious Metals by ICP-OES Spectrometry**; Albert Brennsteiner, *Jobin Yvon Inc*; Geoffrey Tyler, *Jobin Yvon SAS*; Agnès Cosnier, *Jobin Yvon SAS*; Nathalie Le Corre, *Jobin Yvon SAS*

12:15 (269) **Platform-To-Platform Sample Transfer and Handling System with Distribution, Dilution, and Micro-Dosing Via Electrothermal Vaporization And Electrostatic Re-Precipitation*)**; Alexander Trenin, *I. Physikalisches Institut, Ju*; Gerd Hermann, *I. Physikalisches Institut, Ju*; Rudolf Matz, *I. Physikalisches Institut, Ju*; Albert Gilmutdinov, *Department of Physics, Kazan S*; Konstantin Nagulin, *Department of Physics, Kazan S*; Wolfgang Frech, *Department of Chemistry, Analy*; Erik Bjoern, *Department of Chemistry, Analy*

1:15 (270) **In-torch Vaporization (ITV) Sample Introduction as an Alternative to Reaction/Collision Cell ICP-MS**; Vassili Karanassios, *University of Waterloo*; Hamid Badiei, *University of Waterloo*; Greg Sprah, *University of Waterloo*

12:15 (271) **Study of Different Ways of Pre-Concentration for the Determination of Gold, Silver and Copper.**; Maria Ines Toral, *Laboratory of Analytic Chemist*; Libby Morales, *Laboratory of Analytic Chemisty*

1:15 (272) **The Effect of Interface Design Changes on Matrix Effects in ICP-MS**; Phil Shaw, *Thermo Electron*; Jonathan Batey, *Thermo Electron*; Bill Spence

12:15 (273) **Comparison of Rh, Ir and Ru modifiers for in-situ Trapping of Selenium Hydride on W-Coil Electrothermal Atomic Absorption Spectrometry**; Samuel Simao de Souza, *Universidad Federal de Sao Carlos*, Fernando Barbosa Jr; Dario Santos Jr; Francisco Jose Krug, *Centro de Energia Nuclear NA Agricultura*

1:15 (274) **Use of a PFA Nebulizer ICP-MS. Comparison with a Conventional Glass Concentric Micronebulizer for the Analysis of Foods**; José Luis Todoli, *University of Alicante*; Salvador Enrique Maestre, *University of Alicante*; Jean Michel Mermet, *University Claude Bernard*

12:15 (275) **Water Pollution Monitoring Using ICP-AES. Determination of Carbon fractions and Heavy Metals**; José L. Todolí, *Univerisity of Alicante*; Raúl Carbonell, *Univerisity of Alicante*; Salvador E. Maestre, *Univerisity of Alicante*; Juan Mora, *Univerisity of Alicante*

1:15 (276) **Liquid Sample Introduction System Fully Based on Microwave Heating for ICP Spectrometry**; José Luis Todolí, *University of Alicante*; Guillermo Grindlay, *University of Alicante*; Luis Gras, *University of Alicante*; Vicente Hernandis, *University of Alicante*

12:15 (277) **Influence of the Sample Introduction System in the Analysis OF Organotin Compounds by ICP-MS**; José Luis Todolí, *University of Alicante*; Javier Montiel, *University of Alicante*; Juan Mora, *University of Alicante*

1:15 (278) **Chlorine Photometric Speciation in Waters**; José Luis Todolí, *University of Alicante*; Raúl Carbonell, *University of Alicante*; Juan Mora, *University of Alicante*

12:15 (279) **Precise Determination of Alloyed Elements in Steel Samples by Voltage Modulation Glow Discharge Optical Emission Spectrometry**; Kazuaki Wagatsuma, *Institute for Materials Researsh*

1:15 (280) **Comparison of the Phytoestrogen, trans-Resveratrol (3,4',5-trihydroxystilbene) Structures From X-Ray Diffraction and Solution NMR**; Fernando Commodari, *Chemistry & Biochemistry Department*; Abdesslem Khiat, *Hôpital Saint-Luc, Centre Hospital*; Yvan Boulanger, *Hôpital Saint-Luc, Centre Hospital*; Sanae Ibrahimi, *INRS-Institut Armand-Frappier*; Alison Brizius, *Chemistry & Biochemistry Department*; Noah Kalkstein, *Chemistry & Biochemistry Department*

12:15 (281) **Comparison of 17- b-estradiol structures from X-ray diffraction and solution NMR**; Fernando Commodari, *Chemistry Department, One Univ*; Sanae Ibrahimi, *INRS-Institut Armand-Frappier*,; Abdesslem Khiat, *Hôpital Saint-Luc, Centre Hosp*; Yvan Boulanger, *Hôpital Saint-Luc, Centre Hosp*; George Sclavos, *Chemistry Department, One Univ*.

1:15 (282) **Effect of Mutation ON Properties of P53 Tetramerization Domain Observed BY FT-IR Spectroscopy**; Bokkyoo Jun,;Amanda S. Lee; Charles Galea; Richard W. Kriwacki; Christian P. Schultz, *Bruker Optics, Inc.*

12:15 (283) **Cancer Diagnosis and Detection via Infrared Microspectroscopy of Cells and Thin Tissue Sections. What Have we Learned?**; Anthony Shaw, *Institute for Biodiagnostics,*; Sarah Low Ying, *Institute for Biodiagnostics,*; Kimberly McCrae, *Institute for Biodiagnostics,*; Gerald Steiner, *Technische Universität, D-0106*; Rainer Salzer, *Technische Universität, D-0106*; Fernando Guijon, *Technische Universität*

1:15 (284) **Simultaneous Determination of Creatine, Creatinine and Guanidinoacetate in Urine by Ion-Pair High-Performance Liquid Chromatography**; Peter Tang, *Cincinnati Children's Hospital*; Ton DeGrauw, *Cincinnati Children's Hospital*

12:15 (285) **Development of Breath Analyzer for Diabetes Diagnosis Using Cavity Ringdown Spectroscopy**; Chuji Wang, *Mississippi State University*; D. Hossain, *Mississippi State University*; S. T. Scherrer, *Mississippi State University*

1:15 (286) **Chemometrics in Multidimensional High Resolution Luminescence Spectroscopy**; Hector Goicoechea, *Department of Chemistry, Unive*; Shenjiang Yu, *Department of Chemistry, Unive*; Andres Campiglia, *Department of Chemistry*

12:15 (287) **Determination of Pseudo-Rank and Degrees of Freedom for Multivariate Calibration**; John Kalivas; Heather Seipel, *Idaho State University*

1:15 (288) **Using Error Information with the L-Curve for Multivariate Calibration Model Determination**; John Kalivas, *Idaho State University*; Joel Forrester, *Idaho State University*

12:15 (289) **Chromatographic Separations Using Polyelectrolyte Multilayers**; Hassan Rmaile, *Florida State University*; Karyn Usher, *Florida State University*; John Dorsey, *Florida State university*; Joseph Schlenoff, *Florida State University*

1:15 (290) **Controlling Electroosmotic Flow Direction and Rate By Manipulating Surface Charge Property of the Capillary Column Using pH-Responsive Polyelectrolyte Multilayer Coating**; Zhijie Sui, *Florida State University*; David S. Salloum, *Florida State University*; Joseph B. Schlenoff, *Florida State University*

12:15 (291) **Analgesics in Tylenol and Migraine Tablets by the Standard Addition Method**; Huggins Z. Msimanga, *Kennesaw State University*; Jilliann Wiese, *Kennesaw State University*

1:15 (292) **Innovative 90 Degree Reflecting Ion Optics ICP-MS for the Analysis of Environmental Samples**; Shane Elliott, *Varian Analytical, Mebourne*; Stephen Anderson, *Varian Analytical, Melbourne*; Michael Plantz, *Varian Inc*

12:15 (293) **Electrochemical Analysis of Homocysteine Self-Assembled Monolayer Electrode**; Qinshu Sun; Huiyun Wang, *Jining Chemical College*

1:15 (294) **Electrochemical Behavior of Homocysteine-Bridged Superoxide Dismutase Electrode**; Qinshu Sun; Huiyun Wang; Yi Sun, *Jining Chemical College*

12:15 (295) **A Practical Experimental Design to Sweep Current in Polarography without Sacrificing Precision**; Qinshu Sun; Jianmin Xu, *Jining Chemical College*

1:15 (296) **Development of Denerator-Collector for Measurement of Organohalides**; Wisitsri Wiyarat; Werasak Surareuagchai, *Joint Graduate School of Energy & Environment*; Mithran Somasundrum, *Pilot Plant Development and Training*

12:15 (297) **Time-Resolved Optical Imaging, Spectroscopy and Microscopy Using Ultrahigh Rep. Rate, Ultrafast Gated Intensified CCD Cameras**; Ramesh Ahuja, *Tautec LLC*

1:15 (298) **Continuous-Flow Protease Assay Based on Fluorescence Resonance Energy Transfer**; Freek Ariese; Junko Hirata; Hubertus Irth; Cees Gooijer, *Vrije University Amsterdam*

12:15 (299) **Digital Fluorescence Imaging Studies of Controlled Drug Delivery**; Li Chen, *University of New Orleans*; Nsikan Martin, *Xavier University*; Nitsa Rosenzweig, *Xavier University*; Zeev Rosenzweig, *University of New Orleans*

1:15 (300) **Discrimination of Nylon Subclasses using FTIR Microscopy and Multivariate Statistical Techniques**; Elizabeth Enlow, *University of South Carolina,*; Jennifer Kennedy, *University of South Carolina,*; Shana Burnett, *University of South Carolina,*; Christopher Mubarak, *University of South Carolina,*; Alexander Nieuwland, *University of South Carolina,*; Stephen Morgan, *University of South Carolina*

12:15 (301) **A Spectroscopist's View of Lead-Based House Paints**; Gene Hall; Laurie Smith, *Rutgers University*

1:15 (302) **Extraction of Cardiac Troponin I from Muscle Tissue with Carboxylate Magnetic Microparticles**; Dr. Alberto J. Sabucedo, *Florida International Universi*; Dr. Kenneth G. Furton, *Florida International University*

12:15 (303) **Development of a Near-Infrared Spectral Library for the Identification of Umbelliferous Drugs**; Cho Changhee, *Korea Food & Drug Administrati*; Ze Keum-ryon, *Korea Food & Drug Administrati*; Lee Song-Duk, *Korea Food & Drug Administration*

1:15 (304) **Spectroscopic Characterization of Polypropylene Nanocomposites**; Vasilis Gregoriou; Athina Korakianiti, *Foundation of Research & Technology-Hellas*; Vasiliki Papaefthimiou; Theofania Daflou; Stellla Kennou, *Dept. of Chemical Engineering*

12:15 (305) **Study of Micro-Phase Separated Blends of Polystyrene/Polymethyl Methacrylate (PS/PMMA)**; Vasilis Gregoriou; Athina Korakianiti; Georgia Kandilioti; *Foundation of Research & Technology;* Siobhan Walsh, *Dept. of Chemistry - Mass*

1:15 (306) **Determination of Absolute Configuration and Solution Conformation in Aminoalcohols and Tetra-Substituted Alpha-Fluorocyclohexanones: Evidence for Solvent Stabilization of Solution Conformations**; Teresa B. Freedman, *Department of Chemistry, Syracuse*; Laurence A. Nafie, *Department of Chemistry, Syracuse*; Arlette Solladié-Cavallo, *Laboratoire de Stéréochimie*

12:15 (307) **Classification Based on Near-IR Spectra With Application to Cnidium Rhizome**; Ze Keum-ryon, *Korea Food & Drug Administration*; Cho Chang-hee, *Korea Food & Drug Administration*; Sung Rak-sun, *Korea Food & Drug Administration*; Lee Jong-pil, *Korea Food & Drug Administration*; Park Ju-young, *Korea Food & Drug Administration*; Cho So-yean, *Korea Food & Drug Administrati*; Lee Dong-mi, *Korea Food & Drug Administration*; Lee Song-duk, *Korea Food & Drug Administration*

1:15 (308) **Determination of Electrophotographic Paper Fuser Oil Pickup**; Charles Lohrke, *International Paper Company*

12:15 (309) **Low Level Analysis of Arsenic and Selenium in Organic Samples Digested with a Novel Vent and Reseal Approach**; Robert Lockerman, *CEM Corporation*; David Barclay, Ph.D., *CEM Corporation*; Elaine Hasty, *CEM Corporation*; Deborah Kiebach, *CEM Corporation*

1:15 (312) **Formation and Hydration Aluminum Oxide Cluster Ions in a quadrupole Ion Trap**; Anita Gianotto, *INEEL*; Anthony Appelhans, *INEEL*; Gary Groenewold, *INEEL*; Jennifer Rawlinson, *INEEL*; Ravi Pandey, *Michigan Technological Univ.*; Peter de B. Harrington, *Ohio University*

12:15 (313) **Characterization of Organouranyl Complexes using Electrospray Ionization Mass Spectrometry**; Garold Gresham, *INEEL*; Gary Groenewold, *INEEL*; Michael Van Stipdonk, *Wichita State University*; Dorothy Hanna, *Kansas Wesletan University*; Winnie Chien, *Wichita State University*; Victor Anbalagan, *Wichita State University*

1:15 (314) **Generating Electrospray ionization from An Optical Fiber Coated with Gold Nanoparticles and Tungsten Oxide Nanowires on An Tungsten Fiber**; Jingyueh Jeng; Jentaie Shiea, *National Sun Yat-Sen University*

12:15 (315) **Real-Time Chemical Speciation of Selenium Using Gas Chromatography Coupled with Pulsed Glow Discharge Time-of-Flight Mass Spectrometry**; Na Zhang, *Dept. of Chemistry, West Virgi*; Jennifer Robertson, *Dept. of Chemistry, West Virgi*; Lei Li, *Dept. of Chemistry, West Virgi*; Fred King, *Dept. of Chemistry, West Virginia*

1:15 (316) **Target Breast Cancer Marker Proteins with High Resolution Multidimensional Liquid Phase Seapration and Mass Spectrometry**; Kan Zhu; David Lubman, *University of Michigan*; Fred Miller, *Barbara Ann Karmanos Cancer Institute*

12:15 (317) **Trap Effect to Molecular Parameters in Molecularly Doped Polymer System**; Choongkeun Lee, *Chungbuk University*; Won-Jae Joo, *Hanyang University*; Nam-Soo Lee, *Chungbuk University*; Nakjoong Kim, *Hanyang University*

12:15 (319) **Absolute Configuration and Solution Conformation OF Asymmetrically Substituted Biphenyls: Evidence for Unexpected Atropisomeric Stability**; Teresa B. Freedman; Xiaolin Cao; Laurence A. Nafie, *Syracuse University;* Monica Kalbermatter; Anthony Linden; Andreas J. Rippert, *Organisch-Chemisches Institut der University*

1:15 (320) **Metal Cation Concentration determined by Proton NMR and Spectrum Area Integration**; Steven Han, *CSULA*

12:15 (321) **Ab-initio Calculation of Ring Current Effects of Amino Acid Residues to Locate Position of Substrates in Binding Pockets of Enzymes**; Erich Franz Kleinpeter, *Universität Potsdam, Chemische*

1:15 (322) **Characterization of the Chemical Degradation of a Cyanine Dye in NH4OH**; William M. Volcheck; Daniel R. Draney, *LY-COR Biosciences, Inc.*

12:15 (323) **Metadata in Analytical Science**; Stuart Chalk, *University of North Florida*

1:15 (324) **Study of Stability oF 2,6-TADAP and the Formation OF -2,6-Dapema, as New Ligand Chromophore**; César Soto; M. Ines Toral, *University of Chile*

12:15 (325) **Hypernated Liquid Chromatography: A Significant Improvement to Extractalbes Evaluation for Pharmaceutical Container Closure Systems**; David Albert, *NAMSA*

1:15 (326) **Quantitative Raman Measurements at PPB Levels Using Commercially-available SERS Media**; Steven Bell, *Queen's University*; Narayana Sirimuthu, *Queen's University*; Andrew Dennis, *Avalon Instruments*

12:15 (327) **Thermal-Lens Determination of Pyrogenic Substances**; Anton Brusnichkin, *Chemistry Department, M.V. Lom*; Natal'ya Orlova, *Chemistry Department, M.V. Lom*; Vera Samburova, *Chemistry Department, M.V. Lom*; Mikhail Proskurnin, *Chemistry Department, M.V. Lom*.

1:15 (328) **High Throughput Quantitative Raman Spectroscopy for Pharmaceutical QC & Manufacturing**; Andrew Dennis, *Avalon Instruments*; Adrian Boyd, *Avalon Instruments*; Steven Bell, *Queen's University*

1:15 (330) **Sequential Determination of Atapulgite and Nifuroxazide for Derivative Spectrophotometry.**; M. Inés Toral, *Departament of Chemistry. Facu*; Maximiliano Paine, *Departament of Chemistry. Facu*; Patricio Leyton, *Departament of Chemistry. Facu*; Pablo Richter, *National Environmental Center*

12:15 (331) **Multiequilibria Studies of Biomolecules using Multivariate Curve Resolution;** Joaquim Jaumot, *Universitat de Barcelona*; Susana Navea, *Universitat de Barcelona*; Raimundo Gargallo, *Universitat de Barcelona*; Anna de Juan, *Universitat de Barcelona*; Romà Tauler, *IIQAB-CID, CSIC*

1:15 (332) **Fieldable Raman - Issues for Forensic Analysis**; Valerie Cavett, *Federal Bureau of Investigatio*; Justine Brucker-Serrano, *ORISE*; Leslie Duplaga, *ORISE*; Brian Eckenrode, *Federal Bureau of Investigation*

12:15 (333) **Confocal Raman Microscopy of CVD Diamond on Silicon**; Olaf Hollricher, *WITec GmbH*; Wolfram Ibach; Joerg Mueller, ; Klaus Weishaupt

1:15 (334) **Dental Caries Detection Using Multi-modal Optical Methods: A Preliminary Investigation**; Alex C-T. Ko, *Institute for Biodiagnostics,*; Lin-P'ing Choo-Smith, *Institute for Biodiagnostics,*; Mark Hewko, *Institute for Biodiagnostics,*; Lorenzo Leonardi, *Institute for Biodiagnostics,*; Blaine Cleghorn, *Faculty of Dentistry, Universi*; Cecilia Dong, *Faculty of Dentistry, Universi*; Peter Williams, *Faculty of Dentistry*

12:15 (335) **Intermolecular Hydrogen Bonding of Azodicarbonamide in the Pentamer Cluster**; Nam-Soo Lee; Chung-Keun Lee; Sun-Kyung Park, *Chungbuk National University*

1:15 (336) **Temperature Dependence of SERS Intensity Blinking**; Yoshihiro Maruyama, *Research Consortium for Synthetic Nano-Function*; Mitsuru Ishikawa, *Bioanalysis Lab;* Masayuki Futamat, *Nanoarchitectonics Research Center*

4:30 (336a) **Further Reduction of Linear Birefringence in the VCD Measurement With A Rotating Half-Wave Plate and by Orthogally Orientating Sample Cells**; Xiaolin Cao Cao, *Syracuse University;* Laurence Nafie, *Syracuse Univ. & BioTools, Inc.*

12:15 (336b) **Extension of Vibrational Circular Dichroism into the Near-Infrared Region TO 10,000 CM-1**; Xiaolin Cao; Changning Guo, Laurence Nafie; *Syracuse University*

1:15 (336c)**Vibrational Spectroscopic Study of Aminoguanidinium(1+) Dihydrogen Phosphate Phase Transitions**; Ivan Nemec, *Department of Inorganic Chemis*; Zorka Machackova, *Department of Inorganic Chemis*; Karel Teubner, *Department of Inorganic Chemis*; Ivana Cisarova, *Department of Inorganic Chemis*; Premysl Vanek, *Institute of Physics, The Acad*; Zdenek Micka, *Department of Inorganic Chemistry*

12:15 (336d) **Development of a WEB based Teaching and Learning Resource to Support the Teaching of Quality Assurance in Undergraduate Analytical Courses**; Brian Woodget, *UK Analytical Partnership*; Richard Baker, *Uinversity of Reading, UK*; Irene Mueller-Harvey, *University of Reading UK*

Tuesday Afternoon, Room 114
LESTER STROCK AWARD
Presider: George Agnes, *Simon Fraser University*

1:30 (337) **Atomic Plasmas: Key Players in Chromatographic Elemental Speciation**; Peter Uden, *University of Massachusetts*

2:10 (338) **ICP-MS: Metals, Speciation, and More**; Joseph Caruso, *University of Cincinnati*

2:50 **Coffee Break**

3:30 (339) **Inductively Coupled Plasma-Mass Spectrometry (ICP-MS): A Versatile Technique to Identify the Archived Elemental Information in Teeth**; Dula Amarasiriwardena, *Hampshire College*; Ellen Webb, *Hampshire College*; Daniel Kang, *Hampshire College*; Socheata Tauch, *Hampshire College*; Ethan F. Green, *Hampshire College*; Alan Goodman, *Hampshire College*

4:10 (340) **What Can Field-Flow Fractionation - Inductively Coupled Plasma Mass Spectrometry Do for You?**; Ramon Barnes, *University Research Institute*; John Danku, *University of Massachusetts*; Atitaya Siripinyanond, *Mahidol University*; Dula Amarasiriwardena, *Hampshire College*

Tuesday Afternoon, Room 220
ENHANCED RAMAN SPECTROSCOPY FOR BIOANALYTICAL APPLICATIONS
Presider: Nicholas Fell, *U. S. Army Research Laboratory*

1:30 (341) **UV Resonance Raman Studies of Protein Structure and Dynamics**; Sanford Asher, *University of Pittsburgh*

2:10 (342) **UV Raman Detection and Identification of Bacteria, Bacterial Spores, Algae and algae Toxins**; Wilfred Nelson, *URI*; Jay Sperry, *URI*; Ming Wu, *Brookhaven Natnl Lab*; Michael Feld, *MIT*; Qiang Wu, *URI*

2:30 (343) **Surface-Enhanced Raman Detection of Chemical and Biological Agents in Water**; Steven Christesen, *US Army Edgewood Chem Bio Cent*; Kevin Spencer, *EIC Laboratories, Inc.*; Kristina Gonser, *US Army Edgewood Chem Bio Cent*; Michael Lochner, *US Army Edgewood Chem Bio Cent*; James Sylvia, *EIC Laboratories, Inc.*; Susan Clauson, *EIC Laboratories, Inc.*

2:50 **Coffee Break**

3:30 (344) **Nanoparticle Optics for Chemical and Biological Sensing**; Richard P. Van Duyne; Amanda J. Haes; Adam D. McFarland, *1*; Christy L. Haynes, *Northwestern University*

4:10 (345) **Near-infrared Surface-Enhanced-Raman-Scattering (SERS) Mediated Discrimination of single, Optically Trapped, Bacterial Spores**; Troy Alexander, *U. S. Army Research Laboratory*; Paul Pellegrino Pellegrino, *U. S. Army Research Laboratory*; James Gillespie, *U. S. Army Research Laboratory*

4:30 (346) **Investigation of Nanostructures for Reproducible Sers Characterization of Bacterial Spores**; Nicholas Fell, Jr., *U.S. Army Research Laboratory*; James Pendell Jones, *U.S. Army Research Laboratory*; Troy Alexander, *U.S. Army Research Laboratory*; B. Ritz Reis, *United State Military Academy*; Augustus Fountain III, *United States Military Academy*

TECHNICAL PROGRAM - TUESDAY

Tuesday Afternoon, Room 221
PROCESS ANALYTICAL SPECTROSCOPY: DETECTING WEAPONS OF MASS DESTRUCTION
Presider: David Schiering, *SensIR Technology*
Organized by the Coblentz Society

1:30 (347) **Field Detection Of Chemical and Biological Agents**; Alan Samuels, *US Army*

1:50 (349) **Chemical Agent Detection by Surface-Enhanced Raman Spectroscopy**; Stuart Farquharson, *Real-Time Analyzers*; Paul Maksymiuk, *Real-Time Analyzers*; Frank Inscore, *Real-Time Analyzers*; Wayne Smith, *Real-Time Analyzers*; Kate Ong, *U.S. Army, SBCCOM*; Steven D. Christesen, *U.S. Army, SBCCOM*

2:10 (350) **Infrared Microspectroscopy as a Probe for Biological Agents within Solid Mixtures**; Mark Norman; David Schiering; John Reffner; Peter Troost

2:30 (351) **Raman Chemical Imaging for Reagentless BioThreat Detection and Identification**; Patrick Treado, *ChemImage Corporation*; Steve Vanni, *ChemImage Corporation*; Matthew Nelson, *ChemImage Corporation*; Kathy Kalisinsky, *Armed Forces Institute of Path*; Ted Hadfield, *Armed Forces Institute of Pathology*

2:50 **Coffee Break**

3:30 (352) **Detection of Anthrax in Mail by Raman Spectroscopy**; Stuart Farquharson, *Real-Time Analyzers*; Wayne Smith, *Real-Time Analyzers*; Larry Grigely, *Real-Time Analyzers*; Gerald Fenerty, *ID Mail Systems, Inc.*; Jay F. Sperry, *University of Rhode Island*

3:50 (353) **Rapid Detection of Chemical and Biological Warfare Agents Using Surface Enhanced Raman Spectroscopy**; James Sylvia, *EIC Laboratories, Inc*; Kevin Spencer, *EIC Laboratories, Inc*; Jane Bertone, *EIC Laboratories, Inc*; Susan Clauson, *EIC Laboratories, Inc*; Peter Marren, *EIC Laboratories, Inc*

4:10 (354) **New Detection Methods in Ion Mobility Spectrometry**; Andrew Szumlas, *Indiana University*; Gary Hieftje, *Indiana University*

Tuesday Afternoon, Room 222
EMERGING AREAS OF RAMAN SPECTROSCOPY IN SCIENCE AND INDUSTRY
Presider: Fred LaPlant, *Pfizer, Inc.*

1:30 (355) **Chemometrics on the Fly: A Point-and-Shoot Approach to Instantaneous Materials Analysis**; Edward Grant, *Purdue University*

2:10 (356) **Surface-Enhanced Raman Scattering**; Katrin Kneipp, *Harvard Medical School and M.I*;

2:50 **Coffee Break**

3:30 (357) **Nonlinear Optical Molecular Imaging: CARS Microscopy**; Richard Saykally, *University of California, Berkeley*; Kelly Knutsen, *University of California, Berkeley*; Lynn Lee, *University of California, Berkeley*; Justin Johnson, *University of California, Berkeley*; Richard Schaller, *Los Alamos National Laboratory*

4:10 (358) **New Dimensions in Proteomic Sensingi**; Dor Ben-Amotz; Dongmao Zhang; Vladmir Shalaev; Vladmir Drachev

4:50 (359) **Optical-Trapping Raman Microscopy of Single Unilamellar Phospholipid Vesicles**; Daniel Cherney; Travis Bridges; Joel Harris, *Purdue University & Indiana Proteomics Consortium*

Tuesday Afternoon, Room 223
CHIRAL CHROMATOGRAPHY AND DETECTORS II
Presider: Rekha Shah, *Johnson and Johnson*

1:30 (360) **Determination of the Enantiomeric Composition of Pharmaceuticals by Chemometric Analysis of the UV-visible Spectra of Cyclodextrin Inclusion Complexes**; Kenneth W. Busch; Isabel Maya Swamidoss; Sayo O. Fakayode; Marianna A. Busch, *Baylor University*

1:50 (361) **Detection of Chirality in Analytical Processes: From Optical Rotation to Vibrational Circular Dichroism**; Laurence A. Nafie, *Syracuse University* ; Rekha D. Shah, *J&J Pharmaceutical Research*; Rina K. Dukor, *BioTools*

2:50 **Coffee Break**

3:30 (362) **Pseudoconformational Racemates**; Jack Z. Gougoutas, *Bristol-Myers Squibb*

3:50 (363) **Analytical and Semi-prep SFC for Chiral and Achiral Separations with Tandem SFC/MS Monitoring**; Fiona Geiser, *Johnson Matthey*; Jennifer Smith, *AutoChem Berger SFC*

4:10 (364) **Automated Chiral Method Development**; Gary Yanik, *PDR-Chiral Inc.*; Mark Alper, *PDR-Chiral Inc.*; Ron Bopp, *PDR-Chiral Inc.*

Tuesday Afternoon, Room 302
NANOPARTICLES/NANOSTRUCTURES II
Presider: John Green, *University of Alberta*

1:30 (366) **Surface Manipulation of Electronic Properties of Subnanometer-Sized Gold Clusters**; Shaowei Chen, *Southern Illinois University*; Yiyun Yang, *Southern Illinois University*

2:10 (367) **Synthesis and Characterization of Surfactant and Polymer Templated Mesoporous Metal Films**; Roger Campbell, *Department of Chemistry*; Martin Bakker, *Department of Chemistry*; Claude Treiner, *Laboratoire Liquides Ioniques*; Jean Chevalet, *Laboratoire Liquides Ioniques*; François Dardoize, *Laboratoire Liquides Ioniques*

2:30 (368) **One-Dimensional Assembly of Gold Nanoparticles**; Francis Zamborini; Francisco Ibaniez; Zhongqing Wei, *University of Louisville*

2:50 **Coffee Break**

3:30 (369) **Conducting Polymer Nanojunctions: Basic Properties and Chemical Sensor Applications**; Nongjian Tao; Haiqian Zhang, *Arizona State University*

4:10 (370) **Dendrimer-mediated Growth of Magnetic Nanoparticles**; Shane Street, ; Junyan Zhang; M. Shamsuzzoha, *University of Alabama*

4:30 (371) **Electrodeposition of Nanowires in Mesoporous Silica Films**; Martin Bakker, *University of Alabama Department of Chemistry*; Roger Campbell, *Department of Chemistry*; Ravi Sekhon, *Department of Chemistry*

Tuesday Afternoon, Room 304
COLLISION/REACTION CELLS VS. HIGH CELLS VS. HIGH RESOLUTION SECTOR FIELD ICP-MS: A CRITICAL EVALUATION 2. INSTRUMENTATION AND APPLICATIONS
Presider: I.B. Brenner, *Ben Gurion University of the Negev*

1:30 (372) **An Excursion in Complex Environmental Sample Analysis: A Critical Review of ICP-SFMS vs. Collision Cell ICP-MS**; J. Sabine Becker, *Research Centre Julich*

2:10 (373) **HR-ICP-MS/DRC-ICP-MS and Isotope Ratio Determination: Uncertainties Challenges and Limits**; Thomas Prohaska, *University of Natural Resource*; Gerald Schultheis, *University of Natural Resource*; Gunda Köllensperger, *University of Natural Resource*; Stephan Hann, *University of Natural Resource*; Gerhard Stingeder, *University of Natural Resource*

2:30 (374) **SF-ICP-MS - Indispensable for Determination of Radionuclides in the Environment - A Comparison With Other Techniques**; Michael Ketterer, *Northern Arizona University*

2:50 **Coffee Break**

3:30 (375) **A Strategic Approach for Optimizing an ICP-MS for an Application. Part 1: Quadrupoles and Collision Cells;** Simon Nelms, *Thermo Electron*; Martin Nash, *Thermo Electron*; Meike Hamester, *Thermo Electron*; Lothar Rottmann, *Thermo Electron*

3:50 (376) **A Strategic Approach for Optimising an ICP-MS for an Application. Part 2. High Resolution Sector-Field Spectrometers**; Meike Hamester, *Thermo Electron*; Lothar Rottmann, *Thermo Electron*; Simon Nelms, *Thermo Electron*; Martin Nash, *Thermo Electron*

4:10 (377) **Figures of Merit of SF-ICPMS in Comparison with ICP-QMS**; Giulio Cozzi, *University of Venice*; Carlo Barbante, *University of Venice*; Anita Varga, *University of Venice*; Clara Turetta, *IDPA-CNR Venezia*; Paolo Cescon, *University of Venice*

4:30 (378) **Resolution of Spectral Interferences by ICP-SFMS and ICP-RC-MS with Laser Ablation for Sample Introduction**; Bodo Hattendorf, *ETH Zürich*; Christopher Latkoczy, *ETH Zürich*; Detlef Günther, *ETH Zürich*

Tuesday Afternoon, Room 305
PRECONCENTRATION FOR ATOMIC SPECTROMETRY BY SOLID-PHASE EXTRACTION AND CHEMICAL VAPOR GENERATION – 2
Presider: Julian Tyson, *University of Massachusetts*

1:30 (379) **Analysis of Otoliths by Solid Phase Preconcentration ICP-MS: Identification of Resident Habitats of Fish Based on Trace Element Otolith Chemistry**; Zikri Arslan; David H. Secor, *University of Maryland Center*

1:50 (380) **Preconcentration for Flow Injection Atomic Spectrometry--1: Design and Operation of Solid-Phase Extraction Manifolds**; Julian Tyson, *University of Mass. Amherst*

2:10 (381) **Preconcentration for Flow Injection Atomic Spectrometry--2: Design and Operation of Hydride Generation Manifolds**; Julian Tyson, *University of Mass. Amherst*

2:30 (382) **Determination of Lead By Hydride Generation Atomic Absorption Spectrometry With Tetrahydroborate Immobilized on an Anion-Exchange Resin**; Wipharat Chuachuad, *University of Massachusetts,Amherst*; Hans Mentzen, *University of Massachusetts,Amherst*; Julian F. Tyson, *University of Massachusetts,Amhers*t

2:50 **Coffee Break**

3:30 (383) **Recent Advances in Vapour Generation/Nebulization**; Ian Brindle; Roger McLaughlin; Xiao Jing; Min Ding; Adam Ptolemy, *Brock University*

4:10 (384) **Hydride Generation and Preconcentration - Bridging them with Something New**; Ralph Sturgeon, *NRCC - INMS*; Joseph Lam, *NRCC-INMS*; Yong-lai Feng, *NRCC-INMS*

4:30 (385) **Discussion of Preconcentration for Atomic Spectrometry by Solid-Phase Extraction and Chemical Vapor Generation - 1**; Julian Tyson, *University of Mass -Amherst*

Tuesday Afternoon, Room 315
INFRARED IMAGING II
Presider: Andre Sommer, *Miami University*
Organzied by the Coblentz Society

1:30 (386) **Studying the Dynamics of Self-Assembling Monolayers (SAM) Using a Planar Array Infrared Spectrograph (PA-IR) in the Mid-Infrared**; John Rabolt; Christian Pellerin, *University of Delaware*; Julia Liu, *University of Delaware*; Danielle Rockwood, *University of Delaware*; Bruce Chase, *DuPont Central Research*

1:50 (387) **Infrared Imaging for Pharmaceutical Formulation Analysis**; Mark Henson, *Pfizer Global R&D*; Lin Zhang, *Pfizer Globabl R&D*; Sonja Sekulic, *Pfizer Globabl R&D*

2:10 (388) **Near-Infrared Spectroscopic Imaging as a Forensic Screening Tool**; Thomas W. Brueggemeyer, ; Jonathan J. Litzau, *USFDA*

2:30 (389) **FTIR Spectroscopic Imaging with Fast Focal Plane Array Detectors**; Rohit Bhargava, *National Institutes of Health*; Scott W. Huffman and Ira W. Levin, *National Institutes of Health*; Shi-Qing Wang, *University of Akron*

2:50 **Coffee Break**

3:30 (390) **Reflectance Imaging in the Near and Mid-IR Regions**; Richard Spragg; Robert Hoult, *Perkin Elmer*

3:50 (391) **Applications of Infrared Imaging for Polymer Characterizations**; Koichi Nishikida, *Thermo Electron Corporation*; Eric Jiang, *Thermo Electron Corporation*; William McCarthy, *Thermo Electron Corporation*; Simon Nunn, *Thermo Electron Corporation*; Steve Lowry, *Thermo Electron Corporation*

4:10 (392) **Near-IR Imaging for Blend Uniformity Analysis**; James Drennen

4:30 (393) **FT-IR Microimaging of Wood and Wood Composites**; Tim Rials, *University of Tennessee;* Nicole Labbe, *University of Tennessee;* Steve Kelley, *National Renewable Energy Laboratory;* Max Chenge, *University of Tennessee*

TECHNICAL PROGRAM – TUESDAY AND WEDNESDAY

Tuesday Afternoon, Room 317
INNOVATIONS AND APPLICATIONS IN ICP-MS
Presider: Joseph McClellan, *Wyeth Pharmaceutical*

1:30 (396) **Application of Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) to the "Fingerprinting" of Trace Evidence**; Tatiana Trejos; José Almirall, *Florida International University*

1:50 (397) **Elemental Analysis of Environmental Samples by ICP-MS**; Stephen Shuttleworth, *GV Instruments*; Fadi Abou-Shakra, *GV Instruments*

2:10 (398) **Reducing Air Entrainment in the Inductively Coupled Plasma**; Duane Rogers, *Indiana University*

2:30 (399) **Routine Analysis in the PPM to PPQ Range with the New Varian ICP-MS**; Michael Plantz, *Varian, Inc.*; Shane Elliott, *Varian Australia Pty. Ltd.*; Stephen Anderson, *Varian Australia Pty. Ltd.*; Iouri Kalinitchenko, *Varian Australia Pty. Ltd.*

2:50 **Coffee Break**

3:30 (400) **Calibration Strategies for Direct Quantitative Elemental Analysis of Deposited Airborne Particles Using Laser Ablation ICP-TOFMS**; Lloyd Allen, *LECO Corporation*; Solomon Teffera, *South Coast Air Quality Manage*; Jeremy O'Kelley, *South Coast Air Quality Manage*

Tuesday Afternoon, Room 318
SEPARATION SCIENCE: DETECTORS FOR GAS CHROMATOGRAPHY
Presider: Mary Ellen McNally, *Dupont*

1:30 (401) **Investigation of Canis Familiaris as Biological Detectors for Explosives Using Headspace SPME-GC-MS Analysis**; Ross Harper, *International Forensic Research*; Jose Almirall, *International Forensic Research*; Kenneth Furton, *International Forensic Research*

1:50 (402) **Applications of a High Speed Gas Phase Raman Spectrometer**; Peter Chen, *Spelman College*; Rebecca Royster, *Spelman College*; Candace Joyner, *Spelman College*; Kyndra Cottingham, *Spelman College*; Leigha Ingham, *Spelman College*

2:10 (403) **Fluorine-Specific Atomic Emission Detector for GC Analysis of Common Fluorocarbons**; Stephen Bialkowski, ; Sonia Sousa, *Du Pont de Nemours*

2:30 (404) **Determination of Hydrocarbons in Fresh Fish of Lagos Lagoon by GC-FID, Following a Soxtec Extraction.**; Chimezie Anyakora, *University of Lagos*; Anthony Ogbeche, *University of Lagos*; K. O. Olayinka, *University of Lagos*

2:50 **Coffee Break**

SEPARATION SCIENCE MICROSEPARATION TECHNIQUES

3:30 (405) **Capillary-Channel Polymer (C-CP) Fibers: A New Stationary Phase for Liquid Chromatography**; R. Kenneth Marcus; Dwella K. Nelson; Rayman D. Stanelle, *Clemson University*

3:50 (406) **Recent Advances in the Capillary Electrophoretic Separation of Polynuclear Aromatic Hydrocarbons**; Chimezie Anyakora, *University of Lagos*

Wednesday Morning, Room 113
MEASUREMENT ERROR CONSIDERATIONS IN MULTIVARIATE ANALYSIS
Presider: Peter Wentzell**,** *Dalhousie University*

8:30 (407) **An Overview of Error Management Methods in Modeling, and Their Implications for Instrumental, Experimental and Model Design**; Christopher Brown; Bert Davis, *INLIGHT Solutions, Inc.*

9:10 (408) **Generalized Least Squares Preprocessing for Improving and Transfering Calibrations**; Barry M. Wise, *Eigenvector Research, Inc.*; Jeremy M. Shaver, *Eigenvector Research, Inc.*; Harald Martens, *Royal Veterinary and Agricultu*; Martin Hoy, *Norwegian University of Science*

9:30 (409) **Perspectives on Preprocessing in Near Infrared Spectroscopy**; Marc Leger, *Trace Analysis Research Centre*; Peter Wentzell, *Trace Analysis Research Centre*

9:50 **Coffee Break**

10:30 (410) **Variable Scattering Correction of Multispectral Calibrations in Turbid**; David Burns, *McGill University*; Claudia Gributs, *McGill University*

10:50 (411) **Methods for Eliminating Calibration Transfer Errors using Augmented Classical Least Squares ***; David Melgaard, *Sandia National Laboratories*; David Haaland, *Sandia National Laboratories*; Steve Lowry, *Termonicolet*; Christine Wehlburg, *Sandia National Laboratories*

11:10 (412) **Measurement Error Considerations in the Analysis of DNA Microarray Data**; Peter Wentzell, *Dalhousie University*; Tobias Karakach, *Dalhousie University*; Margaret Werner-Washburne, *University of New Mexico*; Juanita Martinez, *University of New Mexico*

11:30 (413) **Incorporating Measurement Error Information into Three-Way Analysis**; Lorenzo Vega-Montoto, ; Peter D. Wentzell, *Trace Analysis Research Center*

Wednesday Morning, Room 204
NEW APPROACHES TO TEACHING ANALYTICAL CHEMISTRY – STUDENT LEARNING
Presider: David Harvey, *DePauw University*

8:30 (414) **The Analytical Science Digital Library**; Cameron Dorey, *University of Central Arkansas*; Ted Kuwana, *University of Kansas*; Stuart Chalk, *University of North Florida*; Cindy Larive, *University of Kansas*; George Long, *Indiana University of Pennsylvania*

8:50 (415) **Teaching Students to Think as Analytical Chemists**; David Harvey, *DePauw University*

9:30 (416) **Forensic Analytical Chemistry: Exposing Students to Explosive Problems**; Stephen L. Morgan, *Unviersity of South Carolina*; William E. Brewer, *Clemson Veterinary Diagnostic*; Stephen J. Lambert, *Forensic Laboratory, State Law*; Scott R. Goode, *University of South Carolina*

9:50 **Coffee Break**

10:30 (417) **Bringing Proetomics into the Undergraduate Laboratory**; Eric Eberhardt, *Vassar College*; Elisa Woolridge, *Marist College*

11:10 (418) **Analytical Chemistry for a Broad Audience: Educating Diverse Groups of Students in Multiple Disciplines**; John Schaumloffel, *SUNY College at Oneonta*

11:50 (419) **Quantitative Determination of Copper: Combining Project-Based Laboratories with Single Analyte Detection**; Mark Richter, *SW Missouri State University*

Wednesday Morning, Room 213
BIOANALYTICAL ELECTROCHEMISTRY
Presider: James Sumner, *US Army*

8:30 (420) **Materials Considerations in Microelectrochemical Systems for Bioanalytical Chemistry**; Ingrid Fritsch, *University of Arkansas*; Zoraida Aguilar, *University of Arkansas*; Eyitayo Fakunle, *University of Arkansas*; Brigitte Factor, *University of Arkansas*

9:10 (421) **Electrochemical Detection of Nucleic Acids Using Catalytic Base Oxidation on Gold-Thiol Monolayers**; Holden Thorp, *UNC Chapel*

9:50 **Coffee Break**

10:30 (422) **Exploiting DNA Mediated Charge-Transfer Dynamics for the Design of a Conformationally Gated DNA Detection Device**; Chad Immoos, *Duke University and Army Resea*; Stephen Lee, *Army Research Office*; Mark Grinstaff, *Duke University*

11:10 (423) **Application of Pulsed Amperometric Detection – Microchip CE to clinical analysis**; Carlos D. Garcia, *Colorado State U*; Charles S. Henry, *Colorado State University*

Wednesday Morning, Room 216
SPECTROSCOPY IN FORENSIC EVIDENCE
Presider: Bruce McCord, *Ohio University*

8:30 (424) **The Use of Infrared and Raman Spectroscopy in the Analysis of Forensic Evidence at the FDA's Forensic Chemistry Center**; Mark Witkowski, *Food and Drug Administration;* JaCinta Batson, *Food and Drug Administration*; John Crowe, *Food and Drug Administration*; A. Caroline Machal Kelley, *Food and Drug Administration*; Jill Loeliger, *Food and Drug Administration*

9:10 (425) **Forensic Analysis by UV-visible-NIR Microspectroscopy**; Paul Martin, *CRAIC Technologies*

9:50 **Coffee Break**

10:30 (426) **Structure Elucidation of Pyrolytic Products and Metabolites of Drugs of Abuse**; Patrick Callery; Diaa Shakleya; Madhu Sanga; Alan Myers; Peter Gannett; Timothy Tracy; Brenda Schuler; Padma Tirumalai; Tina Bland; Sandra Tarr

11:10 (427) **Finding the Needle in the Haystack: Separations by Tandem Mass Spectrometry**; Nik Hubbard, *BS Chemistry*; Cheryl Ehorn, *BS Chemistry and Engineering*

Wednesday Morning, Room 220
PROCESS ANALYSIS IN PHARMACEUTICALS AND BIOTECH
Presider: Chris Hassell, *Los Alamos National Labs*

8:30 (428) **Is NIR Microscopy a Useful Performance Prediction Tool for Pharmaceutical Process Robustness?**; Fiona Clarke, *Pfizer*; Stephen Hammond, *Pfizer*

8:50 (429) **Near Infrared Spectroscopy as a Process Analytical Tool: Implementation and Examples**; Katherine Bakeev, *Foss NIRSystems*

9:10 (430) **Micro X-Ray Fluorescence Imaging of Pharmaceutical Tablet Formulations**; Thomasin Miller, *Los Alamos National Laboratory*; George Havrilla, *Los Alamos National Laboratory*

9:30 (431) **In-situ FTIR Monitoring of Solvent-Drug Matrixes During Displacements and Crystallizations of Potentially Hazardous Intermediates**; Kyle Leeman, *Pfizer*; Paul Ahlijanian, *Pfizer*; John Tucker, *Pfizer*; Matt Weekly, *Pfizer*; Greg Withbroe, *Pfizer*; Anne Serdakowski, *University of Rhode Island*

9:50 **Coffee Break**

10:30 (432) **Rapid Analysis of Pharmaceutical Products via Multiplex Laser Raman Spectroscopy**; Leslie Tack; Bruce True, *Roper Scientific*

10:50 (433) **Demonstration of Novel Raman Sampling Strategies with Applications to Real-Time Reaction Monitoring.**; Brian J. Marquardt, ; David Veltkamp

11:10 (434) **A hybrid Raman System Provides the Stability and Sensitivity Needed for Industrial Applications**; Wayne Smith, *Real-Time Analyzers*; Larry Grigely, *Real-Time Analyzers*; Viktor Khitrov, *Real-Time Analyzers*; Robert Carangelo, *Real-Time Analyzers*; Stuart Farquharson, *Real-Time Analyzers*

11:30 (435) **The Applications of Microspectroscopy to Biopharmaceuticals**; Zai-Qing Wen, *Amgen Inc.*; Gianni Torraca, *Amgen Inc.*

Wednesday Morning, Room 221
NEW APPROACHES TO HELP STUDY CARDIOVASCULAR DISEAS E
Presider: Dana Spense, *St. Louis University*

8:30 (436) **ATP: The Red Blood Cell Link to Local Control of Vascular Resistance**; Randy Sprague; Jeffery Olearczyk; Alan Stephenson, ; Andrew Lonigro, *St. Louis University*

9:10 (437) **Application of Optical Spectroscopy to Measurement of Capillary Oxygen Transport In Vivo**; Christopher Ellis, *University of Western Ontario*

9:50 **Coffee Break**

10:30 (438) **Nanotechnology in the Detection of Nitric Oxide Signaling in the Ischemic Heart and Brain**; Tadeusz Malinski, *Ohio University*

11:10 (439) **Probing Red Blood Cell Properties and Function using Microfluidic Systems as Microcirculation Mimics**; Dana Spence, *St. Louis University*

Wednesday Morning, Room 222
2ND ANNUAL PROFESSOR CHARLES K. MANN MEMORIAL AWARD SYMPOSIUM IN THE AREA OF ANALYTICAL RAMAN SPECTROSCOPY
Awardee: Michael J. Pelletier
Presider: Fran Adar, *JY Horiba*

8:30 (440) **New Fiber Optic Raman Probes Using a Single Zero-Background Optical Fiber**; Michael Pelletier, *Jet Propulsion Laboratory*

9:10 (441) **Probing Biomechanics by Raman Spectroscopy**; Michael D. Morris, *University of Michigan*

9:30 (442) **The Utility of Quantitative Raman Spectroscopy in Pharmaceutical Quality Control and Process Control**; Mark Kemper, *Kaiser Opical Systems*; Paul Luner, *Pfizer Corp.*; Bonnie Avery, *University of Mississippi*; Atul Shukla, *University of Tennessee*

9:50 **Coffee Break**

10:30 (443) **Multivariate Kinetic Fitting of in-situ Raman Spectra From Non-Isothermal Batch Reactions**; Paul Gemperline, *East Carolina University*; Doug Tsao, *East Carolina University*; Patrick Cutler, *East Carolina University*; Marcel Maeder, *Newcastle University*; Graeme Puxty, *Newcastle University*

10:50 (444) **Finding Specificity in Multivariate Curve Resolution**; Jeremy Shaver, *Eigenvector Research Inc.*; Neal Gallagher, *Eigenvector Research Inc.*

11:10 (445) **Structure and Orientation in Fibers: The Power of Polarized Raman Scattering**; Bruce Chase, *DuPont Central Research*; Simon Frisk, *University of Delaware;* John Rabolt, *University of Delaware*; Richard Ikeda, *University of Delaware*

Wednesday Morning, Room 223
HIGHLY AUTOMATED METHODS USING INFRARED SPECTROMETRIC DETECTION
Presider: John Hellgeth, *Hewlett Packard*
Organized by the Coblentz Society

8:30 (446) **Automated in-situ Reaction Monitoring and Data Anlaysis Using Midinfrared Spectrometry**; Jeffrey Sherman, *Mettler-Toledo AutoChem*

9:10 (447) **Applying Technology to Infrared Analysis for High Throughput and Reproducibility**; Allison Toms, *Lubrication and Fluid Power, Inc.*

9:50 **Coffee Break**

10:30 (448) **From Tailored Instruments to Spectral Sensors**; John Coates, *Coates Consulting*

11:10 (449) **Applications of Infrared Analysis of Large Sample Sets for Polymer and Pharmaceutical Industries**; William J. McCarthy, *Thermo Electron*; Scot Ellis; Eric Y. Jiang, ; Koichi Nishikida; N. Simon Nunn

Wednesday Morning, Room 302
FEMTOSECOND – LASER ABLATION IN MATERIAL ANALYTICS
Presider: Roland Hergenroeder, *Institute for Spectochemistry*

8:30 (451) **From Ultrashort to Long Pulse Regime: Role of the Laser Pulse Duration in Laser-Induced Plasma Spectroscopy**; Boris Le Drogoff, *Institution 1*; Mohamed Chaker; Mohamad Sabsabi; Joëlle Margot; François Vidal; Tudor W. Johnston; Stéphane Laville; Olivier Barthélem

9:10 (452) **Femtosecond Laser-Induced Plasmas and Ablation for ICP-MS**; Richard Russo, *Lawrence Berkeley National Lab*; Sam Mao, *Lawrence Berkeley National Lab*; Xianzhong Zeng, *Lawrence Berkeley National Lab*; Chunyi Liu, *Lawrence Berkeley National Lab*; Jong Yoo, *Lawrence Berkeley National Lab*; Jhanis Gonzalez, *Lawrence Berkeley National Lab*; Xianglei Mao, *Lawrence Berkeley National Lab*

9:50 **Coffee Break**

10:30 (453) **Particle Formation and Distrubution in fs-Laser Ablation of Metals**; Roland Hergenroeder, *Institute for Spectrochemistry*; Kay Niemax, *Institute for Spectrochemistry*; Vanja Margetic, *Institute for Spectrochemistry*; Ota samek, *Institute for Spectrochemistry*; Joachim Koch, *Institute for Spectrochemistry*

11:10 (454) **Ultrashort Pulse Micromachining and New Femtosecond Laser Technologies**; Boris Chichkov, *Laser Zentrum Hannover e.V*

Wednesday Morning, Room 304
SPECIATION APPLICATIONS
Presider: Nancy Miller-Ihli, *USDA*

8:30 (455) **Speciation of Cobalamins (Vitamin B12) using Microseparation Techniques Combined with ICP-MS**; Enrique Yanes, *Food Composition Lab, USDA*; Nancy Miller-Ihli, *Food Composition Lab, USDA*

8:50 (456) **Determination of Trace Arsenic Speciation in Aqueous Samples by HPLC and ICP-MS**; Fadi Abou-Shakra, *GV Instruments*; Stephen Shuttleworth, *GV Instruments*

9:10 (457) **Separation of heme Fe, hemoprotein Fe, and non-heme Fe in Meats**; James Harnly; Edith Blackwell; Charmonte Watkins, *USDA*

9:30 (458) **Application of HPLC and ICP-MS for Analysis of Drug Metabolites and Organic Pharmaceutical Compounds.**; Fadi Abou-Shakra, *GV Instruments*; Stephen Shuttleworth, *GV Instruments*

9:50 **Coffee Break**

10:30 (459) **The Development of an In Situ Monitoring Approach for the Determination of Trace Hexavalent Chromium in Surface Water**; Melissa Singer Pressman, *University of WI - Milwaukee*; Joseph Aldstadt, *University of WI - Milwaukee*

10:50 (460) **Speciation with Electrospray Mass Spectrometry and Time Resolved Laser Induced Fluorescence**; Christophe Moulin, *CEA*; Badia Amekraz, *CEA*; Sonia Colette, *CEA*; Gabriel Plancque, *CEA*; Christophe Jacopin, *CEA*; Carole Bresson, *CEA*; Jean Louis Fleche, *CEA*

11:10 (461) **Chemical Speciation of Hydrocarbon Mixtures using Gas Chromatography Time-of-Flight Mass Spectrometry with a Pulsed Glow Discharge Ion Source**; Ruth Waddell, *Chemistry Division, Los Alamos*; Cris L. Lewis, *Chemistry Division, Los Alamos*; D. Christian Hassell, *Chemistry Division, Los Alamos*

Wednesday Morning, Room 315
MICRO- AND NANO-NEBULIZATION: CONCEPTS, DEVICES, FUNDAMENTALS, AND NOVEL APPLICATIONS
Presider: Akbar Montaser, *George Washington University*

8:30 (462) **Application of Micronebulization to Torch-Integrated Sample Introduction Systems With an Emphasis on Torch Design, Transient Signals and Speciation**; Jean-Michel Mermet, *University of Lyon, France*; José-Luis Todoli, *University of Alicante, Spain*

8:50 (463) **A Modified Nukiyama-Tanasawa Model to Predict Droplet Size for Microconcentric Nebulizers**; Kaveh Kahen, *Department of Chemistry, Georg*; Billy Acon, *Department of Chemistry, Georg*; Akbar Montaser, *Department of Chemistry*

9:10 (464) **Micronebulization with High Spectral or Chemical Resolution ICP-MS**; John Olesik

9:30 (465) **Recent Research on Optimizing Spray Chamber by Computer Simulation**; Harald Berndt, *Institute for Spectrochemistry*

9:50 **Coffee Break**

10:30 (466) **New Developments in Isotope Analysis by ICP-MS Using Micronebulization**; J. Sabine Becker, *Research Centre Juelich*

10:50 (467) **Inductively Coupled Plasma Mass Spectrometry with a Demountable Direct Injection High Efficiency Nebulizer**; Craig Westphal, *Department of Chemistry, Georg*; Kaveh Kahen, *Department of Chemistry, Georg*; Akbar Montaser, *Department of Chemistry*

11:10 (468) **Recent Insights into the Electrospray Process Through Studies Involving Single Isolated Droplets with Net Charge**; Agnes George; *Simon Fraser University*

11:30 (469) **Effects of Sample Introduction System on Secondary Discharge and Temperatures in Helium Inductively Coupled Plasma Mass Spectrometry**; Kaveh Jorabchi, *Department of Chemistry, The G*; Menghae Hwang, *Department of Chemistry, The G*; Akbar Montaser, *Department of Chemistry*

11:50 (470) **On-Line Combination of Electrochemistry with ICP-AES and with ICP-MS and Related Applications**; Alfred J. Baca, *CSULA*; Ana De La Ree, *CSULA*; Feimeng Zhou, *CSULA*

Wednesday Morning, Room 317
FLUORESCENCE APPLICATIONS II: BIOANALYTICAL METHODS
Presider: Zeev Rosenzweig, *University of New Orleans*

8:30 (471) **Controlled Fabrication of Fluorescence Based Nanosensors Using Layer by Layer Adsorption of Polyelectrolytes on Gold Nanoparticles.**; Zeev Rosenzweig, *University of New Orleans*; Nguyen Thi Kim Thanh, *University of New Orleans*

8:50 (472) **Luminescent Semiconductor CdSe-ZnS Quantum Dots (QDs) Doped Silica Nanospheres Based Immunosensors**; Yongfen Chen, *University of New Orleans*; Zeev Rosenzweig, *University of new Orleans*

9:10 (473) **Lipobead- Based Nanosensors for Chloride Measurement in Biological Samples**; Aihui Ma, *University of New Orleans*; Zeev Rosenzweig, *University of New Orleans*

9:30 (474) **Using Molecular Beacons as Probes to Monitor Intracellular mRNA from Single Living Cells**; Timothy Drake, *University of Florida*; Zehui Cao, *University of Florida*; Weihong Tan, *University of Florida*

9:50 **Coffee Break**

10:30 (475) **FRET Trap Beads – Model Sensors for Carbohydrate Based Drug Screening**; Gabriela Dumitrascu, *University of New Orleans*; Georgeta Crivat, *University of New Orleans*; Zeev Rosenzweig, *University of New Orleans*

10:50 (476) **Molecular Aptamers as Novel Probes for Protein-Protein Interactions**; Zehui Cao, *University of Florida*; Weihong Tan, *University of Florida*

11:10 (477) **Spectroscopic Characterization of a Glucose Binding Protein**; Rebecca L. Owen, *Duke University*; Linda B. McGown, *Duke University*; Javier Alarcón, *Becton Dickinson Technologies*; Douglas B. Sherman, *Becton Dickinson Technologies*; Kristen Weidemaier, *Becton Dickinson Technologies*; J. Bruce Pitner, *Becton Dickinson Technologies*

11:30 (478) **Cytotoxicity Study of Neutrophils Using Near-Infrared Fluorescent Compounds**; Richard Williams, *Morgan State University, Chemi*; Leonette Cox, *Morgan State University, Chemi*; Dwayne Hill, *Morgan State University*; LaVentrice Taylor, *Morgan State University*

Wednesday Morning, Room 318
MASS SPECTROMETRY AS A TOOL FOR EXPLORATION AND ANALYSIS
Presider: Joseph McClellan, *Wyeth Pharmaceutical*

8:30 (479) **In-Situ Chemical Sensing using Underwater Mass Spectrometry**; R. Timothy Short; Frisco H. W. van Amerom; Peter G. Wenner, ; Ryan J. Bell, ; Karsten Koehn, ; Strawn K. Toler, ; John E. Edkins

9:10 (480) **Mass Spectrometry in the Space Transportation System (STS) Program**; Timothy P. Griffin, *NASA*

9:50 **Coffee Break**

10:30 (481) **IR-Laser Desorption, UV-Resonant Multiphoton Ionization, and Tunable Resonant Photodissociation of Large Molecules in Ion-TrAP MS**; Michael Blades; August Specht; Denis Roland; John Hepburn

11:10 (482) **Examination of the 13C/12C Isotopes in Sparkling Wine with On-line Sampling and Isotope Ratio MS.**; Guy Bilodeau, *GV Instruments*; Francois Fourel, *GV Instruments*; Stephen Shuttleworth, *GV Instruments*

11:30 (483) **Detection of Energetic Materials by Surface Photofragmentation-Fragment Detection Spectroscopy**; Ross Sausa; Jerry Cabalo, *National Research Council*

Wednesday, 2:00 PM – 5:00 PM, Exhibit Hall C
SAS/FACSS SPONSORED POSTER SESSION

Your poster should be put up between 10:00 AM and noon on Wednesday and removed between 5:00 – 6:00 PM. Please leave your poster in place for the entire time. Check below for your presentation time.

3:30 (3) **Milestones in the History and Evolution of the Raman Effect**; Michel Delhaye, *U Lille (retired)*; Wolfgang Kiefer, *U Wurzburg*; Derek Long, *U Bradford*; Edouard DaSilva, *Jobin Yvon*; Jacques Barbillat, *U Lille*; Paul Dhamelincourt, *U Lille*

2:15 (484) **New Approach for Recording Absorption Spectra of Polycyclic Aromatic Hydrocarbons in Shpol'skii Matrixes at Liquid Nitrogen and Helium Temperatures**; Adam Bystol, *Department of Chemistry, Unive*; Andres Campiglia, *Department of Chemistry*

3:30 (485) **An Intrinsic Wavelength Standard for UV/visible Molecular Absorption Spectrophotometry**; John C. Travis, *NIST*; David L. Duewer, *NIST*

2:15 (486) **SRM 2036: a Reflectance Wavelength Standard utilizing Rare earth Oxide Glasses**; Steven Choquette, *NIST*; Leonard Hanssen, *NIST*; Edward Early, *NIST*

3:30 (487) **Mass Spectrometry of Room Temperature Ionic Liquids**; Glen P. Jackson; Sheng Dai; Douglas C. Duckworth, *Oak Ridge National Laboratories*

2:15 (488) **Low Cost Techniques for Speciation and Determination of Arsenic from Pressure-Treated Wood: Application in Middle-School Science Projects**; Richmond Ampiah-Bonney, *University of Massachusetts*; Julian Tyson, *University of Massachusetts*

3:30 (489) **A Comparison of AC and DC Electrodic and EDTA-Enhanced Phytoremediation of Lead using Indian Mustard (Brassica juncea)**; David Butcher, *Western Carolina University*; Jae-Min Lim, *Western Carolina University*

2:15 (490) **Applications of Acousto-Optic Tunable Filter Hyperspectral Imaging (AOTF-HIS) to Examinations of Inductively Coupled Plasma Chemistry**; Jon Carnahan; Ling Bei; Kirk Duffin, *Northern Illinois University*

3:30 (491) **Vapor Detection Utilizing an AOTF Based Near-Infrared Spectrometer**; Jon Carnahan; John Carr; Ling Bei; *Northern Illinois University;* Jack Demergian, *Argonne National Laboratory*

2:15 (492) **UV Raman Spectrometry using Acousto Optic Tunable Filters**; Jon Carnahan; Kaho Kwok, *Northern Illinois University*

3:30 (493) **Design and Modeling Studies of a MicroThetaPinch Plasma Source for Atomic Emission Spectrometry**; Joel Goldberg, *University of Vermont*; Edward Navarre, *Middlebury College*

2:15 (494) **Direct Determination of Selenium in Yeast by Slurry Sampling Electrothermal Atomic Absorption Spectrometry**; Chethaka Kahakachchi, *University of Massachusetts, D*; Iain Mount, *Nottingham Trent University, D*; Julian Tyson, *University of Massachusetts, D*; Peter Uden, *University of Massachusetts*

3:30 (495) **Investigation of the Borohydride Activity of Organoselenium Compounds in a Flow-Injection, Hydride-Generation, Atomic Absorption Spectrometric Procedure**; Chethaka Kahakachchi, *University of Massachusetts*; Julian Tyson, *University of Massachusetts*; Peter Uden, *University of Massachusetts*

2:15 (496) **Identification of organoselenium compounds in Brassica juncea (Indian Mustard) by HPLC-ICP-MS for phytoremediation studies**; Chethaka Kahakachchi, *University of Massachusetts*; Julian Tyson, *University of Massachusetts*; Peter Uden, *University of Massachusetts*

3:30 (497) **Elemental and Isotopic Measures Using Plasma Diode Laser Ringdown Spectroscopy**; Sudip P. Koirala, *Mississippi State University*; S. T. Scherrer, *Mississippi State University*; Chuji Wang, *Mississippi State University*; Yixiang Duan, *Los Alamos National Laboratory*; Christopher B. Winstead, *University of Southern Mississippi*

2:15 (498) **A Comparison of Optical and Mass Spectrometric Measurements of Ion Density Profiles in an Inductively Coupled Plasma**; Jeff Macedone, *Brigham Young University*; Andrew Mills, *Brigham Young University*; Paul Farnsworth, *Brigham Young University*

3:30 (499) **Analysis of Oil Paints by Laser Ablation High Resolution Inductively Coupled Plasma Mass Spectrometry**; Jerzy Mierzwa, *CIF, Tulane University*; Deborah Grimm, *CIF, Tulane University*

2:15 (500) **Investigation of Ionization in a Pulsed Glow Discharge Plasma Using Optical Spectroscopy and Electrostatic Probes**; Jennifer Robertson, *West Virginia University, Depa*; Lei Li, *West Virginia Universit*; Na Zhang, *West Virginia University;* Amy Keesee, *West Virginia University*; Earl Scime, *West Virginia University;* Fred King, *West Virginia University*

3:30 (501) **A Calibration Method for Elemental Speciation Analysis using Liquid Chromatography – Inductively Coupled Plasma – Mass Spectrometry**; Eric Salin; Margaret Antler; E. Jane Maxwell

2:15 (502) **Accurate and Precise Determination of Si and Ge ratio of Si-Ge Chip**; Lee Yu, *NIST*

3:30 (503) **Luminescence Lifetimes of Lanthanide Complexes As Qualitative Tools For Protein Analysis**; Hector Goicoechea, *Department of Chemistry*; Bidhan Roy, *Department of Chemistry*; Adam Bystol, *Department of Chemistry*; Andres Campiglia, *Department of Chemistry;* Sanku Mallik, *Department of Chemistry*

2:15 (504) **Fiber-Optic SPR Sensors for Rapid Detection and Monitoring of Biomarkers for Cardiac and Cerebrovascular Trauma**; Kayla Hamersky, *Arizona State University*; Karl Booksh, *Arizona State University*; Michael Sierks, *Arizona State University*; Stephen Beaudoin, *Arizona State University*

3:30 (505) **Evaluating the Health of Compromised Tissues Using Near Infrared Spectroscopy and Imaging**; Lorenzo Leonardi, *National Research Council Canada*; Michael Sowa, *National Research Council Canada*; Jeri Payette, *National Research Council Canada*; Bernie Schattka, *National Research Council Canada*; Michelle Hastings, *National Research Council Canada*; Elicia Kohlenberg, *National Research Council Canada*

2:15 (506) **MALDI-IM-oTOF MS for the Rapid determination of Secondary Structure in the Gas-Phase: Implications to Solution-Phase Protein Folding.**; Brandon T. Ruotolo; Kent J. Gillig; Holly A. Sawyer; David H. Russell, *Texas A&M University*

3:30 (507) **Raman Chemical Imaging**; Patrick Treado, *ChemImage Corporation*; Steve Vanni, *ChemImage Corporation*; Matthew Nelson, *ChemImage Corporation*; Kathy Kalisinsky, *Armed Forces Institute of Path*; Ted Hadfield, *Armed Forces Institute of Path*

2:15 (508) **Optical Spectroscopy Analysis of Cytochrome c conformations: Impact of Sodium Dodecyl Sulfate**; Qi Xu, *University of Illinois at Chic*; Timothy Keiderling, *University of Illinois at Chicago*

2:15 (559d) **Acids Using Fourier Transform Vibrational Circular Dichroism**; Rosina Lombardi, *Syracuse University*; Xiaolin Cao, *Syracuse University*; Soon Sam Kim, *Jet Propulsion Laboratory*; Rina Dukor, *BioTools Inc.*; Laurence Nafie, *Syracuse University, BioTools*

2:15 (510) **Determination of Biochemical Oxygen Demand of Municipal Waste Water using UV/Vis-NIR Spectroscopy Combined with multivariate Analysis (PLS1)**; Dennis H. Rabbe; Kenneth W. Busch; Marianna A. Busch, *Baylor University*

3:30 (511) **Approaches to Solid-Phase Extraction Using Monolithic Stationary Phases: SPE-LC-MS of Biotoxins**; Jessica L. Ammerman; Joseph H. Aldstadt, *University of Wisconsin - Milwaukee*

2:15 (512) **Real Time Study of Chain Conformation During the Formation of Self-Assembled Monolayers (SAMs) Using Planar Array Infrared (PA-IR) Spectroscopy**; Yujuan Liu, *University of Delaware*; Christian Pellerin, *University of Delaware*; Anand Kalambur, *University of Delaware*; John Rabolt, *University of Delaware*; Bruce Chase, *Central Research and Development*

2:15 (513) **Utilizing an IAM (Immobilized Artificial Membrane) Fast-Screen Mini Cartridge Column for Large Scale DRUG Absorption Screening**; Francis Mannerino, *Regis Technologies*; Ted Szczerba, *Regis Technologies*; Dr. Louis Glunz III, *Regis Technologies*

3:30 (514) **Low-Level Gallium Analysis in Plutonium Oxide**; Jeffrey Miller; Lawrence Drake; David Gallimore; Frances Martin; Alexander Martinez; Joseph Rodriguez, *Los Alamos National Lab*

2:15 (515) **Coherent Anti-Stokes Raman Spectroscopy as a Detector for High Speed Gas Chromatography**; Rebecca Royster, *Spelman College*; Candace Joyner; Kyndra Cottingham; Peter Chen

3:30 (516) **Extending the Limits of the BergerSFC Minigram**; Jennifer Smith, *AutoChem BergerSFC*; Terry A. Berger, *AutoChem BergerSGC*

2:15 (517) **Volatile Selenium Compounds Determination by Solid Phase Micro Extraction and Porous Layer Open Tubular Gas Chromatography with Atomic Emission Detection**; Harriet Totoe, *University of Massachusetts*; Eric Block, *SUNY-Albany*; Julian Tyson, *University of Massachusetts*; Peter Uden, *University of Massachusetts*

3:30 (518) **Data Acquisition in Undergraduate Chromatographic Experiment**; Alexander Nazarenko, *Chemistry Department, SUNY*; Natalie Nazarenko, *Chemistry Department, SUNY*

2:15 (519) **Rotational Invarients for Polarized Raman Spectroscopy**; Simon Frisk, *Dept. of Materials Science & E*; Richard M. Ikeda, *Dept. of Materials Science & E*; D. Bruce Chase, *Central Research & Development*; John F. Rabolt, *Dept. of Materials Science & Eng.*

3:30 (520) **Speciation of V, Cr and Fe by Capillary Electrophoresis Dynamic Reaction Cell Inductively Coupled Plasma Mass Spectrometry**; Ching-Fen Yeh; Shiuh-Jen Jiang, *Department of Chemistry,National Sun Yat-sen Univ*

2:15 (521) **An Electrochemical Investigation into the Behavior of Self Assembled Monolayers (SAMS) of Selected Molecules on both Macro and Nano-gold Electrodes**; Paul Miney; Paula Colavita; Lindsay Taylor; Michael Myrick, *University of South Carolina*

3:30 (522) **Environmental Analysis Using GC-CARS**; Kyndra Cottingham, *Spelman College*; Rebecca Royster, *Spelman College*; Leigha Ingham, *Spelman College*; Candace Joyner, *Spelman College*; Peter Chen, *Spelman College*

2:15 (523) **The Effect of Copper Overlayers on Alkanethiols and Conjugated Oligomers Self-Assembled on Gold**; Paula E Colavita; Michael Doescher; Una Evans; Paul Miney; Annabelle Molliet; John Reddic; Lindsay Taylor; Jing Zhou; Donna Chen; Michael L Myrick, *University of South Carolina*

2:15 (524) **Molecular Sensors for the Base-Specific Detection of Native DNA Nucleotides**; Paula Colavita, *University of South Carolina*; Maria Schiza, *University of South Carolina*; Annabelle Molliet, *University of South Carolina*; Laura Bridgman, *University of South Carolina*; Michael L Myrick, *University of South Carolina*

3:30 (525) **Instrumentation for Multidimensional Luminescence Spectroscopy in Shpol'skii Matrixes at Liquid Nitrogen and Helium Temperatures**; Andres Campiglia, *Department of Chemistry*; Adam Bystol, *Department of Chemistry*; Shenjiang Yu, *Department of Chemistry*

2:15 (526) **A Single Measurement Fiber Optic Chemical Sensing Excitation-Emission Matrix Fluorometer for Remote and In Situ Sensing**; James Jordan, *Arizona State University*; Karl Booksh, *Arizona State University*; Yoon-Chang Kim, *Arizona State University*

3:30 (527) **Luminescence Characteristics of Propranolol and 4-Hydroxypropranolol at Liquid Nitrogen and Liquid Helium Temperatures**; Marina Santos; Andres Campiglia, *University of Central Florida*

2:15 (528) **Design of a Multi-Fluorophore Molecular Beacon Using Conjugated Polymer as its Fluorophore**; Chaoyong Yang; Mauricio Pinto, *Department of Chemistry*; Min Yang; Arup Sen, *GenoMechanix, L.L.C., Gainesvi*; Kirk Schanze; Weihong Tan,*University of Florida*

3:30 (529) **Laser Excited Time-Resolved Shpol'skii Spectroscopy for the Direct Analysis of Polycyclic Aromatic Hydrocarbons in Soil Samples**; Shenjiang Yu; Hector Goicoechea, *Department of Chemistry,* Andres Campiglia, *Department of Chemistry, University of Central Florida*

2:15 (530) **Application of Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry (LA-ICP-MS) to a Population of Automobile Lenses for Forensic Discrimination**; Linda Farr; Jose Almirall, *Florida International University*

3:30 (531) **Analysis of Children's Latent Fingerprints by Infrared Microspectroscopy**; Diane Williams, *FBI Forensic Science Research*; Rebecca Schwartz, *FBI Latent Print Unit*; Edward Bartick, *FBI Forensic Science Research*

2:15 (532) **Stereoview Elemental X-Ray Imaging**; George Havrilla, *Los Alamos National Laboratory*; Thomasin Miller, *Los Alamos National Laboratory*; Robert Morton, *Conoco Phillips*; Ken Huntley, *Conoco Phillips*

3:30 (533) **Application of Micro X-Ray Fluorescence (MXRF) to Chemical and Biological Forensics**; Thomasin Miller, *Los Alamos National Laboratory*; George Havrilla, *Los Alamos National Laboratory*

2:15 (534) **Characterization of Tapered Germanium Waveguide Sensors with Ray Tracing and Synchrotron IR Radiation**; Mark Braiman, *Syracuse University*; Jitraporn Vongsvivut, *Chulalongkorn University*; Sanong Ekgasit, *Chulalongkorn University*; Jason Fernandez, *Syracuse University*

3:30 (535) **Acquisition of Mid-Infrared Spectroscopic Information From Nonrepeatable Events with Sub-100 Microsecond Temporal Resolution**; Chris Snively, *University of Delaware*

2:15 (536) **Simultaneous Acquisition of FTIR Spectral Information From Multiple Liquid Phase Samples**; Chris Snively; Reed Hendershot; Jochen Lauterbach, *University of Delaware*

3:30 (537) **Dual-Wavelength Time-Resolved Resonance Ionization Imaging With Cesium and Mercury Atomic Vapors**; Jamshid Temirov; N. V. Chigarev; Oleg Matveev; Nicolo Omenetto; Ben Smith; James Winefordner, *University of Florida*

2:15 (538) **Laser Ionization Spectroscopy of Cs and Hg atomic vapors**; Jamshid Temirov; Oleg Matveev; Nicolo Omenetto; Ben Smith; James Winefordner, *University of Florida*

3:30 (539) **Development of Sensitive and Inexpensive Sensors Using Fiber Loop Ringdown Spectroscopy**; Chuji Wang, *Mississippi State University*; S. T. Scherrer, *Mississippi State University*; Ping-Rey Jang, *Mississippi State University*; D. L. Monts, *Mississippi State University*

2:15 (540) **Fluorescence Spectroscopy of Molecular Ions Trapped in a Quadrupole Ion Trap Mass Spectrometer**; Keneth Wright; Michael Blades, *University of British Columbia*

3:30 (541) **Examination of the 13C/12C Isotopes in Sparkling Wine with On-line Sampling and Isotope Ratio MS.**; Guy Bilodeau, *GV Instruments*; Francois Fourel, *GV Instruments*; Stephen Shuttleworth, *GV Instruments*

2:15 (542) **Forensic Applications in Continuous Flow IRMS**; Francois Fourel, *GV Instruments*; Andrew Phillips, *GV Instruments*; Lionnel Mounier, *GV Instruments*; Guy Bilodeau, *GV Instruments*; Stephen Shuttleworth, *GV Instruments*

2:15 (543) **Analysis of Bromine in Flame Retardant Plastics Using Pulsed Glow Discharge Mass Spectrometry**; Lei Li, *Department of Chemistry, West*; Chris Barshick, *GE Plastics, General Electric*; Tom Millay, *Department of Chemistry, West*; Fred King, *Department of Chemistry, West*

3:30 (544) **Study of Zinc-Metallothionein Binding Properties by Tandem Mass Spectrometry Using Collision-Induced Dissociation**; Yuchen Lu, *West Virginia University*; Fred King, *West Virginia University*

2:15 (545) **Nanoparticle Beam Deposition as a Novel Technique for the Formation of Organic Thin Films**; Ashley Greer-Reese, *University of South Carolina*; Brian Genge, *University of South Carolina*; Kristen Krantzman, *College of Charleston*; Donna Chen, *University of South Carolina*; Michael Myrick, *University of South Carolina*

3:30 (546) **Investigation of Anti-Arthritic Therapeutic Agents**; Sarka Prochazka, *University of Technology, Sydney*; Mary Mulholland, *University of Technology, Sydney*; Anthea Lloyd-Jones, *University of Technology, Sydney*

2:15 (547) **The Analysis of Ultra-Thin Layers by GD-OES (A comparison with other Surface Techniques)**; Kim Marshall; Kevin Brushwyler; Charles Maul; Joel Mitchell, *LECO Corporation*

3:30 (548) **Application of a Cyclophosphazene Encapsulated in a Porous Silica Matrix as Solid Phase for the Determination of Metalic Complexes**; Miguel Barbosa, *Laboratorio de Química*; Maria Ines Toral, *Laboratorio de Química*; Carlos Diaz, *Laboratorio de Química*

2:15 (549) **Investigations of Thin Polymer Films With Vibrational Spectroscopic Techniques**; Andreas Gupper, *Research Institute for Electro*; Peter Wilhelm, *Research Institute for Electro*; Robert SAF, *Institute for Chemistry and Tech*; Thomas Steindl, *Institute for Chemistry*

3:30 (550) **Solid State S-33 NMR of Inorganic Minerals**; Peter Rinaldi, *University of Akron*; Todd Wagler, *University of Akron*; William Daunch, *University of Akron*; Matt Panzer, *University of Akron*; Wiley Youngs, *University of Akron*

2:15 (551) **Universal Resonantly Enhanced Raman Spectrometer**; LaTasha Amisial, *Spelman College*; Candace Joyner, *Spelman College*; Kristle McBride, *Spelman College*; Peter Chen, *Spelman College*

2:15 (552) **Development of an in-situ Raman Probe to Monitor Hydrothermal Vent Reactions**; Tina Battaglia, *Arizona State University*; Karl Booksh, *Arizona State University*

3:30 (553) **Monitoring the Hydrolysis of Methylmethoxysilanes in an Aqueous Environment by Raman Spectroscopy**; Martin Bennett; Mary Tecklenburg, *Central Michigan University; 1*; Kurt Brandstadt, *Dow Corning Corp.*

2:15 (554) **Use of IR and Raman Spectroscopy to Study Sustained Release Oral Dosage Forms: A Case Study**; Dirk Cleeren, *Johnson & Johnson Pharmaceutic*; Sigrid Stokbroekx, *Johnson & Johnson Pharmaceutic*; Jef Peeters, *Johnson & Johnson Pharmaceutic*; Marcus Brewster, *Johnson & Johnson Pharmaceutic*

3:30 (555) **Anisotropy of Surface-Enhanced Raman Bands and Surface Plasmon Bands of Single Ag nanoparticles**; Tamitake Itoh; Kazuhiro Hashimoto; Akifumi Ikehata; Yukihiro Ozaki, *Kwansei-Gakuin University*

3:30 (556) **Multiplex Resonance CARS in a Flame**; Candace Joyner, *Spelman College*; LaTasha Amisial, *Spelman College*; Kristle McBride, *Spelman College*; Peter Chen, *Spelman College*

2:15 (557) **Ultra-Sensitive Detection of Biological Molecules: The Role of Ionic Effects in Surface-Enhanced Raman Scattering**; Tae-Woong Koo, *Intel Corporation*; Selena Chan, *Intel Corporation*; Lei Sun, *Intel Corporation*; Xing Su, *Intel Corporation*; Andrew Berlin, *Intel Corporation*

3:30 (558) **A Raman Microscopy Investigation of the Distribution Variation caused in Pharmaceutical Tablets by Different Manufacturing Processes**; Fiona C. Thorley, *University of Leeds*; Kurt J. Baldwin, *University of Leeds*; David C. Lee, *GlaxoSmithKline*; David N. Batchelder, *University of Leeds*

2:15 (559) **A Robust HPLC(IC)-ICPMS Method for ?Routine? Speciation Analysis of Ground Waters for Arsenic**; Jonathan Talbott, *Illinois Waste Management and*; John Scott, *Illinois Waste Management*; Buulinh Qaach, *Illinois Waste Management*; Tom Holm, *Illinois State Water Survey*; Steve Wilson, *Illinois State Water Survey*; Marv Piwoni, *Illinois Waste Management*

2:15 (559b) **Enhanced Vibrational Circular Dichroism in Metal Complexes and Metalloproteins with Low-lying Electronic States**; Yanan He; Laurence Nafie; Teresa Freedman, *Syracuse University*

2:15 (559c) **Near-Infrared Vibrational Circular Dichroism of Terpenes, Ephedrines and Polypeptides**; Changning Guo, *Syracuse university*; Taiping Zhao, *Syracuse University*; Xiaolin Cao, *Syracuse University*; Teresa Freedman, *Syracuse University*; Laurence Nafie, *Syracuse University*

Wednesday Afternoon, Room 315
FEEDBACK GENERATION SESSION ON THE DRAFT FDA GUIDANCE ON PROCESS ANALYTICAL TECHNOLOGY
Presider: Gary Zuber, GlaxoSmithKline

1:30 (560) **Feedback Generation Session on the Draft FDA Guidance on Process Analytical Technology**; James Rydzak, *GSK*; Gary Zuber, *GSK*

1:35 (561) **FDA PAT Update: Introduction to the PAT Draft Guidance**; Ajaz Hussain, *FDA*

1:55 (562) **FDA PAT Draft Guidance Presentation**; Ajaz Hussain, *FDA*

2:50 **Coffee Break**

3:10 (563) **Discussion Breakout Groups on PAT Draft Guidance**; Gary Zuber, *GSK*

4:10 (564) **Presentation of Feedback Summaries of Breakout Groups**; Gary Zuber, *GSK*

5:25 (565) **Summary and Closing Remarks**; James Rydzak, *GSK*

TECHNICAL PROGRAM - THURSDAY

Thursday Morning, Room 113
CHEMOMETRICS: SPECTROSCOPIC APPLICATIONS IN PHARMACEUTICALS AND BIOANALYTICAL
Presider: Kathy Alam, *Sandia National Labs*

8:30 (566) **Data Analysis Strategies for Spectroscopic Imaging of Pharmaceutical Tablet**; Lin Zhang, *Pfizer Global R&D*; Mark Henson, *Pfizer Global R&D*; Sonja Sekulic, *Pfizer Global R&D*

8:50 (567) **FT-IR Reflectance Microspectroscopy Study of Bacterial Spores Following the Autoclaving Process**; David L. Perkins, *University of South Carolina*; Charles R. Lovell, *University of South Carolina*; Michael L. Myrick, *University of South Carolina*

9:10 (568) **MCR Analysis of Cellular Changes Detected from ATR-IR Data**; M. Kathleen Alam, *Sandia National Laboratories*; Jerilyn A. Timlin, *Sandia National Laboratories*; Laura E. Martin, *Sandia National Laboratories*; Rick Lyons, *University of New Mexico*; Brian Hjelle, *University of New Mexico*; Kristin Garrison, *University of New Mexico*

9:30 (569) **Determination of Enantiomeric Purity of Samples by Chemometric Analysis of UV/Visible Spectral Data**; Jemima R. Ingle; Dennis H. Rabbe; Marianna A. Busch; Kenneth W. Busch, *Baylor University*

9:50 **Coffee Break**

10:30 (570) **Determination of Hotness Levels in Capsicum Fruits by Chemometric Modeling of UV Spectral Data**; Carolyn Markey; Marianna A. Busch; Kenneth W. Busch, *Baylor University*

10:50 (571) **Optimization of PLS Calibrations for FT-IR Analysis of Various Sugar Sources**; Bruce Thompson, *Brown & Williamson Tobacco Corp*

11:10 (572) **Application of Partial Least Squares Methods to FT-IR Gas Phase Analysis of Sidestream Cigarette Smoke**; Bruce Thompson, *Brown & Williamson Tobacco Corp*; Boris Mizaikoff, *Georgia Institute of Technology*

11:30 (573) **Infrared/Chemometric Monitoring of Water Adsorption onto Type 3A Zeolite***; Anding Zhang, *The University of New Mexico*; Wenxiang Zeng, *The University of New Mexico*; David Haaland, *Sandia National Laboratories*; Thomas Niemczyk, *The University of New Mexico*

Thursday Morning, Room 204
NEW APPROACHES TO TEACHING ANALYTICAL CHEMISTRY – ENVIRONMENTAL CHEMISTRY
Presider: David McCurdy, *Truman State University*

8:30 (574) **The Development of Cross-Discipline Undergraduate Research: Trace Metal Analysis of Snapping Turtles Collected from Erie County, Pennsylvania**; Thomas Spudich, *Penn State Erie, The Behrend C*; David Duberow; Chadwick Knight; Deseree Dupres; Jeanette Schnars,

8:50 (575) **The Environment: Bringing chemistry home**; John Brock, *Warren Wilson College*

9:30 (576) **The Water Project: An Ongoing, "Real-World" Experience for the Undergraduate Analytical Lab**; T. C. Werner, *Union College*

9:50 **Coffee Break**

10:30 (577) **Teaching Analytical Chemistry: A Research Approach using the Local Environment**; Jeffrey Draves, *Monmouth College*

11:10 (578) **Applying CPR to Analytical Students: Pre- and Post-Lab Calibrated Peer Review Writing for AAS Experiments in Environmental Chemistry**; Lawrence Margerum, *University of San Francisco*; Maren Gulsrud, *University of San Francisco*

11:50 (579) **An Environmentally Focused Analytical Curriculum**; David Butcher, *Western Carolina University*; Cynthia Atterholt, *Western Carolina University*; Roger Bacon, *Western Carolina University*

Thursday Morning, Room 216
ELECTROPHORETIC SEPARATIONS IN CAPILLARIES AND MICROCHIPS
Presider: Doug Gillman, *University of Tennessee*

8:30 (580) **Spatially Resolved Multiplexed Detection for Channel Electrophoresis**; Scott A. Shippy, *University of Illinois Chicago*; Jennifer A. McReynolds, *University of Illinois Chicago*

9:10 (581) **In Vitro Evolution of Functional DNA using Capillary Electrophoresis**; Michael Bowser, *University of Minnesota*; Shaun Mendonsa, *University of Minnesota*

9:50 **Coffee Break**

10:30 (582) **Radical Activated Cleavage for Protein Characterization**; Wyatt Barb; Mark Hayes, *Arizona State University*

11:10 (583) **Temperature-Programmed Mixing in Microchannels Using Liposomes**; Laurie Locascio, *NIST*; Wyatt Vreeland, *NIST*

Thursday Morning, Room 220
NEW/NOVEL APPLICATIONS OF IR AND NIR
Presider: Emil Ciurczak, *Integrated Technical Solutions*

8:30 (584) **Noise Covariance Estimation Techniques in the Application of Maximum Likelihood Principal Component Analysis to Near-Infrared Chemical Imaging**; Frederick Koehler, *Spectral Dimensions*; Eunah Lee, *Spectral Dimensions*; Linda Kidder, *Spectral Dimensions*; E. Neil Lewis, *Spectral Dimensions*

8:50 (585) **Industrial Quality Control and High-Throughput Analysis by Near-Infrared, Mid-Infrared and Raman Spectroscopy**; Heinz W. Siesler; Inna Gerber, *University of Duisburg-Essen*

9:30 (586) **Compact NIR Diode Array Spectrometer Systems for Pharmaceutical Manufacturing**; Promit Das, *Control Development, Inc.*; Terrance Kinney, *Control Development, Inc*; Ross Herrold, *Control Development, Inc*

9:50 **Coffee break**

10:30 (587) **Near-Infrared Chemical Imaging and its Connection to Process Analytical Technology**; E. Neil Lewis; Linda Kidder; Ken Haber; Eunah Lee, *Spectral Dimensions, Inc.*

11:10 (588) **Factors Effecting NIR Chemical Images of Solid Dosage Forms**; Fred LaPlant; Steve Arrivo, *Pfizer Global R&D*

11:30 (589) **Mid and Near Infrared Determination of Concentrations in Mixtures of Solid-State Pharmaceutical Compounds**; Yanga K Dijiba, *University of New Mexico*; zhang Anding, *University of New Mexico*; Thomas. M Niemczyk, *University of New Mexico*

TECHNICAL PROGRAM - THURSDAY

Thursday Morning, Room 221
ADVANCES IN VIBRATIONAL SPECTROSCOPY FOR SOLIDS
Presider: John Chalmers, *VS Consulting*

8:30 (590) **Look and Listen – Non-invasive Monitoring of Powder Mixing with NIR Spectrometry**; David Littlejohn, *University of Strathclyde*; Luke Bellamy, *University of Strathclyde*; Alison Nordon, *University of Strathclyde*

9:10 (591) **Real-Time Spectroscopy of Polymer Melt Processsing – Applications and Developements**; S.E Barnes; M.G Sibley; H.G.M Edwards; I.J Scowen; P.D Coates, *IRC in Polymer Engineering*

9:50 **Coffee Break**

10:30 (592) **Applications of PAT to pharmaceutical manufacturing**; Steve Hammond, *Pfizer*; Martin Warman, *Pfizer*; Fiona Clarke, *Pfizer*; Neville Broad, *Pfizer*

11:10 (593) **High-Speed, High-Resolution, Near-Infrared Spectroscopy For Industrial Process Control**; Richard Crocombe; Petros Kotidis; David Nislick; Walid Atia; Steve Fawcett, *AXSUN Technologies*

Thursday Morning, Room 222
MINIATURIZATION OF SERS DETECTION SYSTEMS
Presider: Peter White, *University of Strathclyde*

8:30 (594) **Optical Detection within Microfluidic Systems**; Andrew deMello, *Imperial College*

9:10 (595) **Expanding the Analytical Utility of Surface Enhanced Raman Spectrometry**; Michael Sepaniak; Gerald Devault, *1*; R. Maggie Connatser; Marco DeJesus; Kathleen Giesfeldt, *University of Tennessee*

10:30 (596) **SERRS Immunoassay**; Peter White, *University of Strathclyde*

10:50 (597) **Development of SERS-Based Sensors for Space Cabin Air Quality Monitoring**; Josef Simeonsson, *Advanced Monitoring, Inc.*

11:10 (598) **Bioanalysis using SERRS in Microsystems**; Duncan Graham, *University of Strathclyde*; W. Ewen Smith, *University of Strathclyde*; Jon Cooper, *University of Glasgow*; Frances Docherty, *University of Strathclyde*; Lorna Stevenson, *University of Strathclyde*

Thursday Morning, Room 223
NOVEL APPROACHES TO AND APPLICATIONS OF RAMAN SPECTROSCOPY
Presider: Steve Choquette, *NIST*

8:30 (599) **Inspection of Pesticide Residues on Food by Surface-Enhanced Raman Spectroscopy**; Chetan Shende, *Real-Time Analyzers*; Alan Gift, *Real-Time Analyzers*; Stuart Farquharson, *Real-Time Analyzers*

8:50 (600) **Two-dimensional Vibrational Spectroscopy Study of the Interactions Caused by Changes in Chemical Composition of Rice Flour**; David Himmelsbach, *USDA-ARS-Russell Res. Ctr.*; Franklin Barton, II, *USDA-ARS-Russell Res. Ctr.*

9:10 (601) **Application of Band Target Entropy Minimization (BTEM) to Extraction of Pure Component Spectra from Raman Image Data**; Effendi Widjaja; Michael Morris, *University of Michigan*

9:30 (602) **Modeling Bone Raman Spectra With Substituted Hydroxyapatites**; Mary Tecklenburg; Adam Perala; Amy Marcotte; Robert Buckland, *Central Michigan University*

9:50 **Coffee Break**

10:30 (603) **Novel Application of Raman Spectroscopy to Chemically Characterize and Quantitate Hydrothermal Vent Systems**; Brian Dable, *Center for Process Analytical*; Brian Marquardt, *Center for Process Analytical*; Karl Booksh, *Arizona State University*; Tina Battaglia, *Arizona State University*

10:50 (604) **Automated, Liquid Core Waveguide Raman Spectroscopy for Parametric Studies of Competing Equilibria: Application to Hexafluorosilicate Hydrolysis**; William F. Finney, *University of Michgian*; Michael D. Morris, *University of Michigan*

11:10 (605) **The Importance of Proper Intensity Calibration for Raman Analysis of Low-Level Analytes in Water**; R. Brian Melkowits; Ted L. Williams; Timothy W. Collette, *USEPA*

11:30 (606) **Analysis of Hexavalent Chromium in Groundwater by Surface-Enhanced Raman Spectroscopy**; Stuart Farquharson, *Real-Time Analyzers*; Khris B. Olsen, *Pacific Northwest National Lab*

Thursday Morning, Room 301
INSTRUMENT DEVELOPMENTS STILL NEEDED IN ICP-AES
Presider: J.-M. Mermet, *Universite Claude-Bernard, Lyon*

8:30 (607) **Instrument Developments Still Needed in ICP-AES**; Jean-Michel Mermet, *University of Lyon*

9:10 (608) **Improving the Sample Introduction System for the Analysis of Microsamples Through ICP-AES**; José Luis Todolí, *University of Alicante*; Jean Michel Mermet, *University Claude Bernard*

9:50 **Coffee Break**

10:30 (609) **Direct Solids Analysis With ICP-AES**; Jose A.C. Broekaert, *University of Hamburg*

11:10 (610) **Nano-Particle Sample Introduction for Inductively Coupled Plasma-Atomic Emission Spectrometry**; Vassili Karanassios, *University of Waterloo*

Thursday Morning, Room 302
GLOW DISCHARGE SPECTROSCOPIES: SOLIDS AND BEYOND
Presider: Kenneth Marcus, *Clemson University*

8:30 (611) **Applications of Quantitative GD-OES to Nanometer Layers - Recent Devlopment**; Arne Bengtson; Thomas Björk, *Swedish Institute for Metals Research*

8:50 (612) **Glow Discharge Spectrometries in the National Metrology Institutes**; Michael Winchester, *NIST*

9:10 (613) **Characterization of Surfaces and Thin Films Down to the Nanometer Scale of Conductive and Non Conductive Materials by RF-GD-OES**; Patrick Chapon, *Jobin Yvon SAS*; Richard Payling, *Surface Analytical*; Philippe Hunault, *Jobin Yvon Inc*

9:30 (614) **RF-GD-OES: A Wealth of Options for Powdered Materials**; R. Kenneth Marcus; Wandee Luesaiwong; Timothy Brewer, *Clemson University*

9:50 **Coffee Break**

10:30 (615) **Effect of a Reactive Glow Discharge Environment on Plasma Species**; Elizabeth Hastings, *University of Florida, Gainesville*; W. W. Harrison, *University of Florida, Gainesville*

10:50 (616) **Investigations of Nitrogen Containing Glow Discharge Plasmas**; Lei Li, *Department of Chemistry, West*; Na Zhang, *Department of Chemistry, West*; Jennifer Robertson, *Department of Chemistry, West*; Fred King, *Department of Chemistry, West*

11:10 (617) **Particle Beam Glow Discharge Mass Spectrometry: A Versatile Biomolecule Ion Source**; R. Kenneth Marcus; W. Clay Davis; Jakob L. Venzie; Justin Hensley, *Clemson University*

11:30 (618) **Liquid Matrices Evaluated by AP MALDI and LD APCI**; Kevin Turney; W.W. Harrison, *University of Florida*

Thursday Morning, Room 304
TRACE ELEMENT DETERMINATIONS IN PHOSPHATE-BASED AND ENVIRONMENTAL MATERIALS
Presider: Peter G. Brown, *Leeman Labs, Inc*

8:30 (619) **Determination of Trace Metals in Fertilizer**; William Hall, *IMC Global*; Peter Kane, *Purdue University*

8:50 (620) **Analysis of Fertilizers Using Dual View ICP With Solid State Detection**; Manuel Almeida, *Leeman Labs, Inc.*; Bruce MacAllister, *Leeman Labs. Inc*

9:10 (621) **Analysis of Phosphate in Fertilizer Concentrates and Process Phosphoric Acid**; Sanford A. Siegel, *CF Industries Inc.*; Harold J. Falls, *CF Industries Inc*

9:30 (622) **Orange Juice Classification via ICP-MS and Artificial Neural Networks**; Seif Nikdel; Murat Azik, *State of Florida*

9:50 **Coffee Break**

10:30 (623) **The Determination of Mercury in Fertilizers at the Risk-Based Acceptable Concentration.**; David Pfeil, *Leeman Labs, Inc.*; Bruce MacAllister, *Leeman Labs, Inc.*

10:50 (624) **Determination of Mercury Concentrations in the Range below 1 ng/L. Target in Environmental Analyses, Challenge for the Analyst**; Gerhard Schlemmer; *AJ Uebrlingen;* Thomas Labatzke, *Analytiks-Jena AG*

11:10 (625) **Comprehensive Studies of Mass Spectrometric and Radiation Detection Methods for Measurement of Ultra-Low Level Actinides**; Cynthia Mahan; Wei Hang; Edward Gonzales; Lu Wang Zhu, *Los Alamos National Lab*

11:30 (626) **Mercury in Retail Fish and the Diet of Canadians**; Robert Dabeka, *Health Canada*; Art McKenzie, *Health Canada*

Thursday Afternoon, Room 113
CHEMOMETRICS: GENERAL METHODS AND APPLICATIONS
Presider: Anding Zhang, *University of New Mexico*

1:30 (627) **Fractal Resolve Method: A New Tool for Separating the Overlapped Peaks Signal on the Basis of Estimating the Fractal Dimension**; Chen Xiaoyan, *Zhong*shan University; Bao Lunjun, *Guangzhou Entry-Exit Inspectio*; Mo Jinyuan, *Zhongshan University*

2:30 (628) **A Novel Chemical Detector Using Cermet Sensors**; Susan Rose-Pehrsson, *Naval Research Laboratory*; Mark Hammond, *Naval Research Laboratory*; John Ziegler, *General Atomics*; Dana Gray, *General Atomics*

2:50 **Coffee Break**

3:30 (629) **Decomposition of the Perturbation Domain in Two-Dimensional Correlation Spectroscopy**; Andrew Jirasek, *University of British Columbia*; Georg Schulze; Robin Turner; Michael Blades

3:50 (630) **Near Infrared Spectroscopy: A Tool to Introduce Nondestructive Real-Time Analysis in the Undergraduate Curriculum.**; Anna Cavinato, *Eastern Oregon University*

4:10 (631) **Principal Component Analysis Utilizing Fractional Dimensionality**; Jeff Cramer, *Arizona State University*; Karl Booksh, *Arizona State University*

Thursday Afternoon, Room 216
MICROFLUIDICS IN ANALYTICAL CHEMISTRY
Presider: Mark Hayes, *Arizona State University*

1:30 (632) **Using Microfluidic Devices for the Analysis of Organelles**; Edgar Arriaga; Chris Whiting; Hossein Ahmadzadeh; Karen Olson, *University of Minnesota*

2:10 (633) **From Silicon- and Plastic-Based Micro-Fluidics to Shirt-Pocket Size Micro-Instruments**; Vassili Karanassios, *University of Waterloo*; Bithi Eshaque, *University of Waterloo*; Sathi Eshaque, *University of Waterloo*

2:50 **Coffee Break**

3:30 (634) **Applications of Optically Gated Vacancy Injections in Microchip Devices**; S. Douglass Gilman, *University of Tennessee*; Kristie R. Carter, *University of Tennessee*; Jason L. Pittman, *University of Tennessee*; Charles S. Henry, *Colorado State University*

4:10 (635) **Preparation of Microchip Columns with Immobilized Biomolecules for Self-Interaction Chromatography and Enzyme Reactors**; Charles Henry; Carlos Garcia; Joseph Valente, *Colorado State University*

4:50 (636) **Neurochemical and Clinical Applications of Microchip Electrophoresis with Electrochemical and Laser Induced Fluorescence Detection**; Barbara Fogarty; Walter Vandaveer IV; Nathan Lacher; Stephanie Pasas; Bryan Huynh; Celeste Frankenfeld; Susan M Lunte, *University of Kansas*; R. Scott Martin, *St. Louis University*

Thursday Afternoon, Room 220
APPLICATIONS OF IMAGING SPECTROSCOPY
Presider: Christine M. Wehlburg, *Sandia National Labs*

1:30 (637) **FTIR-Microscope Mapping Software – An Alternative to Focal Plane Array Technology**; Shannon Richard, *Shimadzu Scientific Instrument*; Timothy Alt, *Shimadzu Scientific Instrument*; John Monti, PhD, *Shimadzu Scientific Instrument*; Kimberly Abramo, PhD, *Shimadzu Scientific Instrument*

1:50 (638) **Analysis of Children's Latent Fingerprints by Infrared Microspectroscopy**; Diane Williams, *FBI Forensic Science Research*; Rebecca Schwartz, *FBI Latent Print Unit*; Edward Bartick, *FBI Forensic Science Research*

2:10 (639) **Novel Imaging Systems: Multivariate Optical Computing from UV to NIR**; Ryan Priore, *University of South Carolina*; Ashley Greer, *University of South Carolina*; Fred Haibach, *Detect-X, a division of Dicut,*; Maria Schiza, *University of South Carolina*; David Perkins, *University of South Carolina*; Michael Myrick, *University of South Carolina*

2:30 (640) **A New InGaAs Array for High Resolution NIR Spectroscopy**; Leslie Tack; Bruce True, *Roper Scientific*

2:50 **Coffee Break**

3:30 (641) **Using Raman Imaging to Map Localized Stress Around Osteocyte Lacuna**; Jian Ling, *Southwest Research Institute*; Daniel Nicolella, *Southwest Research Institute*; Donald Moravits, *Southwest Research Institute*; Michael Miller, *Southwest Research Institute*

3:50 (642) **Non-Invasive Determination of Hypovolemic Shock Using Hyperspectral Imaging**; James Mansfield, *Hypermed*; Andriy Batchinsky, *Institute for Surgical Researc*; Neil Lewis, ; Robert Lew, *HyperMed*; Jenny Freeman, *HyperMed*; Lee Cancio, *Institute for Surgical Research*

4:10 (643) **Label Free Detection of Protein and Small Molecule Microarrays**; Mark McDermott, *University of Alberta*; Vishal Kanda, *University of Alberta*; Chris Ggrant, *University of Alberta*; Salome Guchu, *University of Alberta*; Dennis Hall, *University of Alberta*

4:30 (644) **FT-IR Imaging of Solvent-Induced Crystallisation of Syndiotactic Polystyrene**; Sergei Kazarian; Andrew Chan; Andreas Gupper, *Imperial College London*

Thursday Afternoon, Room 222
PHARMACEUTICAL RAMAN SPECTROSCOPY
Presider: Mark Kemper, *Kaiser Optical Systems*

1:30 (645) **Study of Enzyme-Substrate Binding Using Fiber-Optic Ultraviolet Resonance Raman Spectroscopy**; Andrew Jirasek, *University of British Columbia*; Manon Couture; Lindsay Eltis, ; Robin Turner; Michael Blades, *University of British Columbia*; Frederic Vaillancourt; Christopher Barbosa

1:50 (646) **Speeding drugs through clinical trials: Five-minute analysis of drugs and metabolites in saliva**; Alan Gift, *Real-Time Analyzers*; Chetan Shende, *Real-Time Analyzers*; Stuart Farquharson, *Real-Time Analyzers*

2:10 (647) **Characterizing Pharmaceutical Product Polymorphism Using Raman Chemical Imaging**; Matthew Nelson, *ChemImage Corporation*; David Tuschel, *ChemImage Corporation*; Julianne Wolfe, *ChemImage Corporation*; Patrick Treado, *ChemImage Corporation*

2:30 (648) **In-process Raman measurements of Particulate Systems: The Interrelationship between Particle Dimension, Particle Concentration and Raman Spectra**; Paul Barrett, *Lasentec MT*

2:50 **Coffee Break**

3:30 (649) **Evaluation of Surface Enhanced Resonance Raman Scattering (SERRS) For Highly Sensitive and Highly Multiplexed DNA Analysis**; Karen Faulds, *University of Strathclyde*; Duncan Graham, *University of Strathclyde*; W. Ewen Smith, *University of Strathclyde*; Romina Barbagallo, *LGC*; Jacquie Keer, *LGC*

3:50 (650) **Pharmaceutical process applications of Raman spectroscopy**; Stuart Farquharson, *Real-Time Analyzers*; Alan Gift, *Real-Time Analyzers*; Wayne Smith, *Real-Time Analyzers*

Thursday Afternoon, Room 301
WHAT IS NEW IN ATOMIC ABSORPTION SPECTROMETRY
Presider: Greet de Loos, *Delft University of Technology*

1:30 (651) **Continuum Source AAS – Step By Step on the Way to Simultaneous Multielement Analysis**; Helmut Becker-Ross; Stefan Florek; Uwe Heitmann, *ISAS*; Mao D. Huang; Michael Okruss, *GOSe.v.*

2:10 (652) **Diode Lasers for Element Selective Measurements**; Joachim Franzke, *ISAS*

2:50 **Coffee Break**

3:30 (653) **Novel Vapor Generation Approaches for Trace Element Analysis: UV Light Mediated Alkylation of Selenium and Nickel.**; Zoltan Mester, *Institute for National Measure*; Ralph Sturgeon, *Institute for National Measure*; Xuming Guo, *Institute for National Measure*; Graeme Gradner, *Institute for National Measure*

3:50 (654) **Utilizing Surface Response Techniques for Optimization of Graphite Furnace AA Programs**; Doug Shrader, *Varian Inc.*; Jean-Pierre Lener, *Varian S.A.*; Thomas Preuss, *Varian Australia Pty. Ltd.*; John Sanders, *Varian Australia Pty. Ltd.*; Eric Vanclay, *Varian Australia Pty. Ltd.*

Thursday Afternoon, Room 302
ICP-AES APPLICATIONS
Presider: J.-M. Mermet, *Universite Claude-Bernard*

1:30 (655) **Innovative Sampling Techniques for Improved Productivity in Atomic Spectrometry**; Doug Shrader, *Varian Inc.*; John Sanders, *Varian Australia Pty. Ltd.*; Eric Vanclay, *Varian Australia Pty. Ltd.*

1:50 (656) **High Resolution ICP-OES Analysis of Zirconium Metal**; Albert Brennsteiner, *Jobin Yvon Inc*; Geoffrey Tyler, *Jobin Yvon SAS*; Agnès Cosnier, *Jobin Yvon SAS*; Desirée Ahlum, *Jobin Yvon Inc*; Sébastien Velasquez, *Jobin Yvon SAS*

2:10 (657) **Determination of Trace Element in Precious Metals By ICP-OES Spectrometry**; Albert Brennsteiner, *Jobin Yvon Inc*; Geoffrey Tyler, *Jobin Yvon SAS*; Agnès Cosnier, *Jobin Yvon SAS*; Nathalie Le Corre, *Jobin Yvon SAS*

2:30 (658) **Biological and Clinical Micro- and Nano-Samples by Inductively Couled Plasma (ICP) Spectrometry**; Vassili Karanassios, *University of Waterloo*; Blair Gibson, *University of Waterloo*; Hamid Badiei, *University of Waterloo*; William Vander Wilp, *University of Waterloo*

2:50 **Coffee Break**

3:30 (659) **Method Development Strategies for Analysis of Agricultural Samples by Simultaneous ICP-OES**; Michelle Cree, ; Christine Rivera, *Varian, Inc.*; James Barker, *Varian, Inc.*; XueDong Wang, *Varian, Inc.*

3:50 (660) **An Alternative Calibration Method for the Accurate Determination of Mg/Ca**; Andrew Ryan, *Varian, Inc.*; Stephanie de Villiers, *Department of Earth Science*; Mervyn Greaves, *Department of Earth Science,*; Henry Elderfield, *Department of Earth Sciences*; Michelle Cree, *Varian, Inc.*

4:10 (661) **The Investigation of Boron Measurement Using Simultaneous ICP-OES with Ultrasonic Nebulization.**; Michelle Cree, *Varian, Inc.*; Christine Rivera, *Varian, Inc.*; Fred Smith, *CETAC Technologies*