TECHNICAL PROGRAM - SUNDAY

SUNDAY POSTER SESSION
5:00 – 7:00 PM, Rotunda

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

5:00 (1) **Development of a Cold Vapor Generation Atomic Absorption Spectrometry Technique for the Determinataion of Cadmium in Environmental Samples**; Rebecca H. Wack, *Marist College*

5:00 (2) **Thin film, Ultra Thin Film And Surface Analysis fo Conductive and Non-Conductive Materials by RF-GD-OES**; Lisa C. Goldstone, Patrick Chapon, Richard Payling, Phillipe Hunault, Olivier Bonnot, Lisa C. Goldstone, Celia Olivero, *Jobin Yvon SA, Surface Analytical, Jobin Yvon Inc.*

5:00 (3) **Determination of Trace Elements in Whole Blood**; Penelope A.Robin, David Littlejohn, Thomas DB Lyon, U*niversity of Strathclyde, Glsgow Roal Infirmary*

5:00 (4) **Concomitant Metals Analyzer (CMA) for Both Hydride Forming & "NormaL" Elements in ICP-OES –Investigational Parameters & Effects**; Albert Brennsteiner, Geoff Tyler, Andras Bartha, Maria Ballok, *Jobin Yvon SA, 16-18 rue du Canal, 91165 Longjumea,, Hungary Institute for Geological Sciences, Budapest, Hungary, Jobin Yvon Inc, 3880 Park Avenue, Edison, NJ 08820 USA*

5:00 (5) **Low Level Mercury DetermInations:**; David L. Pfeil, Arthur L. Reed, *Leeman Labs, Inc*

5:00 (6) **Speciation And Microanalysis Of Individual Particles By Means Of Micro-Xanes**; Koen H. Janssens, Kristof Proost, Yngvar Thomassen, Ole-Christian Lind, Brit Salbu, Piero Danesi, Gerald Falkenberg, *University of Antwerp, Belgium, National Institute of Occupational Health, Oslo, Norway, Agricultural University of Norway, Aas, Norway International Atomic Energy Agency Laboratories, Seibersdorf, Austria*

5:00 (7) **Elemental and isotopic analysis using ICP-TOFMS**; Lloyd A. Allen, *LECO*

5:00 (8) **Matrix Effect of Solution Micro-Sample Introduction in Double Focusing Sector Field ICP-MS**; Zhongxing Chen; *Laboratory for Isotope and Trace Element Research*

5:00 (9) **Development of a Dual-Source Time-of-Flight Mass Spectrometer for Simultaneous Elemental Analysis and Molecular Weight Determination**; Gary M. Hieftje, Amy L. Rosen, Steven J. Ray, William C. Wetzel, *Department of Chemistry, Indiana University*

5:00 (10) **Interference-free Determination of Trace Elements in Fish Otoliths by Electrothermal Vaporization Inductively Coupled Quadrupole Plasma Mass Spectrometry (ETV-ICP-QMS)**; Zikri Arslan, Anthony J Paulson, *National Oceanic and Atmospheric Administration (NOAA), Northeast Fisheries Science Center (NFSC), James J. Howard Marine Sciences Laboratory, Highlands, NJ 07732 USA*

5:00 (11) **Evaluation of Hydrofluoric Acid Precipitation of Calcium to Eliminate Calcium Oxide Interferences for Analysis of Fish Otoliths by Solution-based ICP-MS**; Zikri Arslan, Anthony J Paulson, *National Oceanic and Atmospheric Administration*

5:00 (12) **Investigation of the Nitrous Oxide/Acetylene Flame for Laser-Enhanced Ionization Spectrometry**; Denis Boudreau, Isabelle Poulin, Philippe Nobert, *Dept. Chemistry, Laval University*

5:00 (13) **Evaluating Robustness of an Ar-N2 mixed gas plasma for ETV-ICPMS**; William J. Balsanek, James A. Holcombe, *University of Texas at Austin*

5:00 (14) **Use of NIST High Performance Calibration Method for Certified Commercial Standards**; Thomas M. Rettberg, Susan Evans Norris, Lenore Coombs

5:00 (15) **In Situ Solid State Chemical Speciation of Some Airborne Metal Species Associated with Atmospheric Particulate Matter of Varying Size**; Marc M Lamoureux, Nicholas Warner, Janelle Samson, Jonathan Enright, Conrad Grégoire

5:00 (16) **Analysis of Oscillatory Enzyme Activity. Systematic Evaluation of Artifact Sources**; Alexander Scheeline, D. James Morre, Dorothy M. Morre, *University of Illinois at Urbana-Champaign, Purdue University*

5:00 (17) **A Clinical Application of In-vivo Near Infrared Spectroscopy in Burn Depth Assessment**; Lorenzo Leonardi, *National Research Council Canada*

5:00 (18) **Infrared Proteomics – New Tool In Protein Structure Analysis**; Christian P Schultz, Bokkyoo Jun, *BRUKER Optics Inc*

5:00 (19) **Analytical Method Development for the Determination of Compacted DNA and Protamine Sulphate Encapsulated in Polylactide and Polylactide-co-glycolide Microparticles**; Joanna C. Jones, Mairead Dunne, Sally Cudmore, Paul Harkin, *Elan Drug Delivery*

5:00 (20) **Considerations on Metal Ion Doped Glasses as Fluorescent Standard Reference Materials**; Paul C. DeRose, Douglas H Blackburn, Gary W Kramer; *National Institute of Standards and Technology*

5:00 (21) **Raman and IR Spectroscopy for the Examination of Polymer Laminates**; Amanda L. Jenkins, Richard A Larsen, *Jasco Inc*

5:00 (22) **DeterminatioN OF No2 Using A Miniaturised Differential Optical Absorption Spectroscopy System**; J. Alberto Morales, James E. Walsh, Jack Treacy, Wendy E. Garland; *Facility for Optical Characterisation and Spectros*

5:00 (23) **Comparing Near IR and mid-IR Reflectance FT-IR Imaging**; Richard Spragg, Robert Hoult, Jerry Sellors; *PerkinElmer Instruments, England*

5:00 (24) **A Multiresolution Approach to Spectrum Imaging**; Michael R. Keenan, Paul G Kotula, *Sandia National Laboratories*

5:00 (25) **Peptide Fluorescent Chemosensors for Divalent Copper**; Roger M. Leblanc, Yujun Zheng; *University of Miami, Chemistry Department*

5:00 (26) **Analysis of Time Resolved 13CO2/12CO2 Ratios by Infrared Spectroscopy for Medical Diagnostics and Cell Culture Metabolic Studies**; Ronald H. Micheels, Patricia I. Stack, Laura K. Toth, David R. Cave, Jonathan D. Kaunitz, Ryo Ohashi, Jean-Francois P. Hamel; *Polestar Technologies, Inc.,St. Elizabeth's Medical Center, Boston MA, West Los Angeles VAMC and Univ. of California, Los Angeles, School of Medicine, Massachusetts Institute of Technology, Dept. of Chemical Engineering*

5:00 (27) **Precision and Reproducibility of Semi-Automated Sample Deposition for FT-IR/ATR Analyses**; Jessica L. Jarman, Shelly I. Seerley, James A. de Haseth, *University of Georgia*

5:00 (28) **The Bounce in Major League Baseballs: FTIR Tells the Story!**; Chris W. Brown, Scott W. Huffman, Kara Lukasiewicz, Edita Botonjic, *University of Rhode Island*

5:00 (29) **Reducing Pixel-to-Pixel Variations in Backgrounds of Infrared Spectral Images**; Chris W. Brown, Scott W Huffman; *University of Rhode Island,, National Institutes of Health*

5:00 (30) **Microsample Analysis Using Evanescent-Wave Sensors Based on Ge Waveguides**; Mark S. Braiman, Jitraporn Vongsvivut, Mark S Braiman; *Syracuse University, Syracuse NY, Chulalongkorn University, Bangkok Thailand*

5:00 (31) **Characterization of Bone Utilizing Contrast Enhanced Microscopy and Infrared Imaging**; Thomas J. Tague Jr., Lisa Miller; *Bruker Optics, Brookhaven National Laboratory*

5:00 (32) **Determination of Total Arsenic In Urine by DRC-ICP-MS: Matrix Effect Issues, Calibration Strategies and the Use Of Reference Materials.**; Patrick J. Parsons, Christopher D. Palmer, *Wadsworth Center, New York State Department of Health*

5:00 (33) **Identification of "Wrong" Active Ingredients in Counterfeit Drug Products using Accurate Mass Mass Spectrometric Techniques and IR Spectroscopy**; Jean-Claude Wolff, Ian R. Lynch, *GlaxoSmithKline*

Monday Morning, Room 552B
ELEMENTAL MS
Presider: Fred King, University of West Virginia

8:50 (34) **Extending Atomization and Ionization Regimes in Pulsed Glow Discharge Mass Spectrometry**; Willard W. Harrison, Joshua J. Coon, Eric S. Oxley, Kevin P Turney, Jorge Pisonero, Elizabeth A. Pierz, *University of Florida, University of Oviedo*

9:30 (35) **Recent Advances in Geochemical Applications of SIMS Techniques**; Nobumichi Shimizu, *WHOI*

10:10 **Coffee Break**

10:40 (38) **Electrospray Mass Spectrometry for Elemental Speciation**; Gary Horlick, Russell Handy, *University of Alberta*

11:20 (39) **Is There Any Research Left in ICP-MS?**; R. S. Houk

Monday Morning, Room 556B
INFRARED IMAGING I: COBLENTZ SOCIETY SPONSORED
Presider: Linda H. Kidder, Spectral Dimensions

8:50 (40) **Using Infrared and Raman Imaging for Improved Materials Design**; Neil Everall, Mike Schaeberle, Ira Levin, Neil Lewis, Linda Kidder, John Chalmers; *ICI PLC, National Institutes of Health, Spectral Dimensions Inc, Nottingham University*

9:10 (41) **Near-Infrared Imaging: Piecing Together the Jigsaw Puzzle**; Fiona C Clarke, Stephen V Hammond; P*fizer GMS*

9:30 (42) **Assessing the Quality of Pharmaceutical Tablets by Near-Infrared Imaging**; Robbe C. Lyon, Everett H. Jefferson, Eunah Lee, E. Neil Lewis, David S. Lester, Ajaz S. Hussain; *Food and Drug Administration, Spectral Dimensions, Inc., Pharmacia Corporation*

9:50 (43) **"Real-Time" Measurements of Dichroic Ratios on Oriented Polymer Films Using a Multibeam Panar Array IR (PAIR) Spectrograph**; John F. Rabolt, Douglas Elmore, Bruce Chase, Mei-Wei Tsao; *University of Delaware, Cargill, DuPont,, Materials Research Services*

10:10 **Coffee Break**

10:40 (44) **Principal Components Analysis in FT-IR Imaging - a Two-Edged Sword**; Richard A. Spragg, Robert A Hoult; *PerkinElmer Ltd, Seer Green, England*

11:00 (45) **Infrared Spectrochemical Imaging: Faster, Simpler, and Better**; Norman A. Wright, John A. Seelenbinder, Donna M Andrauskas

11:20 (46) **Infrared Imaging for Kidney Pathology**; Andre' J. Sommer, Jessica L. Dellomo, Louis G. Tisinger, Andy P. Evan, James C. Williams, Sharon Bledsoe; *Department of Chemistry and Biochemistry, Miami University, Department of Anatomy, Indiana University School of Medicine*

Monday Morning, Room 551B
FROM GENOMICS TO PROTEOMICS: FRONTIERS IN BIOLOGICAL MS
Presider: Kermit Murray, Louisian State University

8:50 (47) **Proteomics: New Applications for Characterizing and Quantifying Proteins**; Steven P. Gygi, Junmin Peng, Scott A Gerber, Larry J Licklider; *Harvard Medical School, Taplin Biological Mass Spectrometry Facility*

9:30 (48) **Mass Spectrometry-Based Proteomics: Toward Processing Intact Proteins as Tryptic Peptides are Today**; Kelleher L. Kelleher, Steven M. Patrie, Fanyu Meng, Jeffrey Johnson, Benjamin J. Cargile, Leah M. Miller, Andrew J. Forbes; *Univ. of IllinoiS*

10:10 **Coffee Break**

10:40 (49) **Ion Mobility-Mass Spectrometry: Challenges and Design Considerations for Future Instrumentation**; David H. Russell, Brandon T. Ruotolo, Kent J. Gillig, Holly A. Sawyer, Earle G. Stone, John A. McLean; *Texas A&M UnversitY*

11:20 (50) **Functional Aspects of Proteomics: Protein-Protein, Protein-Peptide and Protein-Neurotransmitters interactions**; Amina S. Woods, *NIDA IRP, NIH*

Monday Morning, Room 554B
SINGLE MOLECULE DETECTION IN BIOLOGICAL SYSTEMS I
Presider: Alan Van Orden, University of Colorado

8:50 (51) **Studies of Labeling and Transport in Sol-Gel Materials using Single-Molecule Fluorescence Spectroscopy**; Joel M. Harris, David C. Hanley, Karla McCain, Peter Schluesche; *University of Utah*

9:30 (52) **Single-Molecule Study of Efflux Pump Machinery of Single Living Bacteria Cells**; X. Nancy Xu, Jun Chen, Sophia Kyriacou, Qian Wan, William Brownlow

9:50 (53) **Watching Multi-Conformations of a Single Ion Channel in Action**; H. Peter Lu, *Pacific Northwest National Laboratory*

10:10 **Coffee Break**

10:40 (54) **Nanoscale Environments in Sol-Gel-Derived Silicates and Organic Polymer Thin Films**; Daniel A. Higgins, Maryanne M Collinson, *Kansas State University*

11:20 (55) **Size Correlated Nanoparticle Spectroscopy and Imaging: Application to Rare-Earth Ion Luminescence in Doped Nanocrystals**; Michael D Barnes, Adosh Mehta, Thomas Thundat, Ramesh Bhargava, Andy Bartko, Lynn Peyser, Rob Dickson

11:40 (56) **Single-Molecule Enzymology Using Surface-Enhanced Raman Scattering**; Steven R Emory, Teresa Wenda; W*estern Washington University*

Monday Morning, Room 554A
VIBRATIONAL SPECTROSCOPY: PHARMACEUTICALS
Presider: Dave Schiering, SensIR Technologies

8:50 (57) **Applications and Benchmarks for IR and Raman Spectroscopy in the Pharmaceutical Industry**; Richard W. Duerst, Stan Agre, Rodger; *Abbott Laboratories*
9:30 (58) **A Comparison of Infrared and Raman Analysis of Polymorphs in the Lab and in the Reactor**; James W Rydzak, Teresa Head, Dawn Cohen, Gary Zuber; *GlaxoSmithKline*
10:10 **Coffee Break**
10:40 (59) **From Routine to Close to the Cutting Edge: The varied Applications of Vibrational Spectroscopy in the Pharmaceutical Industry.**; Don A. Clark, *Pfizer Global Research and Development*
11:20 (60) **Microscopy and IR Spectroscopy: Synergies in Pharmaceutical**; John A Reffner; *SensIR Technologies*

Monday Morning, Room 557
FRONTIERS FOR RAMAN SPECTROSCOPY
Presider: Mike Pelletier, Kaiser Optical

8:50 (61) **Two-Dimensional (2D) Correlation Analysis and Chemometrics in Vibrational Spectroscopy**; Isao Noda; *The Procter and Gamble Company*
9:30 (62) **Femtosecond Coherent Raman Spectroscopy**; Wolfgang Kiefer, (Institution 1), Michael Schmitt (Institution 1), Torsten Siebert (Institution 1), Mario Heid (Institution 1), Arnulf Materny (Institution 2), Alexander S. Grabtchikov (Institution 3), Valentin A. Orlovich (Institution 3) *(1)Institut für Physikalische Chemie, Universität Wür; (2)International University Bremen, School of Engineering and Science, Campus Ring 1, D-28759 Bremen, Germany, (3)B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Minsk, Belarus*
10:10 **Coffee Break**
10:40 (63) **Coherent Anti-Stokes Raman Scattering Microscopy**; Ji-xin Cheng, Eric O. Potma, Xiaolin Nan, Andreas Volkmer, Lewis D. Book, Sunney X. Xie; *Department of Chemistry and Chemical Biology, Harvard*
11:20 (64) **Laser Raman Spectroscopy of Single Optically Trapped Particles and Biological Cells**; Juergen Popp, Ralph Gessner, Petra Rösch, Michael Schmitt, Wolfgang Kiefer; *Institut für Physikalische Chemie, FSU Jena, Helmh,, Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany*
11:40 (65) **Vibrational Microprobe Integrating Raman and FTIR Technologies**; Fran Adar, Andrew Whitley, Bernard Roussel, Sophie Morel, John Reffner; *Jobin Yvon, Inc., Jobin Yvon, SA, SensIR*

Monday Morning, Room 556A
FLUORESCENCE SPECTROSCOPY
Presider: John Wright, University of Wisconsin

8:50 (66) **A Fluorescence Detection System for Gas-Phase Ions Trapped in a Fourier Transform Mass Spectrometer**; Jill R. Scott, Paul L. Tremblay, Jason E. Ham, Bill Durham; *Idaho National Engineering and Environmental Labor University of Arkansas*
9:10 (67) **Molecular Fluorescence Spectroscopy: Identification of Plants from Extract Solutions**; Gary D. Rayson, Timothy L. Danielson, Dean M. Anderson, Rick Estell, Eric L. Fredrickson, Kris M. Havstad; *New Mexico State University United State Department of Agriculture*
9:30 (68) **Fluorescence Probe Study of Bicelle Structure and Aggregation**; Brad A. Rowe, Sharon L Neal; *University of Delware*
9:50 (69) **Fast And Slow Proton Transfer Processes in 3-hydroxyflavone Derivatives, Studied in a 10 K Shpol'skii Matrix**; Freek Ariese, Arjen N. Bader, Cees Gooije; *Vrije Universiteit Amsterdam, Department of Analyt*
10:10 **Coffee Break**
10:40 (70) **Novel Methods and Instrumentation for the Analysis of Polycyclic Aromatic Hydrocarbons in Low Temperature Matrices**; Andres D.Campiglia, Adam J Bystol, Andres D Campiglia; *North Dakota State Universit*
11:00 (71) **Solid-Liquid Extraction Time-Resolved Fluorescence Line Narrowing for the Analysis of Polycylic Aromatic Hydrocarbons in Water Samples**; Andres D. Campiglia, Adam J Bystol, *Department of Chemistry North Dakota State University*
11:20 (72) **Deep UV Laser Induced Native Fluorescence Detector for Organic Detection and Classification**; William F. Hug, Ray D. Reid, Michael C. Storrie-Lombardi; *Photon Systems, NASA/JPL*

Monday Morning, Room 555A
OPTICAL SENSORS AND PROBES
Presider: David Walt, Tufts University

8:50 (73) **Chemistry of Si Nanocrystals and Photonic Crystals: Applications in Sensors and Medicine**; Michael J. Sailor; *University of California, San Diego*
9:30 (74) **Amplifying Polymers For Ultrasensitive Sensors**; Timothy M. Swager, *Massachusetts Institute of Technology*
10:10 **Coffee Break**
10:40 (75) **Nano-Pebble Sensors Inside Live Cells**; Raoul Kopelman, *University of Michigan*
11:20 (76) **Optical Microsensor Arrays**; David R. Walt, *Tufts University*

Monday Morning, Ballroom B
LESTER STROCK AWARD
Presider: James Rydzak, GlaxoSmithKline

8:50 (77) **Flow-Injection and Sequential-Injection Methods to Identify, Correct, and Overcome Interelement Matrix Effects in ICP Time-of-Flight Mass Spectrometry**; Gary M Hieftje, Denise M. McClenathan; *Department of Chemistry, Indiana University*
9:30 (78) **Sample Introduction: new devices, new analytes**; Ian D Brindle, Roger L McLaughlin; *Brock University*
10:10 **Coffee Break**
10:40 (79) **Speciation Utilizing HPLC-ICP-MS – What are the Challenges and Opportunities?**; Ruth E Wolf, Kenneth R Neubauer; *PerkinElmer Instruments*
11:20 (80) **Flow Injection Atomic Spectrometry: Finding Fundamental Features**; Julian F Tyson; *University of Massachusetts*

TECHNICAL PROGRAM - MONDAY

Monday Morning, Room 555B
COBLENTZ SOCIETY AWARD
Presider: John W. Hellgeth, SRN, Company

8:50 (81) **Two-Dimensional Infrared Spectroscopy: Revealing Molecular Structure and Dynamics in Solution**; Andrei Tokmakoff; *MIT*
9:30 (82) **RaPTORS: A New Two Dimensional Femtosecond Spectroscopy to Probe the Response of Low Frequency Vibrations in Solution**; David A. Blank; *University of Minnesot*
10:10 **Coffee Break**
10:40 (83) **Three Dimensional IR-Raman Spectroscopy**; Dana D. Dlott; *University of Illinois*
11:20 (84) **Coherent Multiple Dipole Excitation and Reorientation in 2D Spectroscopy**; David M. Jonas; *Department of Chemistry and Biochemistry*

Monday Morning, Room 551A
LEARNING THROUGH COMMUNITY SERVICE
Presider**:** David Schrum, University of Redlands

8:50 (85) **Models for Community-Based Undergraduate Research**; Elaine Hoagland; *Council on Undergraduate Research*
9:10 (86) **Service Learning in an Environmental Chemistry Course**; Mary Kate Donais, Amanda DesRoberts, Sarah Lastella; *Department of Chemistry, Saint Anselm College*
9:30 (87) **The Pine River in Action: Hexavalent Chromium and Student Research**; Melissa M. Strait, Derek M Finkbeiner, Heathere E Gott; *Alma College, Western Michigan University*
9:50 (88) **Service Learning in Analytical Chemistry – The Neighborhood as a Laboratory**; David E. Henderson, Janet F Morrison; *Trinity College*
10:10 **Coffee Break**
10:40 (89) **Service-Learning on the Chippewa River, Isabella County, Michigan**; Claudia B. Douglass; *Central Michigan University*

Monday Morning, Room 553A
CHROMATOGRAPHY METHOD DEVELOPMENT IN THE PHARMACEUTICAL INDUSTRY
Presider: Kenneth Norris, Pfizer, Inc.

8:50 (90) **New Stable Chemically Bonded Carbon Stationary Phases for HPLC and their**; Angelos Kyrlidis, L. Toomey, E. Khmelnitskaia, D. Stoll, C. V. McNeff, P. W. Carr; *Cabot Corporation*
9:10 (91) **Selectivity Optimization in Liquid Chromatography Using Tuned Tandem Column (T3C) Concept**; Yun Mao, Peter W Carr; *Merck & Co*
9:30 (92) **Validating an LC-MS/MS System Under 21 CFR 11**; Kevin Lloyd, *Exygen Research*
9:50 (93) **Development and Validation of Residual Solvent Methods**; Edward Szczesny; *Pfizer, Inc.*
10:10 **Coffee Break**
10:40 (94) **Screening of Column Selectivity for Efficient Method Development**; Uwe D Neue, Jeff R. Mazzeo, Diane M Diehl, Alberto Mendez, E. S. Grumbach, K Tran; *Waters Corporation*
11:20 (95) **Systematic Achiral Method Development Strategies in The Pharmaceutical Industry**; Hugh J Clarke, Kenneth J Norris, John P Larman, Dan Wu-Linhares; *Pfizer, Inc*

Monday Morning, Ballroom E
MICRO- AND NANO- NEBULIZATION
Presider: Akbar Montaser, George Washington University

8:50 (96) **Spray Chambers in ICP Spectrochemistry: from a Filtration Device to an Evaporation Cavity**; Jean M. Mermet, José L Todoli; *University of Alicante, Spain*
9:10 (97) **The Effect of Gas Rarefaction on the Calculated Lifetime of Aerosol Droplets in an Inductively Coupled Plasma**; Akbar Montaser, C. M. Benson, K. Kahen, J. X. Zhong, S. F. Gimelshein, D. A. Levin; *George Washington University Department of Chemistry,, Pennsylvania State University Department of Aerospace Engineering*
9:30 (98) **Sample Introduction for ICP-OES and ICP-MS: Fundamental Understanding and Practical Application**; John W Olesik, *Ohio State University*
9:50 (99) **Direct Injection Nebulization for Analysis of Oil**; Kaveh Kahen, Adelitza Strubinger, Akbar Montaser; *The George Washington University*
10:10 **Coffee Break**
10:40 (100) **Structure and Dynamics in Electrified Nanodroplets of Macromolecular Solutions**; Akos Vertes, Vasiliy Znamenskiy; *The George Washington University*
11:00 (101) **Key Fundamental and Diagnostic Issues in Micro-, Nano-, and Pico-sampling with Laser Ablation ICPMS**; Richard E. Russo, Sam S Mao, Xianglei Mao; *Lawrence Berkeley National Laboratory*
11:20 (102) **Sample Introduction System for Micro- and Nano-Samples by Plasma Spectrometry**; Vassili Karanassios; *Department of Chemistry, University of Waterloo, Waterloo, Ontario,, Canada N2L 3G1*
11:40 (103) **Determination of Phosphorus Concentration in Extremely Small Protein Samples Important in Alzheimer Disease**; J. Sabine Becker; *Research Centre Juelich*

Monday Morning, Room 552A
LASER-BASED ATOMIC METHODS
Presider: Ken Marcus, Clemson

8:50 (104) **Discrimination of Ammunition Fragments by Laser Induced Breakdown Spectroscopy**; Scott R. Goode, Andrea A. Thomas, Alex Nieuwland; *University of South Carolina*
9:10 (105) **Trace Metal Analysis by Use of Resonant Laser Ablation – Phenomenological and Analytical Studies**; Robert G. Michel, Jeremy F. Koscielecki, Peter Stchur, Heather K. Molyneux, *University of Connecticut*
9:30 (106) **Influence of Particle Size created by Laser-Induced on the ICP Response for the Analysis of Metals**; Detlef Günther, Hansruedi Kuhn, Marcel Guillong, Ingo Horn, Christopher Latkoczy; *ETH Zürich*
9:50 (107) **Quantitative Relationship of Analytical Performance to Laser Wavelengths for Several Practical Samples Using Laser Ablation ICPMS**; Lawrence M. Neufeld, Richard E. Russo, Samual Mao; *Wave Research, Lawrence Berkeley Labs*
10:10 **Coffee Break**
10:40 (108) **Application of Laser Ablation to Bulk Analysis of Solids by Simultaneous ICP-OES**; Michelle E Cree, Lawrence M. Neufeld; *Varian, Inc., New Wave Research*

TECHNICAL PROGRAM - MONDAY

11:00 (109) **Coupling of Graphite Furnace Vaporization and Laser-Enhanced Ionization for the Determination of Trace Metals**; Denis Boudreau, Karine Herreyre, Philippe Nobert, Denis Boudreau; *Dept. Chemistry, Laval University*

11:20 (110) **Analytical Spectroscopy – Laser Absorption Cavity Ringdown Spectrometry**; George P. Miller, Shiquan Tao, Fabio J Mazzotti, Jerzy Mierzwa, Chuji Wang, Christopher B Winstead; *Mississippi State UniversitY*

11:40 (111) **Development of a VUV-LIPS system**; Ulrich Panne, Igor Radivojevic, Christoph Haisch, Reinhard Niessner, Helmut Becker-Ross, Stefan Florek; *Technical University Munich, ISAS Berlin*

Monday Morning, Room 550A
ELECTROCHEMISTRY I
Presider: Radha Pyati, University of Colorado

8:50 (112) **Detection of DNA Damage From Enzyme-Generated Toxic Metabolites Using Electrochemical Biosensors**; Jing Yang, James F Rusling; *University of Connecticut*

9:10 (113) **Electrochemical Detection of Trace Metals using a Boron-Doped Diamond Electrode**; Carol M. Babyak, Ronald B. Smart, A. Manivannan; *Department of Chemistry, West Virginia University,,*

9:30 (114) **Measurement of Electronic Transport in Conjugated Organic Oligomers via Nanoarrays of Metal-Organic-Metal Junctions**; Paula E. Colavita, Michael S Doescher, *University of South Carolina*

9:50 (115) **Electrochemically-mediated Metal Binding using Immobilized Biopolymers**; Ashley M. Johnson, James A. Holcombe; *The University of Texas at Austin*

10:10 **Coffee Break**

Monday Morning, Room 553B
MATERIALS AND SURFACE CHARACTERIZATION
Presider: Shane Street, University of Alberta

8:50 (116) **NMR Evidence for Formation of Tetrahedral Al and Repolymerization of the Si Network During Dissolution of Aluminosilicate Glass and Crystal**; Natia Tsomaia, Susan L. Brantley, James P. Hamilton, Carlo G. Pantano, Karl T. Mueller; *Department of Chemistry and Materials Research Ins,, Department of Geosciences and Materials Research Institute, Penn State University, University Park, PA 16802, USA*

9:10 (117) **Forensic Applications of Ion Beam Mixing and Surface Spectroscopy of Latent Fingerprints**; Charles H. Koch, Mathew Agustine, Harris Marcus; *Institute of Materials Science University of Connecticut*

9:30 (118) **Optimization of Ablation Parameters for the Elemental Profiling of Automotive Glass and Paints by LA-ICPMS and LIBS**; Andria L Hobbs, Shirly Montero, Tatiana Trejos, Jose R Almirall, *International Forensic Research Institute and Department of Chemistry at Florida International University*

9:50 (119) **Using Two-Dimensional Correlation Spectroscopy to Investigate the f-f transition of Lanthanide Complexes**; Jinguang Wu, Yizhuang Xu, Ying Zhao, Juan Feng, Dongliang Tao, Jun Yang, Yong Li, Guowei Lu, Weiming Du, Duanfu Xu, Jinguang Wu; *Department of Chemistry, Peking University, Institute of Chemistry, Chinese Academy of Sciences, Department of Physics, Peking University*

10:10 **Coffee Break**

10:40 (120) **Development Andand Optimization of a Laser Carbonized Polyimide Film as a Sensor Substrate**; John M Ingram, Mike White, Augustus W Fountain; *Photonics Research Center, United States Military, Photonics Research Center*

11:00 (121) **Detection of Solid State Reaction Chemistry Using Micro X-Ray Fluorescence Imaging And Raman Spectroscopy**; George J. Havrilla, Michael Beckstead, David Morris; *Los Alamos National Laboratory*

11:20 (122) **Analysis of Microbes, Minerals, and Contaminants Using the Laser-based Optical and Chemical Imager (LOCI)**; Jill R. Scott, Mary E. Kauffman, Timothy R. McJunkin, Paul L. Tremblay; *Idaho National Engineering and Environmental Labor*

Monday Afternoon, Room 551A
MASS SPECTROMETRY I
Presider: Aaron Timperman, University of West Virginia

1:30 (123) **Isolation and Characterization of Copper-Complexing Ligands from Marine Waters**; Richard W. Vachet, Myrasol B Callaway, Catherine A Cogut; *University of Massachusetts-Amherst*

1:50 (124) **Detection and Analysis of Selenoproteins and Selenoamino acids in Selenium Enriched Saccharomyces Cerevisiae Cellular Components**; Katie DeNicola, Claudia A. Ponce de Leon, Jospeh A. Caruso; *University of Cincinnati*

2:10 (125) **Trace Level Cesium Analyses by ICP/MS in Environmental Samples**; Gregory C. Eiden, Charles J. Barinaga, May-Lin P. Thomas, Scott A. Lehn, Orville T. Farmer III

2:30 (126) **Determination of Brominated Acetic Acids in Drinking Water Using Solid Phase Extraction and High-Performance Ion-Exchange Chromatography-Inductively Coupled Plasma Mass Spectrometry**; Qiantao Cai, Zhong-Xian Guo, Chunhai Yu, Zhaoguang Yang; *Centre for Advanced Water Technology*

2:50 **Coffee Break**

3:30 (127) **Determination of Mercury, Lead, Cadmium And Arsenic in Urine by ICP-MS - Internal Standard and Matrix Matching Considerations**; Christopher D. Palmer, Patrick J Parsons; *New York State Department of Health, Wadsworth Cen.*

3:50 (128) **Elemental Quantification of Flame Retardant Polymers Using Glow Discharge Mass Spectrometry**; *John T Millay, *Lei Li, **C. M. Barshick, *F. L. King; **West Virginia University, **GE Plastics*

4:10 (129) **Zn – Peptide Bond Energy Determination for Zinc Finger Motif by ESI-MS**; Fred L. King, Yuchen Lu; *West Virginia University*

Monday Afternoon, Room 556B
INFRARED IMAGING II: COBLENTZ SOCIETY SPONSORED
Presider: Linda H. Kidder, Spectral Dimensions

1:30 (130) **Infrared Arrays and Chemical Analysis: Populations, Particles and Planes**; Neil Lewis, Linda Kidder, Eunah Lee, Ken Haber; *Spectral Dimensions, Inc.*

1:50 (131) **Application of Two New Alternating Least-Squares (ALS) Regression Methods to Spectroscopic Image Analysis**; Thomas M. Hancewicz, Shuliang L. Zhang, Ji-hong Wang, Philip K. Hopke; *Unilever R&D US, 45 River Road, Edgewater, NJ, Dept. of Chemical Engineering, Clarkson University, Potsdam, NY 13699 USA*

2:10 (132) **Industrial Applications of Fluorescence Spectral Imaging**; Susan E. Forest, Jeff T. Grothaus, Keith D. Ertel, Charlie Rader, Janyl Plante; *Procter and Gamble*

2:30 (133) **New Opportunities to be Realized from Time Resolved Imaging Spectroscopy**; Quentin S. Hanley, Vinod Subramaniam, Elaine Sullivan; *University of the West Indies, Department of Biology, Advanced Science and Technology Lab, Astra Zeneca R & D Charnwood*

2:50 **Coffee Break**

3:30 (134) **Heating Up Cancer Diagnostics with Infrared Radiation: Search for Markers**; Rina K. Dukor, Gloria M. Story, E. E. Lower, R. S. Yassin, Beth L. Johnson, Curt A. Marcott; *BioTools, Inc., The Procter & Gamble Company, University of Cincinnati Medical Center Central DuPage Hospital*

3:50 (135) **Infrared Spectroscopic Imaging**; Gloria M Story, Curtis Marcott, Elyse E. Lower, Rawia S. Yassin, Beth L. Johnson, Rina K. Dukor; *The Procter and Gamble Company, University of Cincinnati, Medical Center, Central DuPage Hospital, Vysis, Inc.*

4:10 (136) **Effects of Spectral Resolution on Infrared Imaging Experiments and Data Analysis**; Sharon P. Markel, Willem Windig; *Eastman Kodak Company*

4:30 (137) **MCR Analysis of Infrared Hyperspectral Data: An Image of Substance**; Christine M. Wehlburg, Mike Keenan, Mark van Benthem, David M Haaland; *Sandia National Laboratories*

Monday Afternoon, Room 554B
ANALYTICAL CHEMISTRY IN BIOLOGICAL MICROENVIRONMENTS
Presider: Julie Stenken, Rensselaer Polytechnic Institute

1:30 (138) **Conformation and Dynamics of Membrane Peptides and Proteins by Solid-State NMR**; Mei Hong, Daniel Huster, Satoru Yamaguchi, Xiaolan Yao; *Iowa State University*

1:50 (139) **Monitoring D-Serine Dynamics In Vivo Using Online Microdialysis – Capillary Electrophoresis**; Michael T. Bowser, Kylie B. O'Brien, Christina T. Klug; *University of Minnesota, Department of Chemistry*

2:10 (140) **An Electrochemical BioMEMS Platform for Acute Cellular Transport Studies, and a Microscopic Optical Sensor for In Vivo Clinical Monitoring**; Koji Tohda***** , Makoto Yoshida , Jian Yang , Miklos Gratz; *Dept. of Biomedical Engineering, CWRU, Cleveland*

2:50 **Coffee Break**

3:30 (141) **Tissue Spectroscopy and Imaging for Cancer Diagnosis**; Lei Geng, Ed Crowell, Piyanka Desilva; *University of Iowa*

3:50 (142) **Monitoring Macrophage Chemical Signaling During Inflammation with Microdialysis Sampling Techniques**; Julie A. Stenken, Li Sun, Rui Chen; *Rensselaer Polytechnic Institute*

4:10 (143) **Studying Endothelial Cell Attachment Using TIRF Microscopy and AFM**; William M. Reichert; *Duke University*

4:50 (144) **Tissue Spectroscopy and Imaging for Cancer Diagnosis**; Lei Geng, Ed Crowell, Piyanka Desilva

Monday Afternoon, Room 554A
NMR ADVANCES IN PHARMACEUTICAL ANALYSIS
Presider: Andreas Kaerner, Eli Lilly and Company

1:30 (145) **Opportunities for NMR in Accelerated Pharmaceutical Research and Development**; David J Detlefsen, Jeffrey L Whitney, Mark E Hail; *Novatia, LLC, Novatia, LLC*

2:10 (146) **Analysis of Ciprofloxacin Transformation Products in Aquatic Ecosystems by LC-NMR and LC-MS/MS**; Cynthia K. Larive, Laurie A. Cardoza, Valentino Almeida, David W. Graham; *University of Kansas*

2:50 **Coffee Break**

3:30 (147) **Structural Elucidation of Pharmaceutical Impurities and Degradants**; Linda L. Lohr, Karen M Alsante, Thomas R Sharp, Dinos O Santafianos, Todd D Hatajik; *Pfizer Inc*

4:10 (148) **Pharmaceutical Applications of Solid State NMR**; Ales Medek, Russell B Poe, Gregory S. Steeno; *Pfizer*

Monday Afternoon, Room 557
RAMAN IMAGING - IDENTIFYING PROBLEMS & VISUALIZING SOLUTIONS
Presiders: Ken Williams and Rick Bormett, Renishaw

1:30 (149) **Raman Imaging from the NIR to the UV: Solutions Appropriate to the Physical and Materials Constraints**; Fran Adar, Michel Leclercq, HanJuergen Reich, Bernard Rousseau, Andrew Whitley; *Jobin Yvon, Inc. Jobin Yvon, SA*

1:50 (150) **Micro-Raman Spectroscopy And Imaging of Single "Live" Red Blood Cells**; Don McNaughton, Bayden R Wood, Larissa Hammer; *Centre for Biospectroscopy and School of Chemistr*

2:30 (151) **Volumetric Raman Microscopy - The Next Dimension in Chemical Imaging**; Patrick J. Treado; *ChemIcon Inc*

2:50 **Coffee Break**

3:30 (152) **Mineralogical Applications of Raman Microprobe Mapping**; Lutz Nasdala, Ingo Reese, *Johannes Gutenberg-University, D-55099 Mainz, Germ, Jobin Yvon GmbH, D-64625 Bensheim, Germany*

3:50 (153) **Understanding Pharmaceutical Formulations Using Chemical Images**; Rachel H. Brody, Donald A. Clark, John C. Mitchell, Martin J. Snowden; *Medway Sciences, University of Greenwich, Pfizer Global Research and Development*

4:10 (153A) **Applications of Spectroscopic Imaging to Polymer Blends;** K. L. A. Chan, S. G. Kazarian; Imperial College, London UK

Monday Afternoon, Room 556A
VIBRATIONAL SPECTROSCOPY
Presider:Mary Jane Schultz, Tufts University

1:30 (154) **Vibrational Dynamics in 2D Electronic Spectra**; David M. Jonas; *Department of Chemistry and Biochemistry*

2:10 (155) **Three Dimensional Vibrational Spectroscopy of Molecular Liquids**; Dana D Dlott, Zhaohui Wang, Andrei Pakoulev; *University of Illinois*

2:50 **Coffee Break**

3:30 (156) **Probing the Aqueous-Air Interface at the Molecular-Level**; Mary Jane Shultz, Steve Baldelli, Cheryl Schnitzer, Danielle Simonelli; *Tufts University University of Houston, Stonehill College,Intel Corp.*

4:10 (157) **Using Phase Relationships in Nonlinear Optics to Determine Orientation of Adsorbates and Solvent Molecules at the Electrochemical Interface**; Steven Baldelli, Yuen-ron Shen, Phillip N. Ross, Gabor A. Somorjai; *University of Houston, University of California, Berkeley, Lawrence Berkeley National Laboratory*

Monday Afternoon, Room 553A
SPECTROSCOPY ON A BUDGET
Presider: Kimberley Schrum, Whittier College

1:30 (158) **Introducing Spectrophotometry in Grades 6-12 Using a College-based Spectrophotometer Loan Program**; Jill N. Granger; *Sweet Briar College*

1:50 (159) **Applications of Absorption Spectroelectrochemistry in Artificial Blood Research**; Scott C. Dorman; *Birmingham-Southern*

2:10 (160) **Integration of Spectroscopy Throughout the General Chemistry Curriculum**; Jeffrey E. Anderson, Terry W McCreary; *Murray State University*

2:30 (161) **An Inexpensive Laser/CCD Raman Spectrometer**; Carl Salter, Mandy Hennip, Julie M. Jones, Benjamin A. DeGraff, Stephanie A. Schaertel; *Department of Chemistry, James Madison University; Department of Chemistry, Grand Valley State University, Allendale, MI 49401; Department of Chemistry, Moravian College, Bethlehem, PA 18018*

2:50 **Coffee Break**

3:30 (162) **The History of Improving Automobile Emissions: A Laboratory Investigation for Freshman Chemistry Students**; Jane A Ganske; *Pepperdine University*

3:50 (163) **Educational Multiwavelength Flame Atomic Emission Spectrometer**; Alexander Y. Nazarenko; *SUNY, College at Buffalo*

4:10 (164) **Educational Grant Program for Fiber Optic Spectroscopy Systems**; Robert S. Kearton, *Ocean Optics*

Monday Afternoon, Room 551B
PROTEOMICS: SEPARATION BASED APPROACHES
Presider**:** Greg Opiteck, Bristol-Myers Squibb Co.

1:30 (165) **Biomarker Discovery in Plasma and Urine**; Gregory J. Opiteck, James X Pang; *Bristol-Myers Squibb Company*

2:10 (166) **Enrichment of Minor Plasma Components for Biomarker Discovery**; Tom G. Holt, Rose Flick, Elizabeth Birzin, Wanda Chan, Susan Rohrer, John Cummings, John Mehl, Ellen Rohde, Pat Griffin; *Merck & Company*

2:50 **Coffee Break**

3:30 (167) **An LC-MS Approach for Determining Protein and Low-Molecular-Weight Disease Markers**; Chris Becker, Thomas Shaler, Hua Lin, Weixun Wang, Sushmita Roy, Hiahong Zhou; *SurroMed, Inc*

4:10 (168) **Applied Systems Biology: Proteomic Analysis**; Clary B. Clish, Gary Lavine, Jane Nagel, Stephen Naylor; *Beyond Genomics, Inc.*

5:00 (169) **Mass Spectrometry: A Direct Route to Diagnostic Marker Discovery in Disease**; Brad C. Guild, *Millennium Pharmaceuticals*

Monday Afternoon, Room 555A
SEPARATIONS FOR DRUG DEVELOPMENT AND ANALYSIS
Presider: Mark Rose, Merck Research Laboratories

1:30 (170) **Adding Potential to Chromatography-Electrochromatography in Drug Development**; John Stobaugh; *The University of Kansas*

2:10 (171) **Interfacing Liquid Chromatography and Fourier-Transform Infrared Spectroscopy: Deposition Effects and Quantitative Analysis in Polymer Analysis**; Sander J. Kok; *TNO Voeding*

2:50 **Coffee Break**

3:30 (172) **HPLC coupled with CLND and TOF-MS for the On-Line Determination of Relative UV Response Factors.**; Peter D. Angus, Patrick H Lukulay, Matthew Lorenz, David Rossi, *Pfizer Global Research and Development*

4:10 (173) **The Potential of Microchip Separations in Drug Development and Analysis**; Charles S. Henry, Joseph C Fanguy, Yali Jia; *Mississippi State University*

Monday Afternoon, Room 552B
MATRIX EFFECTS IN ICP-AES AND MS
Presider: John-Michael Mermet, University of Lyon-CNRS

1:30 (174) **Mitigation of the Non Spectroscopic Interferences in ICP-AES by Simplifying the Sample Introduction System**; José L. Todolí, Jean M. Mermet; *University of Alicante, University Claude Bernard*

2:10 (175) **Influence of the Analyte Concentration on Matrix Effects in ICP-AES**; Jean M Mermet, Monica Iglesias, Emmanuelle Poussel; *University of Lyon-CNRS*

2:30 (176) **Diagnosis and Correction of Matrix Effects in Inductively Coupled Plasma Mass Spectrometry**; Eric D. Salin, Margaret Antler, Paul Abbyad, John Tromp, Hai Ying, *McGill University*

2:50 **Coffee Break**

3:30 (177) **High-Powered Diagnostic Tools to Characterize and Alleviate Matrix Interferences in ICP Spectrometry**; Gary M Hieftje, Gerardo Gamez, Mao Huang, Scott A Lehn; *Department of Chemistry, Indiana University,Chinese Academy of Sciences, Beijing, China, Pacific Northwest National Lab, Richland, WA 99352*

4:10 (178) **Understanding and Controlling Matrix Effects in ICP-OES and ICP-MS**; John W. Olesik, Savelas Rabb; *The Ohio State University*

Monday Afternoon, Room 552A
ATOMIC SPECTROSCOPY IN THE NATIONAL LABS
Presider: Paul Cable, SRS

1:30 (179) **Characterization of Actinide Removal Mechanisms for High-Level Waste Treatment: Application of X-ray Absorption Fine Structure (XAFS) Spectroscopic Techniques**; Martine C Duff (1), Douglas B. Hunter (1), David T. Hobbs (1), Mark J. Barnes (1), Samuel D. Fink (1), Zurong Dai (2), John P. Bradley (2), N. Dietz (3), Jeffrey Fortner (3); *Westinghouse Savannah River Co., Sav. River Techno, Livermore National Laboratory, Livermore, CA 94551, Argonne National Laboratory, Argonne, IL 60439*

2:10 (180) **Selective Attenuation of Isobaric Interferences in Quadrupole Ion Trap Mass Spectrometry**; Douglas C. Duckworth, Glen P Jackson, Fred L King; *Dept. of Chemistry, West Virginia University, Morg, Chemical Sciences Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-2008*

2:50 **Coffee Break**

3:30 (181) **Laser Ablation ICPMS: Chemical Analysis Applications at Berkeley and other National Labs**; Rick Russo, Richard E Russo, Jhanis Gonzalez, Xianglei Mao, Sam S. Mao; *Lawrence Berkeley National Laboratory, Universidad Central de Venezuela, Facultad de Ciencias, Escuela de Química*

4:10 (182) **VISION: A Vibrational Spectrometer for the Spallation Neutron Source**; John Z. Larese; *University of Tennessee, Oak Ridge National Lab*

Monday Afternoon, Room 553B
INTERFACIAL ELECTROCHEMISTRY AND SPECTROELECTROCHEMISTRY
Presider: Roger Terrill, San Jose State University

1:30 (183) **Spectroscopy with Surface Plasmons**; Roger H. Terrill, Mondona Zangeneh, Nga Doan; *San Jose State University*

1:50 (184) **Spectroelectrochemical Sensing Based on Multimode Selectivity**; John N. Richardson; *Shippensburg University*

2:10 (185) **Nanoparticle Assemblies and Nanoscale Electron Transfer**; Shaowei Chen, Renjun Pei, Yiyun Yang, Fengjun Deng; *Southern Illinois University, Carbondale*

2:50 **Coffee Break**

2:30 (186) **Spectroelectrochemical Characterization of Charge Storage at Thin Films of Nanostructured Mesoporous Oxides**; Jeffrey W. Long, Winny Dong, Amanda L. Young, Lala R. Qadir, Debra R. Rolison; *Naval Research Laboratory*

3:30 (187) **SERS-Based Spectroeletrochemical Investigation of Functionalized Ag Electrode Surfaces: Probing and Controlling Interfacial Structure and Reactivity with Applied Potential**; Joel M. Harris, Vanessa B. Oklejas, Rory H. Uibel, Joel M. Harris; *University of Utah*

4:10 (188) **Active Control of Surface Transport with Electrochemically Generated Chemical Potential Gradients**; Paul W. Bohn, Susan T. Plummer, Brian D. Coleman, Karin M. Balss; *University of Illinois at Urbana-Champaign*

Monday Afternoon, Room 550A
BIOMEDICAL SURFACE SCIENCES AND BIOLOGICAL INTERFACES
Presider: Dave Castner, University of Washington

1:30 (189) **Chemical Characterization and Imaging Using Surface Analysis: Tools for Evaluating Biomaterials and Drug Delivery Systems**; Anna M. Belu; *Medtronic, Inc*

2:10 (190) **Nanometer Scale Characterization of the Physical Properties of Biomolecular Systems: Measurement and Applications**; Gil U Lee

2:50 **Coffee Break**

3:30 (191) **Interrogating the Structure and Composition of Adsorbed Protein Films with XPS and ToF-SIMS**; David G. Castner; *University of Washington*

4:10 (192) **Nonlinear Optical Null Ellipsometry of Biological Interfaces**; Garth J. Simpson, Ryan M. Plocinik, Robert M. Everly; *Purdue University*

4:30 (193) **Measuring the Chirality of Surface Confined Proteins and DNA by Second Harmonic Generation Circular Dichroism Spectroscopy**; John C. Conboy; *University of Utah*

Tuesday Morning, Room 551A
MASS SPECTROMETRY II
Presider: Aaron Timperman, University of West Virginia

8:50 (194) **Internal Energy of Ions Generated by Matrix-assisted Laser Desorption Ionization**; Akos Vertes, Guanghong Luo, Ioan Marginean, Akos Vertes; *Department of Chemistry, George Washington University*

9:10 (195) **Improvements in Quantitative Analysis in Glow Discharge Mass Spectrometry with a Time-of-Flight Mass Analyzer**; Gary M Hieftje, Denise M McClenathan; *Indiana University, Department of Chemistry*

9:30 (196) **Precise Uranium Isotope Ratio Measurements by ICP-QMS**; Gregory C. Eiden, Scott A. Lehn, Orville T. Farmer III, Charles J. Barinaga; *Pacific Northwest National Laboratory*

9:50 (197) **Investigation of Ion Transport in a Reaction Cell ICP-MS**; John W. Olesik, Deanna Jones; *The Ohio State University, The Ohio State University*

10:10 **Coffee Break**

10:40 (198) **Design Considerations for a Dual-Reflectron Time-of-Flight Mass Spectrometer**; Gary M Hieftje, William C Wetzel, David P Myers, Andrew M Leach; *Department of Chemistry, Indiana University, Bloomington, IN 47405,, LECO Corporation, St. Joseph, MI 49085, Department of Chemistry, Stanford University, Stanford, CA 94305,, Department of Chemistry*

11:00 (199) **Correcting ICP-MS Isotope Ratio Measurements for Mass-Discrimination Effects: An Art In Its Own**; Christophe R. Quétel, Ivan Tresl; *EC - Joint Research Center - Institute for Reference*

11:20 (200) **Pseudo-Steady State Signals for the Determination of Trace Elements in Bullets by Flow Injection Inductively Coupled Plasma Mass Spectrometry**; Julian F. Tyson, Emily R. Yourd, Robert D. Koons; *University of Massachusetts*

11:40 (201) **Analytical Performance of a Glow Discharge Ionization Source Mattauch-Herzog Geometry Mass Spectrograph with Focal Plane Camera Detection**; Gary M. Hieftje, James H. Barnes, IV, Roger P. Sperline, M. Bonner Denton, David W. Koppenaal, Charles J. Barinaga; *Department of Chemistry, Bloomington, IN 4740,, Department of Chemistry, University of Arizona, Tuscon, AZ 85721, Pacific Northwest National Lab, Richland, WA 99352*

Tuesday Morning, Room 556A
CHEMISTRY AND THE BIOMEDICAL SCIENCES: THE ANALYTICAL INTERFACE
Presiders**:** Dana Spense, St. Louis University and Douglas Gilman, University of Tennessee

8:50 (202) **Capillary Electrophoretic Enzyme Inhibition Assays**; Doug Gilman, Angela R. Whisnant, Courtney Neel, Kristie Carter; *University of Tennessee, Department of Chemistry*

TECHNICAL PROGRAM - TUESDAY

9:10 (203) **Photonic Nano-Explorers: From Subcellular Chemical Imaging to Cancer Detection and Therapy**; Raoul Kopelman, *University of Michigan*

9:30 (204) **Analysis of Gene Expression in Single Breast Cancer Cells**; Sheri J. Lillard, Jennifer L. Zabzdyr, Sandra Villa, Amisha Shah; *University of California, Riverside*

9:50 (205) **Studies Toward a Fully Integrated Separation-Based Sensor for Monitoring Biological Systems Using Microchip Capillary Electrophoresis**; R. Scott Martin, Susan M. Lunte, Bryan H. Huynh; *University of Iowa, University of Kansas*

10:10 **Coffee Break**

10:40 (206) **Chemical Analysis in Optically Challenging Biological Samples by Using Multi-Photon Excited Fluorescence**; Frank V. Bright, Eric J. Bukowski; *University at Buffalo, The State University of New York*

11:00 (207) **Development of Circulatory Vessel Mimics from Microbore Tubing Reveal Important Information about Hypertension**; Dana M Spence; *Saint Louis University*

11:20 (208) **In Vivo Voltammetry as a Tool for Probing Neurochemical Mechanisms in the Unanesthetized Rat**; Adrian C. Michael, Amina S Khan; *University of Pittsburgh, Department of Chemistry*

11:40 (209) **Noninvasive Analysis of Blood Hematocrit on Human Subjects Using VIS-NIR Spectroscopy and Multivariate Regression**; Patrick O. Idwasi**;** ***University of Massachusetts Medical School***

Tuesday Morning, Room 555A
CHIRAL ANALYSIS I
Presider: Kenneth Busch, Baylor Univeristy

8:50 (210) **Chiral and LC/MS Analysis of Ketoprofen in Plasma from the Asian Elephants (Elephas maximus)**; Robert P. Hunter, David E Koch, Ramiro Isaza; *Department of Anatomy & Physiology, Kansas State University, Department of Clinical Sciences*

9:30 (211) **Chiral Columns or Chiral Detectors? A Question of Importance in HPLC Chiral Methods Development**; Rekha D. Shah, Rekha D Shah; *Johnson & Johnson Pharmaceutical Research & Development*

10:10 **Coffee Break**

10:40 (212) **SFC in Chiral Analysis Using Polysaccharide Columns**; Rodger W Stringham; *Chiral Technologies, Inc*

11:20 (213) **Building a Toolbox for the Determination of Absolute Stereochemistry of Small Molecules in Drug Discovery**; Oliver J. McConnell, Alvin Bach, Vasilios Marathias, Brian Marquez, Donald Herold, Kristi Fan, Douglas Ho, Laurence Nafie, Rina Dukor, Teresa Freedman; *Wyeth Research,, Princeton University, BioTools* & Syracuse University

Tuesday Morning, Room 554A
PHARMACEUTICALS I
Presider: Ed Gump, Boehringer-Ingelheim

8:50 (214) **Time-Resolved NIR/VIS Spectroscopy for Analysis of Solid Pharmaceuticals**; Jonas Johansson, Staffan Folestad, Mats Josefson, Christoffer Abrahamsson, Stefan Andersson-Engels, Sune Svanberg; *AstraZeneca R&D Molndal, Lund Institute of Technology*

9:10 (215) **Development of a Monte Carlo application for investigation of light transport through pharmaceutical tablets**; Jonas Johansson, Christoffer Abrahamsson, Stefan Andersson-Engels, Sune Svanberg, Staffan Folestad, Mats Josefson; *Lund Institute of Technology, AstraZeneca R&D Molndal*

9:30 (216) **Metabonomics: LC/MS Combined with Principle Component Analysis Showes Promise for the Screening of Rat Urine in Drug Development**; Robert S. Plumb, Chris L. Stumpf, Marc V. Gorenstein, Jose Castro-Perez, John N. Haselden; *Waters Corporation, Milford, MA, Micromass LTD, Manchester, UK, GlaxoSmithKline, Ware, Herts, UK*

9:50 (217) **Breaking Through the Barriers with Automation Methods Development**; Michael D. Jones, Michael E. Swartz, Tom Jupille, Lloyd R. Snyder, John W. Dolan, Richard Lee-Berman, Michael D. Jones; *Waters Corporatio, LC Resources*

10:10 **Coffee Break**

10:40 (218) **Determination Of Solid - State forms Of Ephedrine in Mixtures Using Infrared Spectroscopy**; Thomas M. Niemczyk, Yanga K Dijiba, Anding Zhang; *The University of New Mexico*

11:00 (219) **Proving Reference Material Traceability- An Essential Link in the Validation Chain**; Stuart R. Huckins, Martin J. Long, Thomas Sauter, Brian Davies; *PerkinElmer Instruments Ltd*

11:20 (220) **Solid State Analysis of Multicomponent Pharmaceutical Powders by Red-Excitation, Dispersive Raman Spectroscopy**; Reinhard Vehring; *Inhale Therapeutic Systems, Inc*

11:40 (221) **Determining Particle Size Distribution of Active Ingredients In Pharmaceutical Formulations Using Raman Chemical Imaging Analysis**; Matthew P. Nelson, Julianne Ware, Patrick J. Treado; *ChemIcon, Inc*

Tuesday Morning, Room 550A
ENVIRONMENTAL
Presider: Mark Hayes, Arizona State University

8:50 (222) **The Development of a Down-well TCE Sensor for Long-Term Monitoring Applications**; Scott McWhorter, Kimberly R. Powell, Kristine L. Eland, Steven M. Serkiz; *Westinghouse Savannah River Company, Analytical De, Westinghouse Savannah River Company, Waste Processing Technology, SRTC, Building 773A*

9:10 (223) **MicroVessels™: A New Approach to Closed Vessel Microwave Dissolution of Small Samples**; Leslie H. Rhodes; *CEM Corporation*

9:30 (224) **Microwave Digestion of Large Samples: Open and Closed Vessel**; David Barclay; *CEM Corporation*

9:50 (225) **Development of 21 CFR Part 11 Compliant Software for Atomic Spectrometry**; Doug Shrader, Michelle Cree, John Sanders, Eric Vanclay, Filippa Minnelli, Xue Dong Wang; *Varian, Inc., Varian Australia Pty Ltd*

10:10 **Coffee Break**

10:40 (226) **A High-throughput Microwave Digestion System for Ultra-Trace Element Analysis in Micro-Quantitative biological Samples**; Zheng Yang, Bradley T. Jones; *Wake Forest University*

11:00 (227) **Direct Analysis of Calixarene-based Solvent by ICP-MS and ICP-ES during Decontamination of Radioactive Waste**; Frank M. Pennebaker, David P. Diprete, L. C. Johnson, Mira A. Malek, Art R. Jurgensen; *Westinghouse Savannah River Company*

11:20 (228) **The Use of Laser Ablation ICP-MS and Collision Cell Technology for the Analysis of Metal-Containing Particulate Matter**; Marc M Lamoureux, Nicholas Warner, Jonathan Enright

Tuesday Morning, Room 557
RAMAN SPECTROSCOPY IN PHARMACEUTICAL RESEARCH AND DEVELOPMENT
Presider: Forrest Wessner, Thermo Nicolet

8:50 (229) **Drug Product Investigations Utilizing Raman Spectroscopy**; David E. Bugay, Pamela A. Martoglio-Smith, Ruth L. Te, Melissa A. Houghtaling; *SSCI, Inc.*

9:30 (231) **Raman Analysis of Structure Activity Relationships (SAR) in Molecular Binding**; Don E. Pivonka; *AstraZeneca*

10:10 **Coffee Break**

10:40 (230) **Quantitation of Phase Separation in Biopolymer Emulsions: The Use of Confocal Raman Spectroscopy and Self-modeling Curve Resolution**; Thomas M. Hancewicz, Paul D. A. Pudney, Dale G. Cunningham, Carolyn Gray; *Unilever R&D US, Edgewater, New Jersey, 07020 USA,, Unilever Bestfoods R&D Colworth Laboratory, Sharnbrook, Bedford, MK44 1LQ, UK*

11:00 (233) **A Synergistic Approach for the Utilization of Raman Spectroscopy/ Microscopy during Drug Product Development- From Discovery to the Clinic**; Gary McGeorge,; *Bristol-Myers Squibb*

11:20 (234) **Increasing sample throughput for Raman Spectroscopy of pharmaceutical Solids**; Stephen R Lowry, Richard C Wieboldt, Forrest A Weesner; *Thermo Nicolet*

Tuesday Morning, Room 555B
NEAR FIELD OPTICAL MICROSCOPY
Presider: Dan Higgins, University of Kansas

8:50 (235) **Single Molecule Spectroscopy of Interfacial Electron Transfer**; David M. Adams; *Columbia University*

9:30 (236) **Time-Resolved and Polarized Fluorescence Near-Field Scanning Optical Microscopy of Conjuagated Polymer Thin Films**; David A. Vanden Bout; Eun-Soo Kwak, Julie Teetsov, Joseph Imhof; *University of Texas*

10:10 **Coffee Break**

10:40 (237) **Apertureless Infrared Near Field Spectroscopy of Polymers**; Gilbert C. Walker, Boris B. Akhremitchev, Larissa Stebounova; *University of Pittsburgh*

11:20 (238) **Microscopic Investigations of Fluorescent Polyelectrolyte Surfactant Thin Films**; Daniel A Higgins, Xiangmin Liao; *Kansas State University*

Tuesday Morning, Room 556B
DYNAMIC LUMINESCENCE IMAGING
Presider: Lei Geng, Iowa State University

8:50 (239) **Chemiluminescence Imaging of Single Cell Dynamics**; Edward S. Yeung, Craig A. Aspinwall, Jason A. Gruenhagen; *Iowa State University, University of Arizona, Iowa State University*

9:30 (240) **Localization of strong adsorption sites on chromatographic silica**; Mary J. Wirth, Melody D. Ludes; *University of Delaware*

10:10 **Coffee Break**

10:40 (241) **Detection and Imaging of Secretion from Pancreatic Beta Cells and Islets Using Confocal Fluorescence Microscopy**; Robert T. Kennedy, Jennifer L. Peters, Gabriella M. Dahlgren, Weijun Qian, Robert T. Kennedy; *University of Michigan*

11:20 (243) **Observing Molecular Distribution in Chemical Separations with Confocal Fluorescence Imaging**; Lei Geng, Mark Lowry

Tuesday Morning, Ballroom C
MEGGARS AWARD
Presider: James Rydzak, GlaxoSmithKline

8:50 (244) **Picosecond Raman Spectroscopy of Solids: Fluorescence Rejection and Photon Migration**; Neil J. Everall, Thomas Hahn, Pavel Matousek, Anthony Parker, Michael Towrie; *ICI PLC,, National Starch and Chemical, Rutherford Appleton Laboratory*

9:30 (245) **Fluorescence-Suppressed Steady State and Picosecond Time-resolved Resonance Raman Spectroscopy in Solutions**; Pavel Matousek, Michael Towrie, Chensheng Ma, Ming M Kwok, David Phillips, William T. Toner, Anthony W Parker; *Rutherford Appleton Laboratory, Oxfordshire, UK,, Imperial College, London, UK, Oxford University, Oxford, UK,,*

10:10 **Coffee Break**

10:40 (246) **PIRATE- A New Picosecond Time Resolved IR Spectrometer**; Michael Towrie, Michael W. George, David C. Grills, W. M. Kwok, Chensheng Ma, Pavel Matousek, Anthony W. Parker, David Phillips, Naresh Subramaniam, Antonin Vlcek Jnr.; *Central Laser Facility, CLRC Rutherford Appleton L, School of Chemistry, University of Nottingham, NG7 2RD, United Kingdom., Department of Chemistry, Imperial College, Exhibition Road, London SW7 2AY, UK,, Department of Chemistry, Queen Mary and Westfield College, University of London, Mile End Road, London, UK E1 4NS.*

11:20 (247) **Fast and Ultrafast Infrared Studies in Conventional and Supercritical Fluids: From Alkane Activation to Infrared Probes of DNA**; Mike George; *University of Nottingham, UK*

Tuesday Morning, Room 553B
USING TECHNOLOGY TO TEACH ANALYTICAL CHEMISTRY
Presider: Cameron Dorey, University of Central Arkansas

8:50 (248) **The Analytical Sciences Digital Llibrary**; Cameron Dorey, Ted Kuwana, Stuart Chalk, Cynthia Larive, George Long; *University of Central Arkansas, University of Kansas, University of North Florida, Indiana University of Pennsylvania*

TECHNICAL PROGRAM - TUESDAY

9:10 (249) **The Internet as a Medium for Communication and Collaboration in Chemistry Courses.**; George R. Long; *Indiana University of PA*

9:30 (250) **Using Streaming Video and Flash Animation in Teaching Analytical Chemistry**; Mark R Anderson; *Virginia Tech*

9:50 (251) **Teaching Senior-Level Instrumental Analysis Using QuickTime Movies and Flash Animations**; Thomas G Chasteen; *Sam Houston State University*

10:10 **Coffee Break**

10:40 (252) **Using MathCAD in Teaching Analytical Chemistry**; David N. Blauch; *Davidson College, Davidson, NC 28035*

11:00 (253) **Panel Discussion**; Cameron Dory; *University of Central Arkansas*

Tuesday Morning, Room 554B
MINIATURIZED SPEARATIONS: SMALLER IS BETTER
Chris Culbertson, Oak Ridge National Laboratory

8:50 (254) **Single Cell Analysis on Microfluidic Devices**; Christopher T. Culbertson, Maxine A. McClain, Stephen C. Jacobson, J Micheal Ramsey; *Oak Ridge National Laboratory*

9:30 (255) **Controlling Surface Chemistry in Polymer Microfluidic Devices**; Charles S. Henry, Shaofong Gong, Yan Liu; *Colorado State University, Mississippi State University*

10:10 **Coffee Break**

10:40 (256) **Miniaturized Separations Applied to Physiological Problems**; Lisa A. Holland, Alyison Leigh, Roger Joy, Ping Liu; *West Virginia University, Kent State University*

11:20 (257) **Multiplexed Microchip Configurations for High-Throughput Analysis in Proteomics**; Iulia M. Lazar, Lijuan Li, Alexander R. Ivanov, Yang Yu, Marcelo V. Sousa, Barry L. Karger; *Barnett Institute/Northeastern University, Boston; Brazilian Center for Protein Research/University of Brasilia, Brasilia, Brazil*

Tuesday Morning, Room 552A
ICP-MS INSTRUMENTATION
Presider: Ken Marcus, Clemson University

8:50 (258) **Can We Break the Salt Barrier in ICP-MS ? Evaluation of Operating Conditions and Interfaces of ICP-QMS for Geo-Environmental Analysis**; Isaac (Joe) B Brenner, Paul Sigsworth, Phil Shaw, *EAL--BGU, Thermo electron*

9:10 (259) **Trace Analysis of Metal Matrices by ICP-MS**; Ruth E Wolf, Kenneth R Neubauer; *PerkinElmer Instruments*

9:30 (260) **Ion Energy Effects in Hexapole Collision/reaction Cell ICP-MS: Reactivity and the Plasma Potential**; Barry L Sharp, Matthew A. Dexter, Helen J. Reid; *Loughborough University*

9:50 (261) **The Effect of Load Coil Geometry on Ion Transmission Efficiency through the Sampling Orifice of an ICP-MS**; Paul B. Farnsworth, Jeffrey H. Macedone, Rebecca W. Neilson, Paul B. Farnsworth; *Brigham Young University*

10:10 **Coffee Break**

10:40 (262) **Novel High Performance Ion Optics for ICP-MS**; Iouri Kalinitchenko, Barry Sturman, Shane Elliott; *Varian Analytical Instruments*

11:00 (263) **Autodilution And Productivity in ICP-MS, Are They Compatible?**; Phil Shaw; *Thermo Elemental*

11:20 (264) **Using Multiple Collision Cell Settings to Achieve Ultimate Performance in Environmental Analysis**; Bill Spence, Simon Nelms, Karen Lee; *Thermo Elemental*

11:40 (265) **Determination of Trace Elements in Difficult Matrices by Inductively Coupled Plasma – Dynamic Reaction Cell – Mass Spectrometry**; Hakan Gürleyük, Carl Hensman; *Frontier Geosciences*

Tuesday Morning, Room 552B
SPECIATION IN ATOMIC SPECTROSCOPY
Presider: Ken Marcus, Clemson

8:50 (266) **Determination of Mercury Species in Environmental Samples by Ion Chromatography, Post-Column Cold Vapor Generation and Inductively Coupled Plasma Mass Spectrometry**; Qiang Tu, Willie Johnson, Jr., Brian Buckley; *EOHSI, Rutgers University*

9:10 (267) **Volatile selenium and sulfur species in Brassica juncea using SPME/GC-ICP-MS**; Juris Meija, Maria Montes-Bayón, Joseph A Caruso; *University of Cincinnati, Department of Chemistry*

9:30 (268) **Speciation of Arsenic Containing Compounds in Marine Tissues by Multidimensional LC - ICP MS and ESI MS**; Shona McSheehy, Meng Cui, Zoltan Mester, Ralph E Sturgeon; *Institute for National Measurement Standards, National Research Council of Canada*

9:50 (269) **Efficiency of EPA Draft Method 3200 for the Determination of Inorganic and Methylmercury in Soils and Sediments**; Mizanur Rahman, H. M. 'Skip' Kingston; *Department of Chemistry and Biochemistry, Duquesne*

10:10 **Coffee Break**

10:40 (270) **Automated Determination of Mercury Species using Gas Chromatography with Cold Vapor Atomic Fluorescence Detection**; Mary Kate Donais, David Pfeil; *Saint Anselm College,, Leeman Laboratories, Inc*

11:00 (271) **Speciation Measurements Using CE-ICP-MS: Dream or Reality?**; Nancy J Miller-Ihli, Enrique G Yanes; *USDA, BHNRC, Food Composition Laboratory*

11:20 (272) **A Method to Determine the Iron Containing Proteins in Meat Samples Using SEC-HPLC with FAAS Detection**; James Murphy, James M Harnly; *USDA, ARS, BHNRC, Food Comp Lab*

Tuesday Morning, Room 553A
ELECTROCHEMICAL SENSORS FOR BIOANALYSIS
Presider: James Burgess, Case Western Reserve University

8:50 (273) **Detection of Cholesterol Through Electron Transfer to Cholesterol Oxidase In Electrode-Supported Lipid Bilayer Membranes**; James D. Burgess, Anando Devadoss; *Case Western Reserve University*

9:10 (274) **Reaction of Cytochrome c from Different Species with Cytochrome c Oxidase Immobilized in Electrode-Supported Lipid Bilayer Membranes**; Melissa C. Rhoten, , James D. Burgess, Fred M. Hawkridge; *Longwood College,, Case Western Reserve University, Virginia Commonwealth University*

9:30 (275) **A Modified Cytosensor for Multianalyte Microphysiometry and Metabolic Responses to Sub-lethal Toxins**; David E. Cliffel, Sven Eklund, Ales Prokop, Eugeni Koslov, Franz Baudenbacher, John Wikswo; *Vanderbilt University*

10:10 **Coffee Break**

10:40 (276) **NOS-modified Electrodes**; Mekki Bayachou, Jean A Boutros; *Cleveland State University*

11:20 (277) **Electrochemical Toxicity Sensors Based on Toxic Metabolite Generation in Layered Protein-DNA Films**; James F. Rusling, Liping Zhou, Jing Yang, Amos Mugerwu, Bingquan Wang; *University of Connecticut*

Tuesday Morning, Room 551B
SURFACE ANALYTICAL TECHNIQUES
Presider: Shane Street, University of Alabama

8:50 (278) **Spectroscopic and Electrical Characterization of Molecular Diodes**; Greg J. Szulczewski, Jianchang Li, Jia Sun, Kye-Young Kim, Silas C. Blackstock; *The University of Alabama*

9:30 (279) **Dye-Labeled PAMAM Dendrimers as Nanoscale Diffusion Probes in Sol-Gel Films**; Joel M. Harris, Karla S. McCain, Peter Schluesche; *University of Utah*

10:10 **Coffee Break**

10:40 (280) **Physical and Mecahnical Properties of Dendrimer-based Nanocomposites**; Shane C. Street, Michael Curry, Fengting Xu, Judith Yang, John Barnard; *The University of Alabama, The University of Pittsburgh*

11:20 (281) **Frictional Anisotropy at Crystalline Interfaces**; Andrew J. Gellman, Christopher M. Mancinelli, Jeff S. Ko; *Carnegie Mellon University, Merck Co., Inc*

12:00 – 2:00 PM, Exhibit Hall C TUESDAY
UNDERGRADUATE 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 plce for the entire time. Check below for presentation time.

12:15 (282) **Solution Residue Analysis in Glow Discharge Spectroscopies**; Kenneth R. Hess, Jeremy L. Steinbacher, Melissa L. Hansen; *Franklin and Marshall College*

1:15 (283) **The Characterization of a Digital Micromirror Array for Atomic Spectroscopy**; Thomas M Spudich, Jennifer M Kuntz, Charles K Utz; *Penn State Erie, The Behrend College*

12:15 (284) **Reactive Gas Mixtures in Glow Discharge Spectroscopies**; Kenneth R. Hess, Adam S. Myers, Mark B. Rowand; *Franklin and Marshall College*

1:15 (285) **Use of a Catalyzed Microfiber Carbon Electrode in a Magnesium-Hydrogen Peroxide Semi-Fuel Cell**; Michelle Dunnell, Russell Bessette; *Umass Dartmouth*

12:15 (286) **Characterization Of Resorcinol -Formaldehyde Organic Aerogel**; Farnoosh Mehrabi, Mohammad Edrisi

1:15 (287) **Reduction of Fluorescence Interference in the Raman Microspectroscopic Determination of Drugs on Paper Currency**; Katelyn M. Macdonald, Kimberley F Schrum; *Whittier College*

12:15 (288) **An Investigation of Fountain Pen Inks by Capillary Electrophoresis Obtained From Documents Under Various Physical Conditions**; David P. Schrum, Courtney Kruse; *University of Redlands*

1:15 (289) **Electrochemical Synthesis And Characterization Of The Conducting Polymer Polyaniline In Supercritical Carbon Dioxide**; Amanda M. Mendonza, Rachna N. Badlani, Patricia A. Mabrouk; *Northeastern University*

12:15 (290) **Analysis of Blood Constituents Using Multi-variate Analysis**; Richard J. Williams, Stacey A. Bridges, Alvin P. Kennedy, Busolo W. Wabuyele, Guillermo A. Casay; *Morgan State University, Battelle, USP*

1:15 (291) **Coordination of Amino Acid Derivatives to Tungsten**; Rebecca A. Lucht, Timothy P. Curran; *Trinity College*

12:15 (292) **Anomalies in the Ion Transport of Phosphoric Acid in Aqueous Media: A 1H and 31P Nuclear Magnetic Resonance Study**; Song H. Chung, Robert Uriarte, Sophia Suarez-Gustave, Steven G Greenbaum; *Chemistry & Physics, William Paterson University, Wayne, NJ 07470, Physics, Hunter College, NY, NY 10021*

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 plce for the entire time. Check below for presentation time.

1:15 (293) **Electrothermal Atomizers for Analytical Spectrometry: From a Tube to a Thermochemical Reactor**; Albert Kh. Gilmutdinov, Konstantin Yu. Nagulin, Yuri A. Zakharov; *Department of Physics, Kazan State University*

12:15 (294) **Automatic Fluorescence Rejection Using Shifted Excitation Raman Difference Spectroscopy-- Residual Background Removal**; Jun Zhao; *Chromex, Inc*

1:15 (295) **NMR and Vibrational Studies of Analytically Relevant Interfaces**; Scott L. Wallen, Erica D. Dawson, Marc A. A. Blatchford, Michael L. Hurrey; *University of North Carolina*

12:15 (296) **Spin-Lattice Relaxation Investigations of Analytically Relevant Systems**; Scott L. Wallen, Erica D. Dawson; *University of North Carolina*

1:15 (297) **Chemical and Biological Warfare Agent Detection by Surface-Enhanced Raman Spectroscopy**; Stuart Farquharson; *Real-Time Analyzers, Inc*

12:15 (298) **Controlling Trace Metal Contamination around the Bevel and Edge Exclusion Area of Silicon Wafers**; Chris Sparks; *International SEMATECH*

1:15 (299) **A Comparison of Methods for the Determination of Organomercury Content in Tissue and Sediment Samples**; Peter M Grohse, Frank X Weber, Troy D Burnette; *RTI International*

12:15 (300) **Applications of ICP-MS in the Semiconductor and Nuclear Industries**; Simon Nelms, Bill Spence, Karen Lee; *Thermo Elemental*

1:15 (301) **Advances in Spark Ablation ICP-MS and ICP-AES for Specialty Alloys and High-Purity Metals Analysis**; Sergei V. Leikin, George G Glavin, George Kraeger; *Spectro Analytical Instruments, Indium Corporation of America*

12:15 (302) **Molecular Composition and Orientation of Silicon Oxides for Si(111)/SiO2 and Si(100)/SiO2 Surfaces using FT-IR and XPS Spectroscopic Methods**; Vasilis G. Gregoriou, Georgia Kandilioti, Stella Kennou, Aggeliki Siokou, Vassiliki Papaeuthimiou; *ICEHT-FORTH*

1:15 (303) **Determination of 3-Dimensional Sample Compostion by FTIR**; John A. Seelenbinder, Donna Andrauskus, Norman Wright; *Digilab*

12:15 (304) **Age Determination of Bloodstains using Infrared Spectroscopy**; Edita Botonjic, Chris W. Brown, Marc Lamontagne, Mary Tsaparikos*University of Rhode Island*

1:15 (305) **Analysis of Organic Semiconductor Solvents using Ultrasonic Nebulization / Membrane Desolvation with ICP-MS Detection**; Fred G. Smith; *CETAC Technologies*

12:15 (306) **Nuclear-Physical Methods of Investigation of an Element Composition in Samples of Soil and Plants**; Shaimon Hushmurodov, Rashida Temirova; *Samarkand state University, Samarkand Kooperative College*

1:15 (307) **General Model for the Response of Optical Sensors Based on Diffusion and Kinetics**; J. Alberto Morales, John F. Cassidy; *Facility for Optical Characterisation and Spectros*

12:15 (308) **Advanced Clean Chemistry Techniques for Controlling the Analytical Blank in Trace Analysis**; Robert Richter, PhD; *Milestone Inc*

1:15 (309) **Determination of Boron in Silicon Wafer by Laser Ablation-Inductively Coupled Plasma Mass Spectrometry Using On-line Isotope Dilution Technique**; Mo-Hsiung Yang, Po-Hsiang Chi, Wen-Ching Wei; *Department of Nuclear Science, National Tsing-Hua,, QA Dept., QRA Div., ProMOS Technologies Inc., Hsinchu, Taiwan, R.O.C.*

12:15 (310) **Application of TXRF and ICP-MS for the analysis of metallic contamination on silicon wafer surfaces: a correlation study.**; Craig Seeley; *Nasson College*

1:15 (311) **Acid-Stable Electro-Active Self Assembled Protein-Polyion Multilayer Films**; Venkateswarlu Panchagnula, Challa V. Kumar, James F. Rusling; *University of Connecticut*

12:15 (312) **Water Analysis in Actinide Oxides by Thermogravimetric Analysis - Mass Spectrometry (TGA/MS) and Thermogravimetric Analysis - Fourier Transform Spectrometry (TGA/FTIR)**; Arthur R. Jurgensen, Kenneth J. Imrich; *Westinghouse Savannah River Site*

1:15 (313) **Electrokinetic Separation of Alkaloids in Ipecac**; Marc C. Lamontagne, Linda Peterson, *Rhode Island College*

12:15 (314) **Application of ICP-MS for determination of phosphorus and iron in biological microsamples**; Sergei F Boulyga, Sabine Becker; *Central Department of Analytical Chemistry,*

1:15 (315) **Pressure Regimes for a Glow Discharge Mass Spectrometer**; Elizabeth P. Hastings, Kevin P Turney, Jorge Pisonero Castro, W. W Harrison; *Univeristy of Florida, Gainesville, Universidad de Oviedo*

12:15 (316) **Determination of Absolute Configuration and Solution Conformation in Molecules with Chiral Axes by Vibrational Circular Dichroism**; Teresa B. Freedman, Xiaolin Cao, Laurence A. Nafie, Quezia Cass, Andrzej Rajca, Andreas J. Rippert; *Syracuse University, Syracuse, NY 13244-4100 USA, Department of Chemistry, Federal University of Sao Carlos 13565-905, Sao Carlos, SP, Brazil, Department of Chemistry, University of Nebraska, Lincoln, NE,, Organisch-Chemisches Institut der Universität Zürich, Winterthurerstr. 190, CH-8057 Zürich Switzerland*

1:15 (317) **Hyphenation of Liquid Separation Techniques and Surface-Enhanced Resonance Raman Spectroscopy**; Reyer J. Dijkstra, Reza M. Seifar, Freek Ariese, Udo A.Th. Brinkman, Cees Gooijer; *Vrije Universiteit Amsterdam*

12:15 (318) **Scanning Electrochemical Microscopic Imaging of Immobilized DNA Molecules and DNA Hybridization at DNA Microarrays**; Feimeng Zhou, Liang Wang, Jun Wang, Jingbo Hu, Zhuobin Yuan, Feimeng Zhou; *Division of Chemistry, Graduate School, Chinese Ac,, Department of Chemistry and Biochemistry, California State University, Los Angeles, CA90032*

1:15 (319) **The Facile Quantification of the Active Ingredient and the Detection of Degradation in a Topical Pharmaceutical Formulation**; Mark S. Kemper, William J. McCarthy, Matthew Nowakowski, Michael C. Garry, Atul J. Shukla, Napasinee Aksornkoae, Christopher Watts, James L. Johnson, Charles Schmidt; *Thermo Nicolet Corporation, University of Tennessee School of Pharmacy, Thermo Finnigan Corporation*

12:15 (320) **Degradation of poly(vinyl chloride) with Different Additives Studied by Micro Raman Spectroscopy**; Andreas Gupper,, Peter Wilhelm, Michael Schiller; *Research Institute for Electron Microscopy, Graz U,, Chemson Polymer-Additive AG, Industriestrasse 19, A-9601 Arnoldstein, Austria (M.S.)*

1:15 (321) **Evaluation of a Hyperspectral Imaging System for Forensic Analysis**; Brian A. ckenrode, Valerie J. Cavett, Kelly M. Langford, Brian A. Eckenrode; *FB, ProVision Technologies*

12:15 (322) **Solid-State NMR Studies of Aluminosilicate Formation in Weathered Clay Systems**; Garry S. Crosson, Sunkyung Choi, Mary K. Amistadi, Jon Chorover, Karl T. Mueller; *The Pennsylvania State University, University of Arizona*

1:15 (323) **Ultra Trace Determination of Mercury In Environmental Matrices**; Cathleen Zimmerman, Jeff Forsberg; *CETAC Technologies*

12:15 (324) **Analysis of dodecyl-poly(phenyleneethynylene): Examination of Heterogeneous Mesostructure in a Conjugated System Using Near-Field Scanning Optical Microscopy (NSOM)**; David A. Vanden Bout, Joseph M Imhof; *University of Texas at Austin, Texas Materials Institute, Center for Nano- and Molecular Science and Technology*

1:15 (325) **Holographic-Laser Raman Study of Ba1-x SrxTiO3 Solid Solution Ceramics**; Krishna K. Deb, Daniel M. Potrepka, Kevin W. Kirchner; *Army Research Laboratory, Sensors and Electron Dev*

12:15 (326) **Highly Sensitive Protein Detection Method in Sodium Dodecyl Sulfate-Polyacrylamide Gels Using Enhanced Luminescence of Lipophilic Fluorescein Derivatives**; Myungkoo Suh, Hyun-Jung Kim, Donghoon Kang, Duk Young Jung, Chulhun Kang, Freek Ariese; *Department of Chemistry, Sung Kyun Kwan University, Department of Neuroscience, Graduate School of East-West Medicinal School, Kyung Hee University, Suwon 449-701, Korea, Analytical Chemistry and Applied Spectroscopy, Free University Amsterdam, 1081 HV Amsterdam, The Netherlands*

1:15 (327) **Bias and Precision Implications of the Limit of Detection Probability Density Function**; Edward Voigtman, Daniel J Montville; *University of Massachusetts Amherst*

12:15 (328) **Transient Grating Evaluation of Photodynamic Therapy Agents**; Andrew C. Beveridge, Gerald J. Diebold, Barbara A. Bench, Sergiu M. Gorun, Johan E. van Lier; *Department of Chemistry-Brown University, Department of Nuclear Medicine and Radiobiology-University of Sherbrooke*

1:15 (329) **Addressing the Challenges of Geochemical and Environmental Samples by ICP-MS**; Jenny J. Godfrey, Bill J. Spence, J. J. Robinson, S. R. Chenery, J. M. Cook, K. M. Perkins, M. J. Watts; *Thermo Elemental, British Geological Survey*

12:15 (330) **Condensation Reactions of CrxOy- in an Ion Trap Secondary Mass Spectrometer**; Anita K. Gianotto, Brittany D. M. Hodges, Anthony D. Appelhans, John E. Olson, Michael T. Benson, Gary S. Groenewold; *Idaho National Engineering and Environmental Labor*

1:15 (331) **Laser-Excited Time-Resolved Shpol'skii Spectroscopy of dibenzo[a,l]pyrene in Water Samples**; Andres D. Campiglia, Shenjiang Yu, Adam J. Bystol, Andres D. Campiglia; *Department of Chemistry North Dakota State University*

12:15 (332) **An Introduction to Inductively Coupled Plasma Atomic Emission Spectrometry**; Lori B. Allen, Christine Evans, Richard Judge; *University of Wisconsin – Parkside*

1:15 (333) **Fluorescence and Phosphorescence Characteristics of Coumarins and Related Compounds**; Andres D. Campiglia, Nathan Saetveit, Adam J. Bystol; *North Dakota State University*

12:15 (334) **Influence of Solvents on the Extraction of Metal Cations by Donnan Dialysis with Flame Atomic Absorption Spectrophotometry**; Lori B. Allen, Amber Antonia; *University of Wisconsin - Parkside*

1:15 (335) **Polymerized liposome-Tb system for carbonic anhydrase sensing**; Andres D. Campiglia, Marina Santos, Andrea F. Arruda, Bidham C. Roy, Sanku Mallik, *Department of Chemistry North Dakota State University*

12:15 (336) **Using Environmental Chemistry Research Projects in General Education Science Courses**; Catherine D Clark, Gerard Klimbal, Louise Hose; *Chapman University*

1:15 (337) **Extraction and Determination of Hexavalent Chromium in Fish Tissue**; Hakan Gürleyük, Susan Mitchell; *Frontier Geosciences*

12:15 (338) **Certification Measurements of Hg in Tuna for an Inter-Laboratory Comparison Exercise, with Stable Isotope Certified Reference Materials from IRMM**; James P. Snell, Christophe Quétel; *Institute for Reference Materials and Measurements*

1:15 (339) **Probing the Dynamics of Chemical Agent Degradation on Urban Surfaces Using Ion Trap Secondary Ion Mass Spectrometry**; Anthony D. Appelhans, Gary S. Groenewold, John M. Williams, Garold L. Gresham, John E. Olson, Mark T. Jeffery, Brad Rowland; *Idaho National Engineering and Environmental Labor*

12:15 (340) **Comparison of Quadrupole and Magnetic Sector ICP-MS on Certification of the Copper and Cadmium Amount Contents in Synthetic Food**; Cristophe R. Quétel, Emilia T. Vassileva, Ivan P. Petrov, Ivan I. Tresl, Cristophe R. Quétel, Philip D.P. Taylor; *European Commission, Joint Research Centre, Instit*

1:15 (341) **Using High Temperature Programming to Improve HPLC Separations**; Dale Felix, Stephanie J. Marin, Brian A Jones; *Selerity Technologies*

12:15 (342) **Preheating - the Key to Successful Programming in High Temperature HPLC**; Dale Felix, Stephanie J Marin, Brian A Jones; *Selerity Technologies*

1:15 (343) **TOF-SIMS Analysis and Imaging of an Additive in Polyethylene**; Mary Jane Walzak, James T. Francis, Heng-Yong Nie, N. S. McIntyre, Blair A. Graham; *Surface Science Western, University of Western Ont,, Products and Chemicals Division, Imperial Oil*

12:15 (344) **Helium Plasma Source Time-of-Flight Mass Spectrometry**; Yixiang Duan, Yongxuan Su, Zhe Jin; *Analytical Chemistry Science, C-ACS*

1:15 (345) **The conformational analysis and study by NMR of sesquiterpene lactone gaillardine.**; Bakhtiyor F. Rasulev, Nasrulla D. Abdullaev, Kamila Eshbakova; *Institute of Chemistry of Plant substances*

12:15 (346) **Multivariate Curve Resolution in the Presence of Non-specific Spectral Backgrounds**; Michael R. Keenan, Mark H. Van Benthem, Paul G. Kotula; *Sandia National Laboratories*

Tuesday Afternoon, Room 551A
ENVIRONMENTAL MASS SPECTROMETRY STUDIES IN AQUATIC SYSTEMS
Presider: Catherine Clark, Chapman University

2:00 (347) **Recent applications of accelerator mass spectrometry for investigating organic compounds in the environment**; Christopher M Reddy, *Woods Hole Oceanographic Institution*

2:40 (348) **Using Direct Temperature-Resolved Mass Spectrometry to Characterize Size Fractions of Aquatic DOM**; Elizabeth C. Minor, Jean-Paul Simjouw, Jaap J. Boon, Anne E. Kerkhoff, Jerre van der Horst; *Chemistry and Biochemistry, Old Dominion Universit,, OEAS, Old Dominion University, FOM Institute AMOLF*

3:20 **Coffee Break**

4:00 (349) **An Ion Trap Mass Spectroscopy Investigation of Dissolved Organic Matter in Natural Waters**; Erik R. Stabenau, Richard G. Zepp, Rod G. Zika; *University of Miami / RSMAS,, US Environmental Protection Agency*

4:40 (350) **Oceanic halocarbon measurements by in situ GC-MS**; Daniel B. King, James H. Butler, Jurgen M. Lobert, Shari A. Yvon-Lewis; *NOAA/CMDL, Boulder, CO, API, San Diego, CA NOAA/AOML, Miami, FL*

TECHNICAL PROGRAM - TUESDAY

Tuesday Afternoon, Room 550A
PROCESS INSTRUMENTATION AND TECHNIQUES
Presider: Chris Hassel, Los Alamos National Laboratory

2:00 (351) **Designing Temperature-Insensitive Multivariate Optical Elements**; Frederick G. Haibach, David L. Perkins, Ryan J. Priore, Maria V. Schiza, Ashley E. Greer, Michael L. Myrick; *University of South Carolina*

2:20 (352) **Practical Applications of Quantitative Measurements in Scattering Media using Photon Time-of-Flight Profiles with Multiresolution Analysis**; Claudia E.W. Gributs, David H. Burns; *McGill University*

2:40 (353) **Light Emitting Diode Excitation Emission Matrix (LED-EEM) Fluorescence Spectroscopy**; Sean J. Hart, Renee D. JiJi, Sean J. Hart; *Naval Research Laboratory (NRL), NRC-NRL Postdoctoral Associate*

3:00 (354) **Raman Spectroscopic Detection Of Capillary Electrophoresis In A Liquid Core Waveguide**; Obianuju Inya-Agha, Michael D. Morris; *University of Michigan, Ann Arbor*

3:20 **Coffee Break**

4:00 (355) **Reaction monitoring using a novel in situ mid infrared spectrometer**; Colin A McGill, Colin A. McGill, David Littlejohn; *University of Strathclyde/CPACT*

4:20 (356) **Application of Multivariate Calibration Methods to Surface Acoustic Wave Array Data**; Dion Rivera, M. Kathleen Alam, William G. Yelton, Robert J. Simonson, David M. Haaland; *Sandia National Laboratory*

Tuesday Afternoon, Room 555B
ADVANCES IN LAB-ON-A-CHIP TECHNOLOGY
Presider: Adam Woolley, Brigham Young University

2:00 (357) **New Tools and Device Designs for Microfluidic Analysis**; Adam T. Woolley, Melissa Draper, Ryan T. Kelly, Tao Pan, Jason W. Munyan; *Brigham Young University*

2:20 (358) **Plastic Microfluidic Devices and Electrophoretic Reporters for Solution-Phase Multiplexing of Protein and Gene Expression**; Stephen J. Williams, Travis Boone, Tina Tian, Hrair Kirakossian, Ann Wainright, Sharat Singh; *ACLARA BioSciences*

2:40 (359) **Combinatorial Chemistry On-Chip**; Paul S Cremer; *Texas A&M University*

3:00 (360) **Chemical Foundations for Polymeric Microanalytical Devices - Surface Modification**; Robin L. McCarley, Bikas Vaidya, Alison F Smith, Suying Wei, Yun Wang, Steven A Soper; *Louisiana State University*

3:20 **Coffee Break**

4:00 (361) **Lab-on-a-Chip Devices for Small Molecule Clinical Diagnostics**; Charles S. Henry, Christopher J. Easley, Hollie C. McGehee, Joseph C. Fanguy; *Mississippi State University*

4:20 (362) **Meeting the Proteomics Challenge with Microfluidics**; Aaron T. Timperman, Ying Zhang, Zhaoyang Huang, Trust Razunguzwa

4:40 (363) **Experimental Studies of Electroosmotic Flow Dynamics and Vacancy Electrophoresis in Microfluidic Devices**; S. Douglass Gilman, Jason L. Pittman, Kristie Carter, Charles S. Henry; *University of Tennessee, Mississippi State University*

Tuesday Afternoon, Room 553A
SINGLE MOLECULE DETECTION IN BIOLOGICAL SYSTEMS II
Presider: Alan Van Orden, University of Colorado

2:00 (364) **Controlled Lateral Migration of Single DNA Molecules in Capillary Electrophoresis**; Edward S. Yeung, Edward S. Yeung, Jinjian Zheng; *Iowa State University*

2:40 (365) **Multiplexed Observation of DNA-Protein Interactions on a Single-Molecule Level by Means of Flow Stretching Individual DNA Molecules**; Antoine M. van Oijen, Donald J. Crampton, Charles C. Richardson, Tom E. Ellenberger, Sunney X. Xie; *Harvard University, Dept. of Chemistry and Chemica, Harvard Medical School, Dept. of Biological Chemistry and Molecular Pharmacology*

3:00 (366) **Studying Chromatographic Adsorption One Molecule at a Time**; Mary J. Wirth, Derrick J. Swinton, Melody D. Ludes; *University of Delaware*

3:20 **Coffee Break**

4:00 (367) **Single Molecule Studies of Long Lived Spatial Heterogeneities in Polymers and Liquids Near the Glass Transition**; David A. Vanden Bout, Laura A Deschenes; *University of Texas at Austin*

4:40 (368) **Initiating the Conformational Transitions of Single DNAs with Optical Trapping**; Daniel T Chiu; *University of Washington*

5:00 (369) **Single Molecule Fluorescence Spectroscopy and Atomic Force Microscopy in the Study of Biomaterial Interfaces**; Alan K. Van Orden, Lori L. Carillo, Jonathon Gerding, Lisa A. Kolodny, Dale M. Willard; *Colorado State University*

Tuesday Afternoon, Room 555A
CHIRAL ANALYSIS II
Presider: Kenneth Busch, Baylor University

2:00 (370) **Forays into Chiral Analysis**; Kenneth W Busch; *Baylor University*

2:40 (371) **Determination of the Structures of Chiral Molecules in Solution Phase**; Prasad L Polavarapu, Feng Wang; *Vanderbilt University*

3:20 **Coffee Break**

4:00 (372) **Advances in Fourier Transform VCD Instrumentation and Applications of VCD for Determination of Absolute Configuration in Molecules of Pharmaceutical Interest**; Laurence A. Nafie(1,3), Teresa B. Freedman(1), Rekha D. Shah(2), Xiaolin Cao(1), Rina K. Dukor(3); *(1)Department of Chemistry, Syracuse University, S, (2)Johnson & Johnson Pharmaceutical Research & Development LLC, Spring House, PA 19477, (3)BioTools Inc., 950 N. Rand Road, Unit 123, Wauconda, IL 60084*

4:40 (373) **Using Low-Temperature Experimental VCD Spectra in Configurational Studies of Chiral Small Molecules**; Douglas J. Minick, Randy D Rutkowske, Luke A Miller; *GlaxoSmithKline*

Tuesday Afternoon, Room 552A
RAMAN SPECTROSCOPY I
Presider: Rich Bormett, Renishaw

2:00 (374) **Analysis of Toxic Chemicals in Water by Surface-Enhanced Raman Spectroscopy**; Yuan-Hsiang (Vincent) Lee, Stuart Farquharson; *Real-Time Analyzers, Inc*

2:20 (375) **Optimization of Surface-Enhanced Raman Substrates for Spectroscopic Detection of Vegetative Bacteria**; Augustus W. Fountain, Melissa Vellone, Sherwin Cheuk, George Elias, Nicholas F. Fell Jr., Alicia G Smith; *United States Military Academy, U.S. Army Research Laboratory*

2:40 (376) **Automated Solvent Subtraction From Mixture Raman Spectra**; Dor Ben-Amotz, Yvette L Antoni, Ryan Favors, Joshua Black, Jeanette Hanna; *Purdue University*

3:00 (377) **Merging Raman Spectroscopy and Chemometrics for Portable, Inexpensive Instrumentation**; J. D. Winefordner, P. E. Eagan, C. L. Stevenson, I. B. Gornushkin, B. W. Smith; *University of Florida, University of Richmond*

3:20 **Coffee Break**

4:00 (378) **Enhanced Chemical Classification using a New Feature Selection Method**; Dor Ben-Amotz, Dongmao Zhang; *Purdue University*

4:20 (379) **Speciation of Organics in Water with Raman Spectroscopy: Utility of Ionic Strength Variation**; Timothy W. Collette, Ted L. Williams; *U.S. Environmental Protection Agency, National Ex*

4:40 (380) **Raman Probe Head Design for Absolute Intensity and Concentration Measurements**; Dor Ben-Amotz, Ryan Favors N Favors, Dongmao Zhang, Yanan Jiang; *Purdue University*

5:00 (381) **Modular Triple Monochromator for UV Raman and resonance Raman Spectroscopy**; Bruce True, Leslie Tack; *Roper Scientific*

Tuesday Afternoon, Room 556A
INFRARED SPECTROSCOPY
Presider: John Wright, University of Wisconsi

2:00 (382) **FT-IR Microspectropic Mapping of the Effects of Enymatic Treatment of Flax Stems**; David S. Himmelsbach, Sadia; *USDA-ARS-Russell Res. Ctr*

2:20 (383) **Molecular Orientation in Ultrathin Films Using Anisotropic Optical Constants Determined by Infrared Spectroscopy**; Isabelle Pelletier, Daniel Blaudez, Bernard Desbat, Thierry Buffeteau, Michel Pézolet; *Centre de Recherche en Science et Ingénierie des M, Centre de Physique Moléculaire Optique et Hertzienne, Laboratoire de Physico-Chimie Moléculaire*

2:40 (384) **Application of a Narrow Band Optimized IR Microspectrometer to Metabolic Studies Using Deuterated Compounds**; David L. Wetzel; Steven LeVine, *Kansas State University*

3:00 (385) **Detection of Organophosphorous Compounds in Characteristic Near Infrared Regions by Using Multivariate Optical Elements**; Maria V. Schiza, Ashley E Greer, David L Perkins, Frederick G Haibach, Michael L Myrick; *University of South Carolina*

3:20 **Coffee Break**

4:00 (386) **Using Rapid-Scan Fourier Transform Infrared Spectral Imaging for Monitoring Dynamic Processes**; Scott W. Huffman, Rohit Bhargava, Ira W. Levin; *National Institues of Health*

4:20 (387) **"Amplified" Fiber-Optic ATR Probes with Improved Detection Limits in the Mid IR**; Mary Thomson, Peter Melling, Boris Mizaikoff, Manfred Karlowatz; *Remspec Corporation, Applied Sensors Laboratory, Georgia Institute of Technology*

4:40 (388) **Infrared Monitoring of Cellular Changes via Direct Subculturing on ATR Crystal Surfaces**; M. Kathleen Alam, Jerilyn A. Timlin, Laura E. Martin, Rick Lyons, Brian Hjelle, Kristen Garrison

5:00 (389) **Field-based Chemometric Quantitative Analysis of Polychlorinated Biphenyls in Oil Using Portable FT-IR Spectroscopy**; Mark L Norman, David H Dinh, David W Schiering; *SensIR Technologies*

Tuesday Afternoon, Room 557
BUILDING A BETTER IMAGE WITH RAMAN AND IR
Presider: Chieu Tran, Marquette

2:00 (390) **Building a better body image. What Raman imaging tells us about development of calvarial tissue.**; Michael D Morris, *University of Michigan*

2:40 (391) **Vibrational Microscopic Imaging of Bone, Cartilage and Skin**; Richard Mendelsohn,; *Rutgers University*

3:20 **Coffee Break**

4:00 (392) **FTIR imgaing for High-Throughput Screening of Catalysts**; Jochen Lauterbach, *University of Delaware*

4:20 (393) **Significant Real World Applications of Chemical Imaging**; Patrick J. Treado, *ChemIcon Inc.*

4:40 (394) **Biomedical Microspectroscopy and Imaging Using Synchrotron Infrared Light**; Lisa M .Miller, *Brookhaven National Laboratory*

5:00 (395) **Sol-Gel Homogeneity: A Closer Look with Near-IR Imaging**; Chieu D. Tran, Mario Politi; M*arquette University, Dept. of Chemistry*

Tuesday Afternoon, Ballroom C
RAMAN SPECTROSCOPY IN ARCHAEOLOGY, ARTS AND HUMANITIES
Presider: John Chalmers, University of Nottingham

2:00 (396) **Raman spectroscope applied to archaeological biomaterials: A critical review**; Howell G. M. Edwards, *University of Bradford*

2:20 (397) **Resonance Raman Spectroscopy for In Situ Characterization of Dyes in Antique Documents and Textiles**; Steven E. J. Bell, Julien Villaumie, Paul Wyeth, Averil McDonald; *School of Chemistry, Queen's University, Belfast; Textile Conservation Center, Winchester, SO23 8DL, U.K.*

2:40 (398) **Raman Spectroscopy of Mineral Pigments in Mediaeval Illuminated Manuscripts from Castilla y Leon (Spain)**; Fernando Rull; *University of Valladolid*

3:00 (399) **Raman spectroscopic studies of pigments on artworks**; Robert Withnall; *Univesity of Greenwich*

3:20 **Coffee Break**

4:00 (400) **Raman Spectroscopic Examination of Objects of Art: Pigments, Dyes, Binding Media and Supports**; Peter Vandenabeele, Lluc Moens; *Ghent University*

4:20 (401) **ARCHAEORAMAN Research on Geomaterials, and Remote Analytical Operations by Mobile Raman Spectroscopy (MRM): Past, Present & Future**; David C. Smith

4:40 (402) **New Applications of Raman Spectrometry in Gemmology**; Lore Kiefert; *SSEF Swiss Gemmological Institute*

5:00 (403) **The Use of Raman Microscopy for the Study of Corrosion Products on Copper Alloy Artifacts**; Karen A. Trentelman, Lowell I. McCann; *The Detroit Institute of Arts, University of Wisconsin, River Falls*

TECHNICAL PROGRAM – TUESDAY

Tuesday Afternoon,Room 553B
PROBLEM BASED LEARNING IN ANALYTICAL CHEMISTRY
Presider: Tom Wenzel, Bates College

2:00 (404) **CHM 1222 - Bioanalytical Chemistry, A Problem-Based Learning Approach to Undergraduate Analytical Chemistry**; Patricia A Mabrouk, Patricia A Mabrouk; *Northeastern University*

2:20 (405) **PBL and Analytical Chemistry Education**; Preetha Ram; *Emory University*

2:40 (406) **Volatile-Organic-Compounds Finger Print of Urban Air: Introducing Pattern Recognition in Undergraduate Analytical Chemistry**; Wilbert W Hope, Umesh Nagarkatte; *Medgar Evers College*

3:00 (407) **Homework: An Important, But Neglected, Aspect of Problem-Based Learning**; Julian F Tyson; *University of Massachusetts*

3:20 **Coffee Break**

4:00 (408) **Problem-based Learning in the Undergraduate Analytical Laboratory**; Cynthia K Larive; *University of Kansas*

4:20 (409) **Crime Solvers in the Analytical Lab**; Robert Q Thompson; *Oberlin College*

4:40 (410) **Panel Presentation: Problem-Based Learning in Analytical Chemistry**; Thomas J. Wenzel, Wilbert Hope, Cynthia Arive, Pam Mabrouk, Preetha Ram, Robert Thompson, Julian Tyson

Tuesday Afternoon, Room 554A
SEPARATIONS AT THE DISCOVERY INTERFACE
Peter Angus, Pfizer Global Research and Development

2:00 (411) **Bioanalytical Separations in Drug Discovery vs. Drug Development: Different Results, Different Expectations, and Different Regulations**; Mark J Rose; *Merck Research Laboratories*

2:40 (412) **Multidimensional Separations Strategies for High-Throughput**; Nicolas Angell, Richard D Smith; *Human Genome Sciences, Pacific Northwest National Laboratory*

3:20 **Coffee Break**

4:00 (413) **Innovative Separation Strategies for Small Molecule and Peptides**; Lisa A Holland, Roger Joy, Alyison Leigh, Ping Liu; *West Virginia University, Kent State University*

4:40 (414) **Rapid, High Throughput Capillary Electrophoresis Approach for Studying Biological**

Tuesday Afternoon, Room 552B
PULSED AND RADIO FREQUENCY GLOW DISCHARGES FOR CHEMICAL ANALYSIS
Presider: M. Winchester, NIST

2:00 (415) **Modeling of glow discharges: dc, rf and pulsed operation modes: Possibilities and limitations.**; Annemie Bogaerts, Renaat Gijbels; *University of Antwerp*

2:20 (416) **Monitoring Impedance in RF Glow Discharge Optical Emission Spectroscopy (GD-OES)**; Richard Payling, Patrick Chapon, Olivier Bonnot, Philippe Belenguer; *Surface Analytical, Jobin Yvon Emission Horiba, CPAT-UPS*

2:40 (417) **Pulsed Glow Discharges for Thin Film Analysis**; Willard W, Harrison, Eric S, Oxley, Willard W, Harrison; *University of Florida*

3:00 (418) **Quantitative Depth Profiling of Non-Conductive Technical Surfaces Using RF GD-OES**; Arne Bengtson; *SIMR*

3:20 **Coffee Break**

4:00 (419) **RF-GD-OES: Rapid Depth Profiling of Diverse Materials**; R. Kenneth Marcus, Alwyn B. Anfone, Wandee Luesaiwong; *Clemson University*

4:20 (420) **Recent Developments in the Field of RF Powered Glow Discharge Spectrometers**; Michael Analytis; *Spectruma Analytik GmbH*

4:40 (421) **Temporal and Spatial Ionization of Molecular Species in Millisecond Pulsed Glow Discharge Time-of-Flight Mass Spectrometry**; Fred L. King, Lei Li, J. T. Millay; *West Virginia University*

5:00 (422) **New Developments in Glow Discharge Spectroscopy**; Patrick L. Palumbo, Charles Maul, *LECO Corporation*

5:20 (423) **Thin-Film Analysis Using Pulsed and rf Glow Discharge with OES and TOFMS**; Jorge Pisonero(1), Beatriz Fernández (2), Nerea Bordel (1), Elizabeth Hastings (3), Kevin Turney (3), Eric Oxley (3), W.W Harrison (3), Alfredo Sanz-Medel (2); *(1) Department of Physics,University of Ovied,, (2) Department of Physical and Analytical Chemistry, University of Oviedo, (3) Department of Chemistry, University of Florida,,*

Tuesday Afternoon, Room 554B
NANOSTRUCTURES I
Presider: C. J. Zhong, SUNY-Binghamton

2:00 (424) **Scanning Probe Microscopy Studies of Nanoparticles**; Francis P. Zamborini; *University of Louisville*

2:40 (425) **Nanoparticles in Chemistry, Materials, and Biology**; Vincent M. Rotello; *University of Massachusetts*

3:20 **Coffee Break**

4:00 (426) **Nanoparticle Conjugation Chemistry: Strengthening Biomolecules' Grip**; T. Andrew Taton; *University of Minnesota*

4:20 (427) **Molecular Recognition at Cyclodextrin-Modified Metal Nanoparticle Surfaces**; Jian Liu, Angel E Kaifer; *University of Miami*

4:40 (428) **Combining Specific and Nonspecific Forces for Assembly of Metal Nanoparicles**; Christine D Keating, Mahnaz El-Kouedi, Glenn P. Goodrich;, *Penn State University*

5:00 (429) **Nanoparticle-Structured Interfacial Binding and Catalytic Properties**; Chuan-Jian Zhong, Jin Luo, Li Han, Mathew Maye, Nancy Kariuki; *State University of New York at Binghamton*

Tuesday Afternoon, Room 551B
BIOANALYSIS BY SEPARATION, CHROMATOGRAPHY AND MASS SPECTROMETRY (TAIWAN)
Presider: Suh-Jen Jane Tsai, Taiwan Chemistry Society

2:00 (430) **Dual-probe microdialysis and allied techniques in the determination of neurochemicals in gerbils subjected to cerebral ischemia/reperfusion**; Fu-Chou Cheng; *TCV General Hospital*

2:20 (431) **Nanoparticles for bioanalysis**; Huan-Tsung Chang; *National Taiwan University*

2:40 (432) **Enantiomeric Separation of Drugs by Capillary Electrochromatography Using Macrocyclic Antibiotics**; Guor-Tzo Wei, Fu-Ken Liu, Sam S Chang, Daniel W Armstrong; *Chung-Cheng University, ScinoPharm Taiwan, Iowa State University*

3:00 (433) **A Novel Analytical Approach of use of Tetrahydrofuran as a Reagent in Liquid Chemical Ionization Ion Trap Mass Spectrometry**; Yong-Chien Ling, Shin-Hwa Tzing, Anil Ghule, Jia-Yaw Chang; *National Tsing Hua University*

3:20 **Coffee Break**

4:00 (434) **Lab-On-A-Chip and Its Applications for Proteomic Analysis**; Shu-Hui Chen, Wang-Chou Sung, Chun-Che Lin, Lan-Yu Wang, Teli Tai, Pao-chi Liao, Pang-Wei Chen, Gwo-Bin Lee; *Department of Chemistry, National Cheng Kung University, Department of Environmental and Occupational Health, Department of Engineering Science*

4:20 (435) **An On-Line Automatic Sample Clean-Up System for the Quantitative Detection of the Benzene Exposure Biomarkers in Human Urine by ESI-MS/MS**; Pao-Chi Liao, Chien-Ming Li, Lung-Cheng Lin, Chien-Wen Hung; *Department of Environmental and Occupational Health*

Tuesday Afternoon, Room 556B
SPECTROSCOPIC PROBING OF BIOMOLECULES AND ASSEMBILIES
Presider: Mary J. Wirth, University of Delaware

2:00 (478) **Controlling and Measuring Local Composition and Properties in Lipid Bilayer Membranes**; Paul S. Weiss; *The Pennsylvania State University*

2:40 (479) **UV Resonance Raman Studies of Protein Structure and Dynamics**; Sanford A. Asher, *University of Pittsburgh*

3:20 **Coffee Break**

4:00 (480) **Total Internal Reflection with Fluorescence Correlation Spectroscopy**; Nancy L. Thompson, Tammy E. Starr, Alena M. Lieto, Randall C. Cush; *University of North Carolina at Chapel Hill*

4:20 (481) **Simultaneous Photokinetic and Rotational Analyis of PRODAN in Phospholipids Bicelles**; Sharon L Neal; *University of Delaware*

4:40 (482) **Simultaneous Characterization of Multiple Protein Conformers in Solution Using Electrospray Mass Spectrometry and Chemometric Approaches**; Igor A Kaltashov; *University of Massachusetts*

5:00 (483) **Detection of Small Molecules by Receptor Conformational Change and Surface Plasmon Resonance**; Helen V. Hsieh, Jason E Gestwicki, J B Pitner; *BD Technologies; University of Wisc-Madison, BD Technologies*

Wednesday Morning, Room 551B
BIOLOGICAL APPLICATIONS OF MASS SPECTROMETRY
Presider: Richard Yost, University of Florida and Joseph McClellan

8:50 (436) **Identifying the Metal Binding Sites in Metalloproteins Using Metal-Catalyzed Oxidation Reactions and Mass Spectrometry**; Richard W. Vachet, Jihyeon Lim, Richard W Vachet; *University of Massachusetts*

9:30 (437) **Trace level analysis of in vivo formed DNA adducts by capillary HPLC-microelectrospray ionization mass spectrometry**; Paul Vouros, J. R. Soglia, Eric T. Gangl; *Northeastern University*

10:10 **Coffee Break**

10:40 (438) **Clinical Application of Mass Spectrometry for Investigation of Amyloidosis**; Amareth Lim, Mark E. McComb, Tatiana Prokaeva, Lawreen H. Connors, Mary T. Walsh, Martha Skinner, Catherine E. Costello; *Boston University School of Medicine*

11:20 (439) **Qualitative and Quantitative Analysis of Recombinant Glycoproteins by Mass Spectrometry**; Nelly Viseux,; *Biogen, Inc*

Wednesday Morning, Room 553B
ISOTOPE RATIO MS
Presider: Robert Steiner, Los Alamos National Laboratory

8:50 (440) **Development of a Discrete Dynode Multiplier Array for Sector MS**; Charles W Wilkerson, Phil L Jacobson, Robert W Springer, Donald C Gautier, Peter J Todd; *Chemistry Division, Los Alamos National Laboratory, Material Science and Technology Division, Oak Ridge National Laboratory*

9:10 (441) **The Use of Multiple Ion Counting in Isotope Ratio Mass Spectrometry**; Simon Meffan-Main, Zenon Palacz, Sarah Goldsmith; *Micromass UK Ltd,, Micromass UK Ltd, Micromass UK Ltd*

9:30 (442) **Ultratrace Analysis of Actinides by Thermal Ionization Mass Spectrometry: Methods and Results**; Tapas Maiti; *PNRL*

9:50 (443) **Measurements of Actinides in Soil, Sediment, Water and Vegetation Samples Collected in Northern New Mexico**; Deward W. Efurd, Bruce M. Gallaher; *Los Alamos National Laboratory*

10:10 **Coffee Break**

10:40 (444) **Second Interlaboratory Comparison for the Analysis of Pu-239 in Synthetic Urine at the Bq (~ 100 aCi) Level**; D.E. McCurdy; *DE&S*

11:00 (445) **Isotopic Analysis Using Electrochemically Modulated Separations On-Line With Inductively Coupled Plasma Time-Of-Flight Mass Spectrometry**; Douglas C. Duckworth; *Oak Ridge National Laboratory*

11:20 (446) **Pu Isotopic Ratio Determinations in Bioassay Samples**; Paula R. Cable-Dunlap, David Fauth, Thomas Labone, Stephen Lamont, Charles Shick

11:40 (447) **Isotope Ratio Measurements Using Micro-Cavity Source Thermal Ionization Mass Spectrometry**; Lee R. Riciputi, Kristofer B. Ingeneri, P.M.B. Hedberg; *Chemical Sciences Division, Oak Ridge National Lab, P.O. Box 2008, Oak Ridge, TN 37831-6365, Safeguards Analytical Laboratory, IAEA, Wagramer Strasse 5, A-1400, Vienna, Austria*

Wednesday Morning, Room 555B
INDUSTRIAL SUCCESSES WITH CHEMOMETRICS
Presider: Chuck Miller, DuPont

8:50 (448) **Robust Statistical Techniques for Multivariate Calibration**; Randy J Pell; *The Dow Chemical Company*

9:10 (449) **Bridging the Lab-Field Gap in Application Development**; Troy W Francisco; *DuPont Central Research & Development*

9:30 (450) **Feasibility of Process Chemistries Realized using AutoChem's Chemometric**; Veronica A. Bracken, Norm E. Van Order, Jr; *Mettler Toledo AutoChem,, Mettler Toledo AutoChem*

9:50 (451) **Application of Multivariate Calibration Methods to Chemiresistor Array Data**; Kathleen M. Alam, Dion Rivera, Clifford K.Ho, Chad E.Davis; S*andia National Labs*

10:10 **Coffee Break**

10:40 (452) **TBA**; Chuck Miller; D*upont*

11:00 (453) **Prediction of baking quality by chemometric analyses of protein electrophortic patterns.**; Ellen M. Faergestad, Frank Westad, Hans J. Skarpeid, Harald Martens, Ellen M. Magnus; *MATFORSK, Norwegian Food Research Institute, Norwa,, KVL, Denmark*

Wednesday Morning, Room 553A
NEW ADVANCES IN HPLC FOR PHARMACEUTICAL ANALYSIS
Presider: Peter Gavin, Eli Lilly and Company

8:50 (454) **Recent Advances in HPLC Column Technology**; Ronald E. Majors, William E. Barber; *Agilent Technologies*

9:30 (455) **Investigating the Use of Monolithic Columns For HPLC Method Development and High-Throughput Analysis**; Nicholas P Toltl, Russell P. Grant, Wincent Lau, Cheryl Cameron, Malcolm Angod, Yiu-Chung Lee, Timothy J Wozniak, Nicholas E. McDonald, Bernard A. Olsen, Peter F. Gavin; *Eli Lilly and Company*

10:10 **Coffee Break**

10:40 (456) **Chiral Separations of Pharmaceutical Compounds on Polysaccharide Stationary Phases: Manipulation of Retention and Selectivity with Polar Mobile Phase Modifiers**; Thomas F Hooker; *Merck and Co., Inc*

11:20 (457) **Applications of Ultra-Stable Phases for HPLC: High Temperature Ultra-Fast Liquid Chromatography and Thermally Tuned Tandem Column (T3C) Liquid Chromatography**; Gregory T Gaudet, Peter W Carr, Clayton V. McNeff, Angelos Kyrlidis, Jon Thompson, Yun Mao; *ZirChrom Separations, Inc., Cabot Corporation, University of Minnesot,, Merck & Company*

Wednesday Morning, Room 557
BIOMEDICAL RAMAN SPECTROSCOPY
Presider: Steve Barnett, OptoMedical

8:50 (458) **Raman spectroscopy for analysis and diagnosis of disease**; Michael S. Feld; *GR Harrison Spectroscopy Laboratory, MIT*

9:30 (459) **Identification and Classification of Oral Bacteria by Raman Spectroscopy**; Andrew J. Berger, Dahu Qi, Robert Quivey; *The Institute of Optics, University of Rochester, Department of Physics and Astronomy, University of Rochester, Center for Oral Biology*

10:10 **Coffee Break**

10:40 (460) **Cancer Gene Detection Using Surface-Enhanced Raman Scattering (SERS)**; Tuan nmn Vo-Dinh, *Oak Ridge National Laboratory*

11:20 (461) **Protocols for Raman and Correlative Light Microscopic Imaging of Bone Tissue**; Nicole J. Crane, Michael D. Morris, Michael A. Ignelzi, Jr; *University of Michigan*

11:40 (462) **Near Infrared Diffuse Reflectance and NIR-Raman Biospectroscopy of Milk for Composition Analysis and Animal Health Estimation**; David H. Burns, Amila de Silva; *McGill University*

Wednesday Morning, Room 556B
RAMAN SPECTROSCOPY II
Presider: Bruce Chase, Dupont

8:50 (463) **Molecular orientation and strain induce crystallization of syndiotactic polypropylene (sPP) using infrared and Raman spectroscopic methods**; Vasilis G. Gregoriou, Georgia Kandilioti, Costas Gatos, Costas Galiotis; *ICEHT-FORTH,, ICEHT-FORTH, ICEHT-FORTH,, ICEHT-FORTH*

9:10 (464) **Temperature Dependent Raman Spectroscopic Studies of Polymer Composite**; Zhenhuan Chi, Bin Chen, Julie P Harmon, Alan M Cassell, Patricia Anne O Muisener; *Renishaw Inc., 5277 Trillium Blvd., Hoffman Estate, NASA Ames Research 2Center, Moffett Field, CA 94035, Department of Chemistry, University of South Florida, 4202 E. Fowler Avenue, Tampa, Fl 33620*

9:30 (465) **Raman Spectroscopy of Molecular Spin-States in Cyanide-Bridged Iron(II) Spin-Crossover Coordination Polymers**; John J. McGarvey, Gabor Molnar, Virginie Niel, Jose-Antonio Real, Antoine Zwick, Azzedine Bousseksou; *School of Chemistry, Queen's University Belfast, N,, Laboratoire de Chimie de Coordination, CNRS UPR-8241, Toulouse, France, Departamento de Quimica Inorganica, Universidad de Valencia, Spain,, Laboratoire de Physique des Solides, CNRS UMR-5477, Toulouse, France*

9:50 (466) **Raman Strain Imaging of MEMS Components For Quality Control**; John D. Baker, David D Tuschel, Patrick J Treado; *ChemIcon, Inc*

10:10 **Coffee Break**

10:40 (467) **Molecular Orientation and Crystallinity of some Commercial Polypropylene Products studied by Micro Raman Spectroscopy**; Andreas Gupper, Peter Wilhelm, Markus Gahleitner, Goulnora Yu. Nikolaeva, Kirill A. Prokhorov, Sergey A. Gordeyev; *Forschungsinstitut fuer Elektronenmikroskopie und,, Borealis GmbH, St. Peter Straße 25, 4021 Linz, Austria (M.G.), General Physics Institute of Russian Academy of Sciences, 38 Vavilov St., 119991 Moscow, Russia (G.N. and K.P.),, Department of Chemical & Process Engineering, University of Strathclyde, 75 Montrose St., Glasgow G1 1XJ, UK (S.G.)*

11:00 (468) **Raman Spectroscopic Characterization of Temperature Dependent Polymer Structure**; Zhenhuan Chi, Zhenhuan Chi, Hugh Gotts, Bin Chen; *Renishaw Inc., 5277 Trillium Blvd., Hoffman Estate, Analytical Services Group, Santa Clara, CA 95054, NASA Ames Research Center, Moffett Field, CA 94035*

11:20 (469) **Kinetic Study of the Decomposition of Notrite to Nitrate in Acid Samples Using Raman Spectroscopy**; Makhapa A. Makhafola, Jacobus F. van Staden, Danita de Waal; *University of Pretoria*

Wednesday Morning, Room 556A
INDUSTRIAL APPLICATIONS OF ADVANCED INFRARED SPECTROSCOPY
Presider: Eric Jiang, Nicolet Instruments

8:50 (470) **Monitoring Photopolymerisation Initiators Using Fast Time-Resolved Infrared Spectroscopy**; Michael W. George; *Nottingham University*

9:10 (471) **Depth Resolution via Time Resolution in FT-IR Photoacoustic Spectroscopy of Layered and Gradient Materials**; John F. McClelland, Roger W Jones; *MTEC Photoacoustics, Inc., Ames Laboratory-USDOE, Iowa State University*

9:30 (472) **Self Modeling Curve Resolution Analysis of On-Line ATR/FT-IR**; Yukihiro Ozaki, Slobodan Sasic, Toru Amari, Heinz W Siesler; *Kwansei Gakuin University, Center for Analytical Chemistry and Science, Inc., University of Essen*

9:50 (473) **MACROSCOPIC SPECTRAL IMAGING**; Curtis Marcott, Gloria M Story, Anthony E. Dowrey; *The Procter & Gamble Company*

10:10 **Coffee Break**

10:40 (474) **Chemical Imaging of Coated Syhthetic Fibers, Polymer Resins and Films by IR-FPA, IR-Microscopy and Raman Microscopy: A comparative study**; Francis V. Acholla, Kenneth B. Laughlin, Scott T. Wills, Wei Xie; *Rohm and Haas Company*

11:00 (475) **Improving the Quality of Information Obtained from a Sample with Hyperspectral Imaging**; Stephen R. Lowry, William C McCarthy, Koichi Nishikida; *Thermo Nicolet*

11:20 (476) **Pharmaceutical Applications of Mid-Infrared and Near-Infrared Chemical Imaging**; Linda H. Kidder, E. Neil Lewis, Eunah Lee, Frederick W Koehler; *Spectral Dimensions, Inc*

11:40 (477) **High Throughput Heterogeneous Catalyst Screening via FTIR Imaging**; Christopher M. Snively, Jochen Lauterbach; *Purdue University, University of Delaware*

SPECTROSCOPIC PROBING OF BIOMOLECULES AND ASSEMBILIES
Papers 478 – 483 can be found on Tuesday afternoon

Wednesday Morning, Room 552B
LIPPINCOTT AWARD
Presider: Mike Pellitier, Kaiser Optical

8:50 (484) **Adventures in UV Resonance Raman Spectroscopy: Big Photons Yield Lots of Information**; Sanford A. Asher; *University of Pittsburgh*

9:30 (485) **Femtosecond Coherence Spectroscopy of Biomolecules**; Paul M Champion; *Northeastern University*

10:10 **Coffee Break**

10:40 (487) **Intensity Enhancement in VCD and ROA due to Resonance with Excited Electronic States of Magnetic Dipole Character**; Laurence A. Nafie, Yanan He, David A. Dunmire, Teresa B. Freedman; *Department of Chemistry, Syracuse University*

11:20 (488) **The Scale of Things: Spectroscopy and Scaling Laws in Bioenergetics**; William H. Woodruff

Wednesday Morning,Room 555A
CHEMOMETRICS IN BIOTECHNOLOGY
Presider: Renee JiJi, NRL

8:50 (489) **Soft Modelling In Bioinformatics By PLSR**; Harald Martens, Ib Søndergaard, Bjørn Alsberg, Martin Høy, Arnar Flatberg, Lars H. Gidskehaug, Endre Anderssen, Lars Munck, Åsmund Bjørnstad; *Technical Univ. of Denmark, Norwegian Univ. of Sci. and Technol., Royal Vet. and Agric. Univ. Denmark, Norwegian Agric. Univ.*

9:30 (490) **Phenotypics: Spectral covariate phenotypic gene and environment indicators in biotechnology**; Lars Munck; *The Royal Veterinary and Agricultural University*

10:10 **Coffee Break**

10:40 (491) **Rapid analysis of Complex Biological Systems Using Advanced Spectroscopies and Machine Learning**; Royston Goodacre, Seetharaman Vaidyanathan, Douglas B. Kell; *University of Wales*

11:20 (492) **Optimization Strategies for Immobilized Biomolecular Arrays**; Jonathan E. Forman, Christina Ho, Jac Luna, Nicole Lunceford, Audrey D. Suseno, Hui Zhou

12:00 (493) **Plenary Discussion: Impact of Chemometrics on Biotechnology in the Future;** Lars Munck**;** ***The Royal Veterinary and Agricultural University***

Wednesday Morning, Room 554A
SEPARATIONS FOR THE REAL WORLD
Presider: Phyllis Brown, University of Rhode Island

8:50 (494) **Designing New Phases for Separations in the 21st Century**; Patrick D McDonald; *Waters Corporation*

9:30 (495) **Analytical to Preparative HPLC: Methods Development, Scale-up and Production**; Prabha Painuly; *Varian, Inc*

9:50 (496) **The Capillary Electrophoresis of Peptides**; Lenore Martin; *University of Rhode Island*

10:10 **Coffee Break**

10:40 (497) **Mass Spectral Characterization of Tetracyclines by Electrospray Ionization, Hydogen/Deuterium Exchange, and Multiple Stage Mass Spectrometry**; Amin M. Kamel, Hassan G. Fouda, Phyllis P. Brown, Burnaby Munson; *Pfizer Global Res. and Dev., Dept. of Drug Metabolism, Department of Chemistry, University of Rhode Islan,, Department of Chemistry and Biochemistry, University of Delaware*

Wednesday Morning, Room 554B
SPECIATION
Presider: Joe Caruso, University of Cincinnati

8:50 (498) **Selenium Speciation in Urine AT Physiological Levels by HPLC-ICP-MS**; J. A. Caruso, K. Wrobel, S. Kannamkumarath; *University of Cincinnati*

9:10 (499) **The Analytical Chemistry of Anticarcinogenic Organoselenium Compounds**; Peter C Uden; *University of Massachusetts*

9:30 (500) **Capillary Electrophoresis With the Parallel ICP MS and ES MS/MS Detection for Metalloproteins Analysis**; Sandra N. Mounicou, Kasia Polec, Dirk Schaumloeffel, Joanna Szpunar, Andreas Prange, Ryszard Lobinski; *Group of Bionorganic Analytical Chemistry, CNRS UM,, Institute for Coastal Research, Department of Physical and Chemical Analysis, GKSS-Research Centre, Max-Planck-Staße, D-21502 Geesthacht, GERMANY, Department of Analytical Chemistry, Faculty of Chemistry, Warsaw University of Technology, ul. Noakowskiego 3, 00-664 Warszawa, POLAND*

9:50 (501) **Compound Independent Calibration of Pesticides and Herbicides by GC-ICP-MS**; Steve M. Wilbur, Randy Cummings; *Agilent Technologies, US EPA Region 10 Laboratory*

10:10 **Coffee Break**

10:40 (502) **Unique Species Information by Field-Flow Fractionation Inductively Coupled Plasma Mass Spectrometry**; Ramon M. Barnes, Atitaya Siripinyanond; *University Research Institute for Analytical Chemistry, University of Massachusetts, Department of Chemistry*

11:00 (503) **Evaluation of Methods for the Extraction and Speciation of Arsenic Present in Various Raw and Processed Food Products**; Nohora P. Vela, Douglas T. Heitkemper, Barbara S. Barnes, Tyre D. Grant, Pamela R. Keating; *U.S. Food and Drug Administration, University of Cincinnati*

11:20 (504) **ICP-MS and ES-MS for the Determination of Se Species in Accumulating Plants**; Maria Montes-Bayon, Danika L. LeDuc, Norman Terry, Joseph A Caruso; *Department of Physical and Analytical Chemistry, Department of Plant and Microbial Biology.University of California Berkeley. Berkeley. CA, Department of Chemistry. University of Cincinnati. Cincinnati. OH*

Wednesday Morning, Room 552A
ICP-OES INSTRUMENTATION AND METHODS
Presider: Ken Marcus, Clemson University

8:50 (505) **On-line Construction of Control Charts for Atomic Spectrometry**; Doug Shrader, Michelle Cree, John Sanders, Eric Vanclay, Glyn Russell; *Varian, Inc,, Varian Australia Pty Ltd.*

9:10 (506) **Trace Determinations & High Precision In Various Matrices by High Resolution ICP-OES Spectrometry**; Albert Brennsteiner, Geoff Tyler, Agnes Cosnier, Nathalie Le Corre, Celia Olivero; *Jobin Yvon S.A., 16-18 rue du Canal, 91165 Longjumeau, Cedex, France, Jobin Yvon Inc., 3880 Park Avenue, Edison, NJ 08820 USA*

9:30 (507) **Improving Sample Throughput and Accuracy in ICP-OES**; Glyn Russell, Ingrid Szikla, Michelle E. Cree, Michael B. Knowles; *Varian Australia Pty Ltd*

9:50 (508) **Designing an Echelle Optical system for an Inductively Coupled Plasma Emission Spectrometer (ICP-OES) to Improve the Quality of Results**; Manuel C. Almeida, David Pfeil, Peter Brown; *Leeman Labs, Inc*

10:10 **Coffee Break**

10:40 (509) **Performance Enhancements Beyond the Latest Generation CID**; Stuart Georgitis, Jim Batchelor, Michael Corvese, Peter Bradley; *Thermo Elemental*

11:00 (510) **Analysis of High-Purity Metals and Semiconductor Grade Specialty Chemicals by Axial ICP-AES with CCD detection**; George G. Glavin, Sergei V Leikin; *Spectro Analytical Instruments*

11:20 (511) **Background Phenomena in Inductively Coupled Plasma Optical Emission Spectrometry**; Greet de Loos, *Delft University of Technology*

Wednesday Morning, Room 551A
NANOSTRUCTURES II
Presider: C. J. Zhong, SUNY-Binghamton

8:50 (512) **Theoretical and Experimental Design of Novel Apertureless Probes for High Resolution Optical Imaging**; Xiaoliang S. Xie, John T. Krug, II, Erik J. Sánchez, X. Sunney Xie; *Department of Chemistry and Chemical Biology, Harvard*

9:30 (513) **Combinatorial Approaches Using Scanning Probe Microscopy**; John-Bruce D. Green; *University of Alberta*

9:50 (514) **Patterned Thin Films of PAMAM Dendrimers Formed Using Microcontact Printing**; Shane C. Street, David Arrington, Michael Curry, Shane Street; *The University of Alabama*

10:10 **Coffee Break**

10:40 (515) **Langmuir Monolayers of Gold Nanoparticles: From Ohmic to Rectifying Charge Transfer**; Shaowei Chen, Siyuan Liu

11:00 (516) **Organic Monolayers on Silicon: Microprinting, Micromachines, and Microarrrays**; Xiaoyang Zhu; *University of Minnesota*

Wednesday, 2:00 PM – 5:00 PM, Exhibit Hall C
SAS 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 plce for the entire time. Actual presentaiton times are staggered. Check your presentation time on the following pages

2:15 (517) **Orientation Study of Thick Poly(ethylene terephthalate) Films by Transmission Infrared Spectroscopy**; Christian Pellerin, Marie-Eve Rousseau, Robert E. Prud'homme, Michel Pezolet; *Department of Chemistry, Laval University, Quebec*

3:30 (518) **Picomole Analysis on Nanoparticles in Microchannels:**; Stuart Farquharson, Paul Maksymiuk, Llord Burgess, Yuan-Hsiang Lee, Stuart Farquharson; *University of Rhode Island, University of Washington, Real-Time Analyzers*

2:15 (519) **Infrared Spectroscopy, Differential Scanning Calorimetry, and X-Ray Diffraction Studies on Structure and Thermal Behavior of Poly(hydroxyalkanoate)**; Adchara Padermshoke, Harumi Sato, Sanong Ekgasit, Isao Noda, Yukihiro Ozaki; *Department of Chemistry, School of Science and Tec,, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand, The Procter and Gamble Company, 8611 Beckett Road, West Chester, Ohio 45069, USA,,*

3:30 (520) **Dynamic FT-Raman Spectroscopy of Polymeric Fibers**; Simon Frisk(1), Richard M. Ikeda (1), Bruce D. Chase (2), John F. Rabolt (1); *Dept. of Materials Science and Engineering, Central Research and Development, DuPont Experimental Station*

2:15 (521) **Development of Novel Metal-Pliable Polymer Composites as Surface-Enhanced Raman Spectroscopy Substrates for Use in Capillary Electrophoresis of Environmentally Relevant Analytes**; Michael J. Sepaniak, R. Maggie Connatser, Kathleen S. Giesfeldt, Nickolay V. Lavrik, Gerald L. DeVault, Michael J. Sepaniak; *Department of Chemistry, University of Tennessee*

3:30 (522) **Characterization of Metal-Pliable Polymer Composites**; Kathleen S. Giesfeldt, R. Maggie Connatser, Nickolay Lavrik, David C. Joy, Michael J. Sepaniak; *University of Tennessee, Knoxville*

2:15 (523) **Selenium Speciation by Gas Chromatography with Element Specific detection and Mass Spectral Identification**; Harriet Totoe (1), Eric Block (2), Julian F Tyson (1), Peter C Uden (1); *Department of Chemistry, University of Massachuset, Department of Chemistry, SUNY at Albany, Albany NY 12222*

3:30 (524) **Enhanced Vibrational Circular Dichroism in Ligand-Bound Metmyoglobins**; David A. Dunmire,, Xiaolin Cao, Teresa B. Freedman, Laurence A. Nafie; *Department of Chemistry, Syracuse University*

2:15 (525) **Improved Performance of a Dual Circular Polarization Raman Optical Activity Spectrometer**; David A. Dunmire, Teresa B. Freedman, Laurence A. Nafie; *Department of Chemistry, Syracuse University*

3:30 (526) **Solid Phase Extraction: A Simple and Promising Organic Matrix Elimination Approach for Trace Element Analysis**; Zheng Yang, Bradley T Jones; *Wake Forest Univ*

2:15 (527) **The Quantification Of Accessible Hydroxyl Sites In Fiberglass Materials Using Solid State NMR Spectroscopy**; Natia Tsomaia, Roderick A. Fry, Karl T. Mueller; *Department of Chemistry and Materials Research*

3:30 (528) **Electrodic and EDTA-Enhanced Phytoremediation of Lead using Indian Mustard (Brassica juncea)**; David J. Butcher, Jae-Min Lim, Arthur Salido, *Western Carolina University*

2:15 (529) **in-vitro Determination of Tissue pH and Lactate Concentration Using Near-Infrared Spectroscopy on Excised Human Atherosclerotic Plaques**; Tania Khan, Morteza Naghavi, Babs R Soller; *University of Massachusetts Worcester, Texas Heart Institute, Center for Vulnerable Plaque Research, University of Massachusetts Worcester*

3:30 (530) **Enantiomeric Excess Determination using Near-Infrared Vibrational Circular Dichroism (NIR-VCD) Spectroscopy**; Changning Guo (1), Xiaolin Cao(1), Rekha D. Shah(2), Teresa B. Freedman(1), Rina K. Dukor(3), Laurence A. Nafie(1,3); *(1)Department of Chemistry, Syracuse University, S,, (2)Johnson & Johnson Pharmaceutical Research and Development LLC, Spring House, PA 19477, (3)BioTools, Inc., 950 N. Rand Road; Unit 123, Wauconda, IL 60084*

2:15 (531) **Membrane Desolvation For HPLC He-MIP Atomic Emission Spectroscopy**; Glenn I Dennis, Debashis Das, Jon W Carnahan; *Northern Illinois University*

3:30 (532) **Identification and Characterization of Organoselenium Compounds in Yeast and Mushrooms by HPLC-ICP-MS and ESI-MS**; Chethaka L Kahakachchi, Chethaka L Kahakachchi (1), Julian F Tyson (1), Peter C Uden (1), Eric Block (2), Philip D Whanger (3); *Department of Chemistry, Lederle Graduate Research, Department of Chemistry, SUNY-Albany, Albany NY 12222, Department of Environmental and Molecular Toxicology, Oregon State University, Corvallis, OR 97331*

2:15 (533) **Investigations of Passive Uranyl Ion Binding to Datura innoxia Cell Walls**; Debbie D. Martinez, Gary D Rayson; *New Mexico State University*

3:30 (534) **Manipulation of Transportation Efficiency of the Aerosol Particles Generated from the ETV to the ICP-MS.**; Nikhilesh K Desai, James A Holcombe; *University of Texas at Austin*

2:15 (535) **Quantitative Microscopic Analysis of Filled Newsprint Handsheets**; Fern S. Mancosky, Timothy Patterson; *Institute of Paper Science and Technology*

3:30 (536) **Determination of the pki of the Ethanolic Extract of Cola Acuminata Using UV-VIS Spectrophotometer**; Chimezie A. Anyakora; *University of Lagos*

2:15 (537) **Spectroscopic and Microscopic Characterizations of Nanostructured Interfacial Sensing Materials**; Li Han, Li Han, Chuanjian Zhong; *State University of New York at Binghamton*

3:30 (538) **Isolation and Characterization of NAD Dimer and Its Photo-Degradation Products**; Laurel A. Luckey, Alexander Scheeline; *University of Illinois Urbana-Champaign*

2:15 (539) **An Inductively Coupled Plasma Carbon Emission Detector for Native L-Amino Acid Separations by Aqueous Reverse Phase Liquid Chromatography**; Bradley T. Jones, Heather L. Peters, Xiandeng Hou, Bradley T. Jones; *Department of Chemistry, Wake Forest University, College of Chemistry, Sichuan University, Chengdu, Sichuan 610064, P.R. China*

3:30 (540) **Improved Spectral Resolution of a Cs Resonance Fluorescence Detector by Electromagnetically Induced Transparency**; James D. Winefordner, Tiffany L. Correll, Nathan C. Pixley, Dimitri Pappas, Nicolo Omenetto, Benjamin W. Smith; *University of Florida*

2:15 (541) **Automating Near- and Mid-Infrared Calibration Development and Testing for Quantitative Analysis.**; James B Reeves, III, Stephen R Delwiche; *AMBL, ANRI, USDA,, ISL, ANRI, USDA*

3:30 (542) **The Analytical Chemistry Division of the International Union of Pure and Applied Chemistry**; David S. Moore, *Los Alamos National Laboratory*

2:15 (543) **Elemental Analysis of Platinum-Iridium Alloys (90/10, 80/20, 75/25, and 70/30) and Pure Pt by ICP**; Elizabeth A. Jones, Steve Johnson; *Medtronic, Inc.*

3:30 (544) **Studies on Flow-Injection In Situ Trapping of Volatile Species of Gold in Graphite Furnace and Atomic Absorption Spectrometric Determination**; Shukun Xu, Hongbing Ma, Xiaofeng Fan, Huanying Zhou; *Research Center for Analytical Sciences*

2:15 (545) **Detection of Contaminants in Water Using Membrane Inlet Mass Spectrometry**; Frants R. Lauritsen, Tenna Aggerholm; *Department of Biochemistry and Molecular Biology*

2:15 (547) **Electrodecomposition of Organic Pollutants and Analysis of its Derivatives by Standard Method, GC-MS and HPLC in an Inorganic Membrane Reactor.**; Angwafor Fru Chi F Chi, Alvin M. Maluleke, Vladimir C Linkov; *University of the Western Cape*

3:30 (548) **A Novel Quantification Methodology for the Determination of Serum Sex Hormone Profile Using LC/MS/MS with Stability Assurance of Catechol Estrogens**; Yu-Chen Chang, Chien-Ming Li, Hsin-Yi Kao, Louis W Chang, Pao-Chi Liao; *National Health Research Institutes, Taiwan, National Cheng Kung University Medical College, Taiwan*

2:15 (549) **The Role of Elemental and Molecular Speciation in Achieving Discharge Limits for Toxic Trace Metals**; Carl E. Hensman, Philip Kilner, Hakan Gurleyuk; *Frontier Geosciences Inc,*

3:30 (550) **Simultaneous Determination of Hydroxyl Value, Ethylene Oxide Content and Primary Hydroxyl Content for Polyetherpolyol by Infrared Spectroscopy**; Kiyoshi Yamamoto, Reiko Kakita, Chitoshi Suzuki, Masanori Meno, Yoko Nozawa; *Asahi Glass Co., Ltd., Asahi Glass Urethane Co., Ltd., Yokogawa Electric Co., Ltd.*

2:15 (551) **Correlation of the Molecular Orientation and Photonic Properties of Rigid-flexible Polymers using FT-IR Linear Dichroism and Photoluminescence Spectroscopic Techniques**; Vasilis G Gregoriou, Christos Chochos, Georgia Kandilioti, Valandoula Deimede; *ICE/HT-FORTH*

3:30 (552) **Materials Characterization Using Micro X-Ray Fluorescence Elemental Imaging**; George J. Havrilla, Thomasin C. Miller, Martha R. Joseph; *Los Alamos National Laboratory, Department of Chemistry, Westminster College*

2:15 (553) **Condensation Nucleation Light Scattering Detection with Ion-exchange Chromatography for Direct Determination of Glyphosate and Aminomethylphosaphonic Acid in Water**; John A. Koropchak, Jing You; *Department of Chemical and Biochemistry Southern Illinois University*

3:30 (554) **Development of a New Air-Cooling Torch for Argon and Helium ICP**; Hidekazu Miyahara, Hironobu Yabuta, Yasushi Hayashi, Masato Watanabe, Eiki Hotta, Akitoshi Okino; *Department of Energy Sciences Tokyo Institute*

2:15 (555) **GC/MS Analysis of Volatile Components of Echinacea Species**; Nirmalendu Datta-Gupta, Xing Dong Yao, Nirmalendu Datta-Gupta; *South Carolina State University*

3:30 (556) **Determination of Trace Metals in Tissues using Collision Cell Inductively Coupled Plasma Mass Spectrometry (ICP-MS)**; Frank X. Weber, Peter M. Grohse, Beatrice M. Wilson; *Research Triangle Institute*

2:15 (557) **Modification of Vitamin E Analysis Method for Routine Use**; Qinglong Chang, Qinglong Chang, Rob Massatti, John Parsen, Sherry Combs; *Soil and Plant Analysis Lab, University of Wisconsin*

3:30 (558) **Mass and Optical Spectroscopy of PAH Cations Measured Using an Ion-Trap Mass Spectrometer**; Michael W. Blades, August Specht, Dennis Rolland, John Hepburn; *University of British Columbia*

2:15 (559) **Application of HPLC-ICP-MS for In Vitro Studies on Biomethylation Oo Arsenic Compounds**; Sasi Kannamkumarath, Katarzyna Wrobel, Kazimierz Wrobel, Joseph A Caruso; *University of Cincinnati,OH, USA, Universidad de Guanajuato, Mexico*

3:30 (560) **A New Glow Discharge Source For Time-of-Flight Mass Spectrometry**; Kevin P. Turney, Elizabeth P. Hastings, J. Pisonero, W. W Harrison; *University of Florida, Universidad de Oviedo*

2:15 (561) **Two-Photon Crossed Beam Optical System for Use of 3-D ORAM Raidation Dosimeter**; Tuan Vo-Dinh, Joon Myong Song, Brian M Cullum, Joel Mobley, James S Bogard, Marko Moscovitch, Gary W Phillips, Tuan Vo-Dinh; *Oak Ridge National Laboratory, Georgetown University Medical Center*

3:30 (562) **Determination of Cobalamins (Vitamin B12) Using CE-ICP-MS**; Nancy J Miller-Ihli, Enrique G Yanes; *USDA, BHNRC, Food Composition Laboratory*

2:15 (563) **Development of an Accurate and Precise Method for Determining Arsenic Species in Various Contaminated Soils Using HPLC-ICP-MS**; Bryan L. Parker, Kazmierz Wrobel, Sasi Kannamkumarath; *University of Cincinnati*

3:30 (564) **Advances in the Instrumentation and Studies of FT-Near Infrared Vibrational Circular Dichroism Spectroscopy**; Xiaolin Cao, Teresa B. Freedman, Laurence A. Nafie; *Department of Chemistry, Syracuse University*

2:15 (565) **Oil and Other Organic Samples by Inductively Coupled Plasma Optical Emission Spectroscopy: Direct Injection or Digestion Methods**; James D. Osborne, Karen J. Jones, Robert A. Massing, Robert M. Montgomery, William F. Vermillion; *Eli Lilly and Company*

3:30 (566) **Determination of Physical Properties and Natural Contaminants**; Brian Wm. Corbett, Mary Kate Donais; *Saint Anselm College*

2:15 (567) **Measurement of Atmospheric Particle-Phase Mercury by Laser Aerosol Mass Spectrometry**; Giuseppe A. Petrucci, Bryan J. Holmes; *University of Vermont*

3:30 (568) **Use of Synchrotron Infrared Spectromicroscopy as a Rapid, Direct, Non-Destructive Method for the Study of Inks on Antique Stamps**; Dale L. Perry, Tommy J. Wilkinson, Michael C. Martin, Wayne R. McKinney; *Lawrence Berkeley National Lab*

2:15 (569) **The Analytical Sciences Digital Library**; Cameron Dorey, Ted Kuwana, Stuart Chalk, Cynthia Larive, George Long; *University of Central Arkansas, University of Kansas, University of North Florida, Indiana University of Pennsyvania*

3:30 (570) **Novel Chemometric Algorithms Applied to Chemical Imaging Data**; Robert C. Schweitzer, Arjun S. Bangalore, Patrick J. Treado; *ChemIcon, Inc*

2:15 (571) **As and Se Determination in Blood and Animal Tissues by FI-HG-AAS With In-Situ Trapping on Rhodium-Coated W-Coil Atomizer**; Fernando Barbosa Jr, Samuel S. de Souza, Francisco J. Krug; *Centro de Energia Nuclear na Agricultura- Usp*

3:30 (572) **Surface Studies of Corrosion of Steel by Lead-Bismuth Eutectic**; Dale L. Perry, Daniel Koury, Allen L. Johnson, Brian Hosterman, Denise Parsons, John W. Farley; *Department of Physics, University of Nevada, Las Vegas, Lawrence Berkeley National Laboratory*

2:15 (573) **The Development of Miniaturized Surface Plasmon Resonance Probes for In-Situ Moisture and Gas Monitoring**; Kristine L. Eland; *Westinghouse Savannah River Company*

3:30 (574) **Advances in VOC Monitoring by On-Line Mass Spectrometry**; Colin A. McGill, Robert Wright, David Littlejohn; *University of Strathclyde/CPACT, ThermoOnix*

2:15 (575) **Fiber-Optic Surface Plasmon Resonance Probes for In-Vivo Biochemical Monitoring**; Karl Booksh, Jean-Francois Masson; *Arizona State University*

3:30 (576) **Fibre Optic Based SPR Analysis of Marine and Hydrothermal Environments**; Karl S. Booksh, Darcy J. Gentleman, Louis A. Obando, John R Holloway; *Dept. of Chemistry and Biochemistry, ASU, Dept. of Geological Sciences, ASU*

2:15 (577) **EEM Spectrofluorometer Followed by Photocatalytic Induced Kinetic Changes**; Karl S. Booksh, Yoon-Chang Kim; *Department of Chemistry & Biochemistry, Arizona State*

3:30 (578) **Molecularly-Imprinted, Polymer-Coated Fiber-Optic SPR Probes for the Detection of PAHs**; Karl S. Booksh, Yoon-Chnag Kim; *Department of Chemistry & Biochemistry, Arizona State*

2:15 (579) **EEM spectrofluorometer followed by photocatalytic induced kinetic changes**; Karl S. Booksh, Yoon-Chang Kim; *Department of Chemistry & Biochemistry, Arizona State*

2:15 (581) **Raman Spectra of Model Bone: Substituted Hydroxyapatites**; Mary M. J. Tecklenburg, Robert Buckland, Amy Marcotte, Adam Perala; *Central Michigan University*

3:30 (582) **Single Particle Analysis of Submicron Particles via Capillary Electrophoresis**; Mitchell E Johnson, Jason C Stokes; *Duquesne University*

2:15 (583) **Micro-Raman studies of as-grown and thermally annealed HgCdTe epitaxial thin films**; Krishna K Deb, Silvue Velicu, Paul Boieriu, Nibir Dhar, Gregory Brill; *Army Research Laboratory, SEDD, 2800 Powder Mill R, SPI, Inc, Bolingbrook, IL 60440, EPIR Ltd, Bolingbrook, IL 60440*

3:30 (584) **FT-IR Studies of Uniaxially Drawn Poly(Ethylene Terephthalate)**; Vasilis G. Gregoriou, Giannis Govaris, Georgia Kandilioti; *ICEHT-FORTH*

2:15 (585) **Raman Microscopy at the Arts/Science Interface**; Gregory D. Smith, Tracey D. Chaplin, Robin J. H. Clark, David Jacobs; *National Synchrotron Light Source, University College London, University College London, British Library*

3:30 (586) **Raman Microscopy and Remote Laser Raman Spectroscopy in Art History and Conservation Science: Three Illuminated Gutenberg Bibles**; Gregory D. Smith, Tracey D. Chaplin, Robin J. H. Clark, Kristian Jensen, David Jabobs; *C. Ingold Lab- Univ. College London,, The British Library*

2:15 (587) **Solution Conformations of Tripeptides and Cyclosporins Using Vibrational Circular Dichroism**; Laurence A. Nafie, Louise A .Bodack, Teresa B. Freedman, Monika Plass, Babur Z. Chowdhry; *Department of Chemistry, Syracuse University, Syracuse, NY 13244-4100 USA, Department of Chemistry, Martin-Luther-University, D-06099, Halle (Saale), Germany, School of Biological Sciences, University of Greenwich, Woolwich, London SE186PF, UK*

Thursday Morning, Room 552B
HIGH PERFORMANCE MASS SPECTROMETRY: FROM FUNDAMENTALS TO BIOLOGICAL APPLICATIONS
Presider: David Muddiman, VA Commonwealth

8:50 (588) **High Sensitivity and Mass Accuracy of Large Nucleic Acids**; David C. Muddiman; *Virginia Commonwealth University*

9:30 (589) **Integrating Top-Down and Bottom-Up Mass Spectrometry for Comprehensive Proteome Characterization**; Robert L. Hettich, Nathan VerBerkmoes, Joshua Sharp, Keiji Asano; *Oak Ridge National Laboratory / University of Tennessee Genome Science and Technology School*

10:10 **Coffee Break**

10:40 (590) **A Proteomics Approach to Understanding Protein Ubiquitination**; Steven P Gygi, Junmin Peng, Carson C. Thoreen, Dongmei Cheng, Joshua E. Elias, Steven P. Gygi; *Harvard Medical School*

11:20 (591) **Adding Meaning to Complex Data Sets; Implementation of Multi-Tiered Database Searching and Spectral Interpretation for Multidimensional LC/MS/MS data**; Roy Martin; *Micromass*

Thursday Morning, Room 554A
LC/MS FOR THE ANALYSIS OF PHARMACEUTICALS
Presider: Thomas Hooker, Merck and Company, Inc.

8:50 (592) **Development of a System for Automatic Processing and Posting of Data from Open-Access LC/MS Instruments to the Web**; Kenneth L. Ray, Scott A. Miller, Brent L. Kleintop; *Bristol-Myers Squibb*

9:30 (593) **LC-MS: A Critical Tool for Metabolite Identification**; Cornelis E .Hop; *Merck Research Laboratories*

10:10 **Coffee Break**

10:40 (594) **Improving Analytical Ability to Address Chemical Diversity: Multi-mode Ionization for LC/MS**; Michael P Balogh; *Waters Corporation*

11:20 (595) **Recent Advances in LC/MS/MS Analysis of Warfarin**; James T Kapron

Thursday Morning, Room 555B
NANOTUBES AND NANOTECHNOLOGY
Presiders: Fan Adar and Andrew Whitley, JY Horiba

8:50 (596) **Raman Scattering From Confined Phonons in Semiconducting Nanowires**; Peter C. Eklund, *Department of Physics, Pennsylvania State University*

9:30 (597) **Charge Transer and Selective Interactions Between Conjugated Polymers andCarbon Nanotubes Probed by Surface Enhanced Raman Spectroscopy**; Alan Dalton; *University of Texas*

9:50 (598) **Raman Spectroscopy of Noncovalently Functionalized Carbon Nanotubes**; Wayne A. Weimer, Rishi Gupta, Jian Chen; *Zyvex Corporation*

10:10 **Coffee Break**

10:40 (599) **Device Fabrication Using Nanotubes with Molecular Recognition Function and Their Spectroscopic Studies**; Hiroshi Matsui, Yung-fou Chen; *City University of New York, Hunter College*

11:00 (600) **Use of Raman Spectroscopy to Characterize the Catalytic Production of Single-walled Carbon Nanotubes (SWNT)**; Daniel E. Resasco, Jose E. Herrera, Leandro Balzano, Francisco Pompeo; *University of Oklahoma, CEMS*

Thursday Morning, Room 556A
MOLECULAR AND VIBRATIONAL SPECTROSCOPIES I
Presider: John Wright, University of Wisconsin

8:50 (601) **Molecularly Imprinted Polymer Sensors for Pesticide Detection**; Amanda L. Jenkins; *Jasco Inc*

9:10 (602) **Polarization Studies of Biological Tissues Using Synchrotron Infrared Microspectroscopy**; David L. Wetzel, John A. Reffner, Lisa L. Miller, Steven M. LeVine, *Kansas State University, SensIR Technologies, Inc., Brookhaven National Laboratory, University of Kansas*

9:30 (603) **Biofilm Monitoring by Photoacoustic Spectroscopy**; Ulrich Panne, Thomas Schmid, Christoph Haisch, Reinhard Niessner

9:50 (604) **Monitoring Adsorption Kinetics of NH3 and NH3/H2O Mixtures on Type 3A Zeolite Using Infrared Spectroscopy**; Thomas M. Niemczyk, Anding Zhang, Yanga K. Dijiba, David M. Haaland; *The University of New Mexico, Sandia National Laboratories*

10:10 **Coffee Break**

10:40 (605) **Spectral Profiling of Biological Microorganisms by Specular Reflectance and Chemometrics**; David L. Perkins; *The University of South Carolina*

11:00 (606) **Leveraging Measurement Traceability in Dispersive Molecular Absorption Spectrophotometry**; John C. Travis, Gary W. Kramer, David L. Duewer; *National Institute of Standards and Technology*

11:20 (607) **Compact, High Sensitivity System for the Detection of Bacterial Endospores**; Nicholas F. Fell, Jr., Paul M Pellegrino, James B Gillespie; *U.S. Army Research Laboratory*

11:40 (608) **Atmospheric Trace Gas Measurements Using Thermo-Electrically Cooled Quantum Cascade Lasers: Line Width and Pulse Shape Characterization for Optimal Detection**; Mark S. Zahniser, David D. Nelson, Mathew Taubman, Joanne S. Shorter, Richard Williams, Quan Shi, J. Barry McManus, Mark S. Zahniser; *Aerodyne Research, Inc, Pacific Northwest National Laboratory*

Thursday Morning, Room 554B
RECENT DEVELOPMENT AND APPLICATIONS OF TWO-DIMENSIONAL CORRELATION SPECTROSCOPY I
Presiders: Wei Zhao, University of Arkansas and Isao Noda, Procter and Gamble

8:50 (609) **Recent Advances in 2D Correlation Spectroscopy**; Isao Noda; *Procter & Gamble Co.*

9:30 (610) **Dynamic Filtering And 2D-IR Correlation Spectroscopy of State to State Transitions**; Hugh H Richardson; *Ohio University*

10:10 **Coffee Break**

10:40 (611) **Infrared Spectra Evaluation of a New Polymer: Poly(phenoxy phenylene vinylene) by Dynamic Two-Dimensional Infrared Spectroscopy**; Georgia A. Arbuckle-Keil, Bing Hsieh, James Wilking; *Rutgers, The State University of New Jersey, Canon R & D, Rutgers*

11:20 (612) **Investigation of the f-f transitions of Lanthanide Complexes by Using Two-Dimensional Correlation Spectroscopy**; Yizhuang Xu, Ying Zhao, Juan Feng, Dongliang Tao, Jun Yang, Yong Li, Guowei Lu, Weiming Du, Duanfu Xu, Jinguang Wu; *Department of Chemistry, Peking University, Beijin, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, P. R. China, Department of Physics*

Thursday Morning, Room 556B
BIOMEDICAL APPLICATIONS OF VIBRATIONAL SPECTROSCOPY: ROYAL SOCIETY OF CHEMISTRY, ANALYTICAL DIVISION
Presider: John Chalmers, University of Nottingham

8:50 (613) **Fourier Transform Infrared Spectroscopic Imaging Methods for Biomedical Diagnostics**; Rohit Bhargava, Daniel C. Fernandez, Scott W. Huffman, Michael D. Schaeberle, Ira W. Levin; *Laboratory of Chemical Physics, NIDDK, NIH*

9:30 (614) **Raman Spectroscopy for the Diagnosis of Epithelial Cancer**; Nicholas Stone, C. A. Kendall, H. Barr; *Cranfield Medical School and Gloucestershire Royal*

10:10 **Coffee Break**

10:40 (615) **Evolutionary computing for the interpretation of vibrational data**; Royston Goodacre; *University of Wales*

11:20 (616) **Single Cell Analysis of Biomedical and Clinical Samples Using Synchrotron FT-IR Microspectroscopy**; Mark Tobin; *Daresbury Laboratory*

Thursday Morning, Room 557
ANACHEM AWARD I
Presiders: Bruce Chase, DuPont and James Rydzak, GlaxoSmithKline

8:50 (617) **Spectroscopy, Microscopy, and Imaging: Polymer Structure from Infrared and Raman**; Bruce Chase, John Rabolt, Stephan Stranick; *DuPont, University of Delaware, NIST*

9:30 (618) **Ultra-Rapid Scanning FT-IR Spectroscopy for the Study of Time-Resolved Adsorption**; Peter R. Griffiths, Husheng Yang, Benjamin Weinstock, Kenneth H. Shafer, John B. Paine, Christopher J. Manning; *University of Idaho, Philip Morris USA, Manning Applied Technology*

10:10 **Coffee Break**

10:40 (619) **Approaches to Infrared and Visible Reflectance Spectroscopic Imaging**; Ira W. Levin, Daniel C. Fernandez, Michael D. Schaeberle, Scott W. Huffman, Karel J. Zuzak, Rohit Bhargava; *National Institutes of Health*

11:20 (620) **Investigating the Structure and Dynamics of Self Assembly in Thin Films Using Planar Array IR (PAIR) Spectroscopy**; John F. Rabolt; *University of Delaware*

Thursday Morning, Room 555A
CHEMOMETRICS IN BIOANALYTICAL AND BIOTECHNOLOGY
Presider: Renee JiJi, NRL

8:50 (621) **Multivariate Curve Resolution Applied to the Detection and Modelling of Intermediate Conformations in Protein Folding Processes.**; Anna de Jaun, Susana Navea, Romà Tauler; *University of Barcelona*

9:30 (622) **Prediction of Baking Quality by Chemometric Analyses of Protein**; E. M. Færgestad, F. Westad, H. Martens, H. J. Skarpeid; *Matforsk*

10:10 **Coffee Break**

10:40 (623) **Multi-Way Models for Four-Way Kinetic Fluorimetric Data – Quantification of Catecholamines.**; Rikke P.H. Nikolajsen, Karl S. Booksh, Åse M. Hansen, Rasmus Bro; *Mikroelektronik Centret (MIC), Technical Universit,, Dept. of Chemistry and Biochemistry, Arizona State University, AZ, USA, National Institute of Occupational Health, DK,, Chemometrics Group, Royal Veterinary and Agricultural University, DK*

11:20 (624) **Multiway Data Analysis of a Number of Chlorophyll Biosynthetic Intermediates in Pigment Extracts from Wild Type and Chlorophyll Deficient Cyanobacteria.**; Karl S. Booksh, Renee D. JiJi, Jason W. Cooley, *Naval Research Laboratory, Chemistry Division, University of Pennsylvania, Department of Biology, Arizona State University, Department of Chemsitry and Biochemistry*

11:40 (625) **Calibration of a Fiber Optic, Surface Plasmon Resonance based Immunosensor for Monitoring Heart Attack Proteins.**; Karl S. Booksh, Jean-Francois Masson, Louis A. Obando

TECHNICAL PROGRAM - THURSDAY

Thursday Morning, Room 553A
SEPARATIONS I
Presider: Lisa Hollan, University of West Virginia

8:50 (626) **Determination of Allicin in Garlic by Standard Addition of Alliin and Supercritical Fluid Extraction**; James M. Harnly, Michael E. Rybak, Elizabeth M. Calvey; *United States Department of Agriculture, Agriculture, Agricultural Research Service, Beltsville Human Nutrition Research Center, Food Composition Laboratory, Beltsville, MD 20705, United States Food and Drug Administration, Center for Food Safety and Applied Nutrition, College Park, MD 20740*

9:10 (627) **Comparison Of HPLC Analyses Of Anthocyanins And Their Hydrolyzed Anthocyanidins In Grape Skin Extracts**; Zhe Zhang, Xiaolan Kou, Ken Fugal, Jerry Mclaughlin; *Nature's Sunshine Products,, Nature's Sunshine Products, Nature's Sunshine Products,, Nature's Sunshine Products*

9:30 (628) **Separation of Fatty Acid Amides by Gas Chromatography Coupled with Mass Spectrometry (GC-MS)**; Mitchell E. Johnson, Tamanna Sultana, Mitchell E. Johnson; *Department of Chemistry and Biochemistry, Duquesne University*

9:50 (629) **Aromatic Specific Laser Ionization Detector Coupled with Fast Gas Chromatography or Rapid Extraction of Aqueous Aromatic VOCs**; Melissa J. Meyer, Anthony J. Borgerding, Orven F. Swenson, Christopher J. Walls, Jeremy Brodersen; *University of North Dakota - Chemistry Department,, North Dakota State University - Physics Department*

10:10 **Coffee Break**

10:40 (630) **Cellular Analysis With Microfluidic Micellar Electrochromatography**; Andrew M. Leach, Aaron R. Wheeler, Keisuke Morishima, Richard N Zare; *Department of Chemistry, Stanford University*

11:00 (631) **Recovery Optimization Considerations for EPA Method 525.2**; Robert B Stiles, Yang, Eileen Murphy, Lee Lippincott, Brian Buckley; *Environmental and Occupational Health Science Inst, New Jersey Department of Environmental Protection (NJDEP)*

11:20 (632) **Continued Optimization and Characterization of a Glass Nebulizer CE/FT-IR Interface for Transmission Analyses**; Jessica L. Jarman, James A. de Haseth; *University of Georgia*

Thursday Morning, Room 553B
MINATURIZATION AND MICROPLASMAS
Presider: V. Karannasios, University of Waterloo

8:50 (633) **Discrete Sample Introduction System for a Battery-Operated, Micro Plasma Device (MPD) On-A-Chip**; Vassili Karanassios; *Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1*

9:10 (634) **The Liquid Sampling Atmospheric Pressure Glow Discharge (LS-APGD): A Practical Plasma for Microsamples and Capillary LC**; R. Kenneth Marcus, W. Clay Davis; *Clemson University*

9:30 (635) **Development and Application of Capacitively Coupled Microplasmas**; Michael W. Blades, Alan Sagan; *University of British Columbia*

10:10 **Coffee Break**

10:40 (636) **Microfabricated Inductively Coupled Plasma Generator as an Optical Emission Source**; Jeffrey A. Hopwood; *Northeastern University*

11:00 (637) **The Dielectric Barrier Discharge and the Hollow Cathode-Type Microdischarge, Suitable Microplasmas for Analytical Applications?**; Kay Niemax; *Institute of Spectrochemistry and Applied Spectroscopy*

11:20 (638) **A New Microchip-Size Radio Frequency Plasma in Optical Emission Spectrometry**; Volker Siemens, *VTT Processes*

Thursday Morning, Room 552A
SAMPLE PREPARATION AND INTRODUCTION
Presider: Ken Marcus, Clemso University

8:50 (639) **Effect of Edta on the Determination of Zinc in Copper and Nickel Matrices by Graphite Furnace Atomic Absorption Spectrometry**; Suh-Jen Jane Tsai, Chia-Ni Chang, Shi-Yang Chen; *Department of Applied Chemistry, Providence University*

9:10 (640) **Supported Liquid Membranes or Packed Bed Reactor for the Separation and Preconcentration of Metals in Flow Injection Systems?** Julian F Tyson, Emily R Yourd, Julian F Tyson; *University of Massachusetts Chemistry Department*

9:30 (641) **Phytoremediation for Arsenic using Brake Ferns (Pteris vittata)**; David J. Butcher, Arthur Salido, Jae-Min Lim, Kelly Hasty; *Western Carolina University*

9:50 (642) **Characterization of Transition Metal and Metal Oxyanion Extraction in FIA Systems Using Short Chain Tethered Bio-Homopolymers for Water Remediation**; Lisa L. Malachowski, Lisa L. Malachowski, James A. Holcombe; *University of Texas*

10:10 **Coffee Break**

10:40 (643) **Templating of Immobilized Short-Chain Metal Chelators to Enhance Selectivity in Remediation and Preconcentration**; Jacqueline L. Stair, James A Holcombe; *University of Texas at Austin*

11:00 (644) **Investigating the Generation of Free Atoms in Solution by Reduction using NaBH4**; John L Molloy, John L. Molloy, James A. Holcombe; *The University of Texas*

11:20 (645) **The Benefits of Temperature Control on a Graphite Block Digestion System.**; Arthur Ross, *SCP SCIENCE*

Thursday Morning, Room 550A
ENVIRONMENTAL SURFACE CHEMISTRY
Presider: Howard Fairbrother, Johns Hopkins University

8:50 (646) **Surface Chemistry, Salt and the Atmosphere: How are they Connected?**; John C. Hemminger, John T. Newberg, Koji Inazu; *University of California, Irvine*

9:30 (647) **Surface Structure and Crystal Growth at the Mineral-Water Interface: In-situ STM and Hydrothermal AFM**; Carrick M. Eggleston, Andrew G. Stack, Kevin M. Rosso, Steven R. Higgins, Sherry D. Samson, Kevin G. Knauss; *Department of Geology and Geophysics, University of Colorado, Boulder, William R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352, Lawrence Livermore National Laboratory, Livermore, CA 94550*

10:10 **Coffee Break**

10:40 (648) **Preparation and Characterization of Transition Metal Nanoparticles Grown on Planar Supports**; Simon J. Garrett, Heather A. Bullen, Anne E. Fischer; *Michigan State University*

11:00 (649) **Adsorption and Photochemistry on Carbon Aerosol Particle Surfaces**; Simon J. Garrett, Michael J. Dorko, Stefano V. Giacomantonio, Jason K. Oman, *Michigan State University*

11:20 (650) **Applications of Surface Analysis in the Environmental Sciences: Dehalogenation of Chlorocarbons with Zero-Valent Iron and Iron-Containing Mineral Surfaces**; D. Howard Fairbrother, Molly M. McGuire, Daniel L. Carlson, Peter J. Vikesland, Tamar Kohn, Adam Grenier, Laura A. Langley, A. Lynn Roberts, D. HowardFairbrother; *Johns Hopkins University, Department of Chemistry, Johns Hopkins University, Department of Geography and Environmental Engineering*

Thursday Afternoon, Room 551A
MS IN PROTEOMICS
Presider: David Han, University of Massachusetts

1:30 (651) **Multi-Dimensional Separations of Complex Mixtures from In-Gel Digestions Using Automated Vented-Column Nanoliquid Chromatography / Tandem Mass Spectrometry**; Larry Licklider; *Harvard Medical School*

2:10 (652) **Mass Spectrometric Analysis of Protein Modifications: High-Resolution Fragment Ion Selection for Precursor Ion Scanning**; Hanno Steen; *Harvard Medical School*

2:50 **Coffee Break**

3:30 (653) **Analysis of Complex Protein Mixtures by Three-Dimensional Chromatography, Isotope Coded Affinity Tags, and Mass Spectrometry**; David Han; *University of Connecticut Health Center*

4:10 (654) **Parallel Peptide Tandem Mass Spectrometry on a Time-of-flight Mass Analyzer**; David Robinson; *Institute for Systems Biology*

Thursday Afternoon, Room 551B
SINGLE CELL MASS SPECTROMETRY
Presider: Jonathan Sweedler, University of Illinois

1:30 (655) **Decoding the Chemical Messengers in a Small Nervous System: A MS-Based Multidisciplinary Approach**; Lingjun Li, Wayne P. Kelley, Jonathan V. Sweedler, Eve Marder; *Brandeis University, University of Illinois*

2:10 (656) **On-line CE-MS Analysis of Intact Cells**; Mehdi Moini, Hsiaoling Huang; *University of Texas at Austin*

2:50 **Coffee Break**

3:30 (657) **Mitochondrial Resolution Chemical Imaging of Single Cells with SIMS Ion Microscopy for Studies of Ion Transport and Anticancer Drugs**; Subhash Chandra; *Department of Chemistry and Chemical Biology*

4:10 (658) **From Single Cells to Single Organelles: Direct MS of the Neuropeptides in a Neuronal Network**; Jonathan V Sweedler; *University of Illinois*

Thursday Afternoon, Room 550A
PROCESS ANALYSIS IN PHARMACEUTICALS
Presider: Chris Hassel, Los Alamos National Laboratory

1:30 (659) **Fermentor Vent Gas Analysis by On-Line Process Mass Spectrometry**; Peter J. Traynor; *Thermo Electron*

1:50 (660) **Improved Bioprocess Monitoring Using In-Line and Non-Invasive Measurements**; Colin A McGill, Colin A McGill, Alison S Dann, Mark D Richardson, Paul A Jeffkins, David Littlejohn; *University of Strathclyde/CPACT, GlaxoSmithKline, Worthing*

2:10 (661) **At-line and On-line Hydrate State Detection in Pharmaceuticals by Near-IR Spectroscopy**; John P Higgins, Steven M Arrivo, Robert L Green, Robert A Reed; *Merck Research Laboratories, Merck and Co., Inc, Pfizer Global Research & Development*

2:30 (662) **Demonstration of a High Precision Immersion Probe for Effective Sampling of Solids by Raman Spectroscopy**; Brian J Marquardt, David J Veltkamp; *CPAC*

2:50 **Coffee Break**

3:30 (663) **Process Analytical in the Early Phase of Pharmaceuticals**; James W. Rydzak, Teresa Head, Dawn Cohen, Gary Zuber

3:50 (664) **Comparison of Near-IR and Laser Induced Breakdown Spectroscopy for Determination of Mg:stearate in Pharmaceutical Powders and Solid Dosage Forms**; Robert L Green, John P. Higgins, Mark Mowery, Julie Good, Robert A. Reed; *Merck Research Laboratories, Merck and Co. Inc..*

4:10 (665) **Creating Knowledge from Data: Applications of Process Analytical Measurements in Pharmaceutical Chemical Process Development**; Paul A. David, Bob T. Roginski, Steve J. Doherty; *Pharmacia Corporation*

4:30 (666) **Online Non-Invasive Analysis of Fluorocarbon Gas in the Headspace of Glass Vials**; James F. Castner, Allan J. Rilling, Luc F. Boudreau; *Bristol-Myers Squibb Medical Imaging (author 1),, ABB Bomem (author 2 and 3)*

Thursday Afternoon, Room 555B
CHEMOMETRICS APPLICATIONS
Presider: Chris Hassel, Los Alamos National Laboratory and Renee JiJi, NRL

1:30 (667) **MAGIK - A New Tool for the Study of Dynamic Heterogeneous Equilibria**; Morris Bader; *Scientific Programmers*

1:50 (668) **Multivariate Curve Resolution Techniques Applied in the Quantitative Analysis of Diffuse Reflectance Near-IR Chemical Image Data**; Frederick W. Koehler, Linda H.. Kidder, E. Neil Lewis; *Spectral Dimensions, Inc*

2:10 (669) **Online Design Reoptimization Algorithm for the Production of Multivariate Optical Elements**; Ashley E. Greer, Frederick G. Haibach, Maria V. Schiza, Ryan J. Priore, Olusola O. Soyemi, Michael L. Myrick; *University of South Carolina*

2:30 (670) **Nonlinearities, How Well Do Multivariate Calibration Methods Handle Them?***; David K Melgaard, David M Haaland; *Sandia National Laboratories*

2:50 **Coffee Break**

3:30 (671) **Signal to Noise Ratios in Multivariate Optical Computing: A Reprise and Extension to the Transmission-Reflection Filter Spectrometer**; Frederick G. Haibach, Michael L Myrick; *University of South Carolina*

3:50 (672) **Novel Imaging Systems: Multivariate Optical Computing from UV to NIR**; Ryan J. Priore, Ashley E. Greer, Fred G. Haibach, Maria V. Schiza, David L. Perkins, Michael L. Myrick; *University of South Carolina*

Thursday Afternoon, Room 554B
NANOPARTICLES IN BIOANALYTICAL CHEMISTRY
Presider: Chris Keating, Penn State University

1:30 (673) **Designer Metal Particles for Multiplexed Bioanalysis**; Michael J. Natan, *Nanoplex Technologies, Inc.*
2:10 (674) **Nanosphere Lithography: Nanoparticle Optics, Biosensors, and Surface-Enhanced Spectroscopy**; Richard P. Van Duyne, Amanda J Haes, Christy L. Haynes, Adam D. McFarland
2:50 **Coffee Break**
3:30 (675) **Highly-Paralleled and Miniaturized Detection of Biomolecular Interactions Based on Nanoparticle Labeling**; Wolfgang Fritzsche, Andrea Csaki, Robert Möller; *Institute for Physical High Technology Jena, Germany*
4:10 (676) **Designing Nanostructured Materials as Sensors of Chemical Transport Across Cell Membranes**; Alexander Wei, Beomseok Kim, Bryce Sadtler, Steven L. Tripp; *Purdue University*

Thursday Afternoon, Room 553B
RECOMBINANT PROTEIN CHARACTERIZATION
Presider: Wei Zhang, Wyeth BioPharma

1:30 (677) **Manufacturing and Analytical Characterization of rhuTNFR:Fc (Enbrel)**; Wayne Gombotz, *Amgen, Inc*
2:10 (678) **Analytical Issues in the Development of Herceptin**; Reed Harris; *Genentech, Inc*
2:50 **Coffee Break**
3:30 (679) **Characterization of recombinant human Bone Morphogenetic Protein-2 (rhBMP-2)**; Thomas J. Porter, Suman Rathore; *Wyeth BioPharma*
4:10 (680) **Analysis of Recombinant Glycoprotein Hormones - Making the Connection Between Structure and Function**; Kate Zhang; *Genzyme Corporation*

Thursday Afternoon, Room 556B
RAMAN SPECTROSCOPY IN PHARAMCEUTICAL SCIENCE
Presider: Ian Lewis, Kaiser Optical

1:30 (681) **In-situ Monitoring of Crystallizations in Pharmaceutical Development**; David C. Lee, Wendy I. Cross, Christopher J. Price, Clare L. Anderton, Kevin H. Jennings; *GlaxoSmithKline*
2:10 (682) **Exploring the Use of Surface Enhanced Raman Scattering for High Throughput Analyses**; Michael J. Sepaniak, Marco Dejesus, Shannon Fox, Maggie Connatser, Roderic Cole, Michael Rooney; *University of Tennessee, Knoxville,, Arqule, Inc.*
2:30 (683) **Raman Spectroscopy for the Development of Crystallization Process of Drug Substances**; George X. Zhou; *Merck & Co*
2:50 **Coffee Break**
3:30 (684) **Advantages of Macro Raman for Pharmaceutical Analysis**; Andrew C. Dennis, Steven E. Bell, Adrian R. Boyd; *Avalon Instruments, Queens University Belfast*
3:50 (685) **Relative Intensity Correction Standards for Raman Spectroscopy with 532nm, 785 nm and 1064 nm Excitation Sources.**; Steven J. Choquette, Edgar Etz, Wilbur Hurst, Douglas Blackburn; *National Institute of Standards and Technology*

Thursday Afternoon, Room 556A
MOLECULAR AND VIBRATIONAL SPECTROSCOPIES II
Presider: John Wright, University of Wisconsin

1:30 (686) **Nanodroplet Quantification: Pushing the Detection Limits of Micro X-Ray Fluorescence**; Thomasin C. Miller, George J. Havrilla; *Los Alamos National Laboratory*
1:50 (687) **Molecular Sensors for the Detection and Identification of Single Native DNA Nucleotides**; Paula E. Colavita, Annabelle C. Molliet, Maria V. Schiza, Michael L. Myrick; *University of South Carolina*
2:10 (688) **Combinatorial Analysis in Catalysis Research: Novel Approaches in Transmission Infrared Spectroscopy**; Anne Leugers, David Neithamer, Larry Sun, Jack Hetzner, Sean Hilty, Sam Hong, Matthew Krause, Ken Beyerlein; *Dow Chemical*
2:30 (689) **Enhanced Spatial Resolution and Spectral Range for Synchrotron Infrared Microscopy at the NSLS**; Gregory D. Smith, Larry Carr; *National Synchrotron Light Source*
2:50 **Coffee Break**
3:30 (690) **Investigation of Near-Infrared Light Propagation in Fish Tissue By Photon Time-Of-Flight Analysis**; Anna G. Cavinato, Carl A. Fahlstrom, Zheming Wang, David M.. Mayes, Mengshi Lin, Barbara A. Rasco; *Eastern Oregon University, Pacific Northwest National Laboratory, Environmental Molecular Science Laboratory, DSquared Development, Inc., Department of Food Science & Human Nutrition, Washington State University*
3:50 (691) **Spectral Imaging of Latent Fingerprints**; Edward G Bartick, *FBI Laboratory*
4:10 (692) **Raman spectroscopic study of Martian Meteorite EETA79001**; Alian Wang, *Washington University*
4:30 (693) **Development of Method for Determination of Nanogram Amounts of Copper(II) by Its Catalytic Effect on Hexacynoferraate(III)-Citric Acid Indicator Reaction**; Surendra Prasad; *The University of the South Pacific*

Thursday Afternoon, Room 550B
RECENT DEVELOPMENT AND APPLICATIONS OF TWO DIMENSIONAL CORRELATION SPECTROSCOPY II
Presiders: Wei Zhao, University of Arkansas and Isao Noda, Procter and Gamble

1:30 (694) **Two-Dimensional Fluorescence Correlatioin Spectroscopy in Protein Folding and Chemical Separations**; Lei Geng, Gufeng Wang; *University of Iowa*
2:10 (695) **Sample-Sample and Statistical 2D Correlation Spectroscopy**; Slobodan Sasic, Yukihiro Ozaki; *Massachusetts Institute of Technology, G. R. Harri, Kwansei-Gakuin University, Dept. of Chemistry, 2-1 Gakuen, Sanda 669-1337 Japan*
2:50 **Coffee Break**

3:30 (696) **Study of Protein Denaturation Using 2D Infrared Correlation Spectroscopy**; Thierry Lefèvre, Karin Arseneault, Michel Pézolet; *CERSIM - Laval University*

4:10 (697) **Molecular Interactions between Single-Walled Carbon Nanotubes and A Biological Matrix Probed by 2D IR Correlation Spectroscopy**; Wei Zhao, Chulho Song, Eric M Tee; *Department of Chemistry, University of Arkansas*

Thursday Afternoon, Room 557
ANACHEM AWARD II
Presiders: Bruce Chase, DuPont and James Rydzak, GlaxoSmithKline

1:30 (698) **Development of Advanced Nanoscale Chemical Characterization Tools for Real World Samples**; Stephan J. Stranick, Bruce Chase, Chris A. Michaels; *NIST, DuPont*

2:10 (699) **Bridging the Surface Resolution Gap between Raman Spectroscopy and High Vacuum Techniques**; Neil Everall, Ewen Smith, Gerry McAnally, Colin Bain, Phillip Greene; *ICI PLC, University of Strathclyde, University of Oxford*

2:50 **Coffee Break**

3:30 (700) **Select Examples of Raman Applications to Forensic and Archeological Science**; Ian Lewis; *Kaiser Optical Systems, Inc*

4:10 (701) **Industrial Research Through Outside Connections**; Curtis Marcott; *The Procter & Gamble Company*

4:50 (702) **Near-Infrared Spectroscopy in Surgery**; William Fateley; *Kansas State University*

Thursday Afternoon, Room 555A
CHEMOMETRICS IN THE GOVERNMENT LAB
Presider: Scott McWhorter, Westinghouse Savannah River Company

1:30 (703) **On-Line Chemometric Analysis of Uranium and Nitric Acid in Nuclear Processing**; Robert Lascola, Gary A. Cooper, Ronald R. Livingston; *Westinghouse Savannah River Cor*

2:10 (704) **Plutonium Aqueous Complexation Equilibria Studied by Multivariate Curve Resolution And Classical Modeling Of Visible Absorption Spectra**; John M. Berg, Steven D. Conradson, John H. Matonic, Mary P. Neu, Sean D. Reilly; *Los Alamos National Laboratory, NM*

3:30 (705) **Use of NIR and Raman Spectrosopies with Chemometrics for Grain Quality Analysis**; David S Himmelsbach, Franklin

4:10 (706) **Chemometrics, Making Government Systems Smart**; Susan L. Rose-Pehrsson, John H. Callahan, Mark H. Hammond; *Naval Research Laboratory*

4:50 (707) **Hyperspectral Fluorescence Image Scanning of Microarrays for Improved Genome Expression Analyses**; David M. Haaland, Jerilyn A. Timlin, Michael B. Sinclair, Mark H. Van Benthem, Juanita Martinez, Angelina Rodriguez, Anthony Aragon, Angelina Rodriguez, Jose Weber, Margaret Werner-Washburne; *Sandia National Laboratories, University of New Mexico, Biology Department, Albuquerque, NM 87131*

Thursday Afternoon, Room 553A
SEPARATIONS II
Presider: Lisa Hollan, University of West Virginia

1:30 (708) **Capillary-Channel Polymer Fibers: A Novel (and Exciting) Stationary Phase for Liquid Chromatography**; R. Kenneth Marcus, W. Clay Davis, Rayman D. Stanelle, Dwella K. Nelson

1:50 (709) **New Techniques for Advanced Detection and Integration**; Patricia A. Fowler, Michael E. Swartz; *Waters Corporation*

2:10 (710) **Protein Separation Using Aqueous Micellar Systems**; Dick van Roosmalen, C.H.J.T. Dietz, M.P.J. Dohmen, L.J.P. van den Broeke, J.T.F. Keurentjes; *Eindhoven University of Technology*

2:30 (711) **Size Exclusion Chromatography ICP-MS Studies on Elements Binding to Humic Substances in Compost Obtained From Urban Solid Waste**; Baki M. Sadi, Juan Castillo, Kazimierz Wrobel, Katarzyna Wrobel, Maria Montes-Bayon, Joseph A Caruso; *Authors 1, 5 and 6: Department of Chemistry, Unive,, Author 2: Universidad de Zaragoza, Spain, Authors 3 and 4: At the University of Cincinnati while on the leave from Instituto de Investigaciones Cientificas, Universidad de Guanajuato, Mexico*

2:50 **Coffee Break**

3:30 (712) **Trace Level Drug Impurity Analysis by Capillary HPLC**; Peter G Alden, Michael Swartz; *Waters Corporation*

3:50 (713) **Biochip System with Capillary Array Electrophoresis for Bioassays**; Tuan Vo-Dinh, Joon Myong Song, Joel Mobley, Tuan Vo-Dinh; *Oak Ridge National Laboratory*

Thursday Afternoon, Room 552A
HIGH RESOLUTION ICP-MS
Presider: Chuck Douthitt, Thermo Finnigan

1:30 (714) **Determination of Co and V in SRM 2783, Air Particulate on Filter Media by using HR-ICP-MS**; Lee L Yu; *National Institute of Standards and Technology*

1:50 (715) **State-of-the-art in precise and accurate isotope ratio measurements**; Sabine J. Becker,; *Research Centre Juelich*

2:10 (716) **Determination of 22 Trace Elements in Geological Materials Using Quadrupole and Double Focusing Sector Field ICP-MS: A Comparison**; Zhongxing Chen, Alan M. Shiller; *Laboratory for Isotope and Trace Element Research, Department of Marine Science, University of Southern Mississippi, Stennis Space Center, MS 39529*

2:30 (717) **Detection and Quantification of Depleted Uranium in Urine using Sector Field ICPMS**; Chuck B. Douthitt, Meike Hamester; *ThermoFinnigan MAT,, ThermoFinnigan*

2:50 **Coffee Break**

3:30 (718) **Applications of HR-ICPMS for Uranium Analysis**; Joachim Hinrichs, Torsten Lindemann, Meike Hamester, Julian D Wills; *Thermo Finnigan*

3:50 (719) **Determination of trace levels of arsenic in whole mouse blood using sector-field ICPMS**; Stefan Sturup, Linda R Klei, Aaron Barshowsky; *Dartmouth College, Department of Earth Science, Dartmouth Medical School, Department of Pharmacology and Toxicology*

4:10 (720) **Spectral Overlaps and Isotope Ratio Measurements: Sector ICP-MS and Reaction Cell Quadrupole ICP-MS**; John W. Olesik; *The Ohio State University*

Thursday Afternoon, Room 554A
DIRECT ANALYSIS TECHNIQUES FOR SOLID MATERIALS
Presiders: Roland Hergenroder and Amy Hunter, ISAS

1:30 (721) **Micro, Nano and Teleanalysis of Advanced Materials Using Laser-Induced Plasma Spectrometry**; Javier J. Laserna; *University of Málaga*

2:10 (722) **Direct Analysis of Solids by Laser-Induced Breakdown Spectroscopy**; Mohamad M. Sabsabi, Vincent Detalle, Louis St-Onge, René Héon, André Hamel; *NRC_IMI*

2:50 **Coffee Break**

3:30 (723) **Direct Elemental Analysis of Soil and Other Solids with Spark-Induced Breakdown Spectroscopy**; Amy J. Ray Hunter, Richard T. Wainner, Lawrence G. Piper, Steven J. Davis; *Physical Sciences Inc*

3:50 (724) **Depth Profile Analysis by LA-ICP-MS – Potentialities and Limitations**; Carla Vogt, Alexei Plotnikov, Klaus Wetzig; *University of Hannover, Institute of Inorganic Chem, IFW Dresden, IFW Dresden*

4:30 (725) **In-Depth Profiling of Multi-Layer Samples with Femtosecond Laser**; Roland Hergenroeder, Kay Niemax, Vanja Margetic;*Institute for Spectrochemistry and Applied Spectroscopy*

4:50 (726) **Direct Analysis of Liquid and Solid Metals Under Reduced Ambient Pressure by Laser-Induced Breakdown Spectroscopy**; Johann Gruber, Johannes Heitz; *Johannes-Kepler-University Linz*