Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS 2015)

The Great SCIentific eXchange SCIX2015

And the National Meeting of the Society for Applied Spectroscopy (SAS)

Providence, Rhode Island, USA
27 September – 2 October 2015

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SUNDAY WORKSHOPS, see page 42 for a list

SUNDAY PROGRAM AND EVENTS

What's Hot Vendor Presentations. Presider: Brian Dable, *Arete Associates, Ballroom B/C*

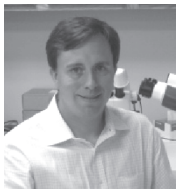
4:10 **Hamamatsu** "Microspectrometers – High Performance, Rugged, the Size of a Lego™"
4:20 **nanoPlus** "Single-Mode Interband Cascade Lasers for Gas sensing applications"
4:30 **artPhotonics** "From Fiber Spectroscopy to Fiber Sensors for 0.3-16μm range"
4:40 **LECO** "Hot to the Touch: Application of the Touch User Interface in the Modern Industrial Laboratory"
4:50 **Tofwerk** "icpTOF from TOFWERK: Multi-Element Detector for Individual Particles and High Speed Laser Ablation Imaging"
5:00 **Viavi Solutions** "MicroNIR PAT for On-line Process Monitoring"
5:10 **Rigaku**
5:20 **AIST-NT** "THE Hot Spot: AFM/Raman and TERS made easy"
5:30 **OPOTEK** "Allowing Science to Determine the Optimal Wavelength: New Developments in Broadly Tunable Optical Parametric Oscillators"
5:40 **Bruker** "Bruker introduces the first FTIR spectrometer capable of scanning from the THz to the NIR in a Single Scan with the New VertexFM"
5:50 **Horiba** "Elemental Analysis: A full line of Products for Direct Solid Samples Analysis, Bulk Elemental Analysis and Depth Profile Analysis."

6:15 **Keynote Lecture;** *Ballroom B/C*
(1) Pre-adaptation: How Basic Research Helps Oceanographers Meet Global Challenges; **Robert S.C. Munier**; Woods Hole Oceanographic Institute

Dr. Munier is the Vice President for Marine Facilities & Operations at The Woods Hole Oceanographic Institution (WHOI) in Rhode Island

7:15 **Welcome Mixer**
SAS Sponsored Student Poster Session • Coblentz Student Awards • FACSS Student and Tomas Hirschfeld Scholar Awards – *Ballroom A*

TECHNICAL PROGRAM – MONDAY
Welcome 7:50 am and Keynote Lecture – 8:00 am; *Ballroom B/C*
Presider: Glen P. Jackson



8:00 am Keynote Lecture

(2) Forensic Microscopy and the Lost Art of Observation; **Christopher Palenik**; Microtrace LLC

Dr. Chris Palenik is a Research Microscopist and Vice President of Microtrace where he enjoys answering practical questions through the examination and characterization of microscopic evidence. Chris has carried out research in various forensic laboratories around the world including the Bundeskriminalamt in Germany (the German Federal Police Crime Laboratory), the Internal Revenue Service National Forensic Laboratory, and a post-doctoral fellowship at the Federal Bureau of Investigation. Chris earned Bachelor of Science degrees from the University of Chicago in chemistry and geology. He completed his master's degree and doctoral studies at the University of Michigan in the department of Geological Sciences on the subject of a naturally occurring nuclear reactor in Gabon, Africa. He has been appointed to the North Carolina Forensic Science Laboratory Advisory board as well as the recently formed United States Forensic Science Standards Organization (OSAC).

Orals 9:15 – 10:55 am

Monday Morning, *Room 554A/B*
RSC/ACS SYMPOSIUM – ANALYSIS WITH PHOTONS – LASER & SYNCHROTRON SPECTROSCOPY SCIENCE & APPLICATIONS
Organizers: David Koppenaal and Rebecca Brodie;
Presider: Doug Duckworth

9:15 (3) **Photons as Reporters of Fundamental Activity in the ICP-MS: Using Lasers to Answer the Five W's**; Paul Farnsworth[1], Lance Moses[1], Jessica Ramsey[1]; [1]Brigham Young University

9:35 (4) **All-Optical Laser Ablation-based Analytical Techniques: Status, Achievements and Directions**; Vassilia Zorba[1], Jhanis Gonzalez[1], Huaming Hou[1], George Chan[1], Xianglei Mao[1], Richard Russo[1]; [1]Lawrence Berkeley National Laboratory

9:55 (5) **Laser SIMS Advancements**; David Willingham[1], Benjamin Naes[1], Mindy Zimmer[1]; [1]Pacific Northwest National Laboratory

10:15 (6) **Recent Advances in Quantifying Actinide Isotope Ratios by RIMS**; Brett Isselhardt[1], Michael Savina[1, 2], Andrew Kucher[1]; [1]Lawrence Livermore National Laboratory; [2]Argonne National Laboratory

10:35 (7) **Real Time Isotopic Analysis of Atmospheric Greenhouse Gases Using Mid-IR Laser Spectroscopy**; David Nelson[1], Barry McManus[1], Joanne Shorter[1], Tara Yacovitch[1], Scott Herndon[1], Mark Zahniser[1]; [1]Aerodyne Research

Monday Morning, *Room 550A/B*
FUNDAMENTALS AND NOVEL APPLICATIONS OF LA-ICP-MS: I
Organizer and Presider: Jorge Pisonero

9:15 (8) **LA-ICPMS: Embracing Challenges of Space and Time**; Bodo Hattendorf[1], Marcel Burger[1], Luzia Gyr[1], Gunnar Schwarz[1], Alexander Gundlach-Graham[1], Hao Wang[1], Detlef Günther[1]; [1]ETH Zurich, Laboratory for Inorganic Chemistry

9:35 (9) **Advances in High Repetition Rate Femtosecond Laser Ablation**; Fanny Claverie[1], Ariane Donard[1, 2], Amélie Hubert[2], Fabien Pointurier[2], Nagore Grijalba[1,3], Nora Unceta[3],Christophe Pécheyran[1]; [1]LCABIE, IPREM UMR UPPA/CNRS 5254, University of Pau and Pays de l'Adour, Pau, France; [2]CEA-DIF, Bruyères le Châtel, Arpajon; [3]Department of Analytical Chemistry, Faculty of Pharmacy, University of the Basque Country, Vitoria-Gasteiz, Spain

9:55 (10) **Novel Forensic Applications Using LA-ICP-MS and LIBS**; Jose Almirall[1], Tricia Hoffman[1]; [1]Florida International University

10:15 (11) **High-resolution for Direct Isotopic Analysis**; Martin Resano[1], Esperanza García-Ruiz[1], Maite Aramendía[1], Eduardo Bolea-Fernandez[2], Frank Vanhaecke[2], Flavio Nakadi[2],Marcia Veiga[2]; [1]University of Zaragoza; [2]Department of Analytical Chemistry, Ghent University, Belgium; [3]Universidade de Sao Paulo

10:35 (12) **Expanding LA-ICP-MS Capabilities with Simultaneous LIBS and LAMIS**; Richard Russo[1,2], Jhanis Gonzalez[1, 2], Xianglei Mao[1,2], George Chan[1], Vasillia Zorba[1], Jong Yoo[2], Alexander Bol'shakov[2], Derrick Quarles[2]; [1]Lawrence Berkeley National Laboratory; [2]Applied Spectra, Inc

Monday Morning, *Room 551B*
BEYOND PCA AND PLS: NEW FRONTIERS IN CHEMOMETRICS
Organizer and Presider: Peter de B. Harrington

9:15 (13) **Topological Data Analysis: A New Tool for Big Data Exploration.**; Ludovic Duponchel[1]; [1]Lille University

9:35 (14) **Multi-block Data Analysis: New Extensions and Applications in Chemometrics**; Douglas Rutledge[1], Delphine Jouan-Rimbaud Bouveresse[1]; [1]AgroParisTech

9:55 (15) **Classical Least Squares Methods for Target Detection in Hyperspectral Imaging**; Neal Gallagher[1]; [1]Eigenvector Research, Inc.

10:15 (16) **Homeopathic ICA: A Simple Approach to Expand the Use of Independent Component Analysis**; Willem Windig[1], Michael Keenan[2], Barry Wise[1]; [1]Eigenvector Reseach, Inc.; [2]8346 Roney Rd. Wolcott, NY 14590

10:35 (17) **Comparative Study of Classification Trees for the Authentication of Marijuana**; Peter Harrington[1], Xinyi Wang[2], Steve Baugh[1]; [1]Ohio University; [2]Cannaprint

Monday Morning, *Room 551A*
ANALYSIS OF COUNTERFEIT DRUGS AND NEW PSYCHOACTIVE SUBSTANCES
Organizer: Oliver Stucliffe; Presider: Glen Jackson

9:15 (18) **High Pressure Studies of Illicit Materials**; Iain Oswald[1], Oliver Sutcliffe[2], Niamh Nic Daeid[3]; [1]University of Strathclyde; [2]Manchester Metropolitan University; [3]University of Dundee

9:35 (19) **Evaluation of Two Wavelengths, 785 and 1064 nm, for the Identification of New Psychoactive Substances using Handheld Raman Spectroscopy**; Amira Guirguis[1], Sarah Girotto[1], Benedetta Berti[1], Jacqueline Stair[1]; [1]University of Hertfordshire

9:55 (20) **Forensic Examinations to Determine Illicit Drugs Commonly Seized in the Philippines: From Evidence to Judgment**; Ronald Jefferson Narceda[1]; [1]Philippine Drug Enforcement Agency

10:15 (21) **Improved Identification Algorithms for Detection of Counterfeit Medicines by Raman Spectroscopy**; Latevi Lawson[1], Jason Rodriguez[1]; [1]FDA

10:35 (22) **Drug Quality and Dissolution Testing at All Points in the Supply Chain: Integration of Scalable Technology in the Health System**; Muhammad Zaman[1], Nga Ho[1], Darash Desai[1]; [1]Boston University

Monday Morning, *Ballroom E*
INDUSTRIAL LIBS
Organizer and Presider: François R. Doucet

9:15 (23) **LIBS Outside the Lab**; Christian Bohling[1], Jens-Uwe Günther[1], Angelika Feierabend[1], Andreas John[1]; [1]Secopta GmbH, Berlin

9:35 (24) **Stimulated Emission and Lasing in a Laser-Induced Plasma**; Lev Nagli[1], Michael Gaft[1]; [1]Laser Distance Spectrometry Ltd

9:55 (25) **The Determination of Bioavailability Concentrations of Nutrients in Soils using Chemometric Analysis of LIBS Data**; Josette El Haddad[1], Aissa Harhira[1], Luc English[2], Gilles Clément[2], Charles Nault[2], Alain Blouin[1],Mohamad Sabsabi[1]; [1]National Research Council Canada - Energy, Mining and Environmentt; [2]LOGIAG Inc.

10:15 (26) **LIBS Process Analyzer**; Francois Doucet[1], Lutfu Ozcan[1]; [1]ELEMISSION Inc.

10:35 (27) **Laser Induced Breakdown Spectroscopy for Gold Analysis in Ore Samples**; Kheireddine Rifai[1,2], Marcel Laflamme[1], Marc Constantin[1], Mohamad Sabsabi[2], Alain Blouin[2], François Vidal[3],Paul Bouchard[2], Konstontinos Fytas[1]; [1]Université Laval; [2]National Research Council Canada - Energy, Mining and Environment; [3]IRNS - Energie matreriaux et telecommunication

Monday Morning, *Room 552B*
SENSING TECHNIQUES FOR COUNTERFEIT DRUG DETECTION
Organizer: Anna Luczak; Presider: Ravi Kalyanaraman

9:15 (28) **Organic and Inorganic Techniques and Strategies for Analysing Illegal Generic Medicines**; Neville Broad[1,2]; [1]Authenticate Limited (UK); [2]University of Kent (UK)

9:35 (29) **Combating Adulterated Drug Products**; Connie Ruzicka[1], Kelly Park[1], Katherine Alejo[1]; [1]US Food and Drug Administration

9:55 (30) **Challenges of Counterfeit Drug Detection in the Field**; Pauline Leary[1], John Reffner[2]; [1]Smiths Detection; [2]John Jay College of Criminal Justice

10:15 (31) **The Creation of Paper-based Devices to Detect Select Pharmaceuticals**; Toni Barstis[1]; [1]Saint Mary

10:35 (32) **Rapid Identification of Counterfeit Medicines from the World Market using Dual Laser Handheld Raman Spectroscopy**; Sulaf Assi[1]; [1]Bournemouth University

Monday Morning, *Room 555B*
SERS
Organizer and Presider: Duncan Graham

9:15 (33) **Point-of-Care Tumor Detection with Biomarker-Targeted SERS Nanoparticles Topically Applied on Fresh Tissues**; Jonathan Liu[1]; [1]University of Washington

9:35 (34) **New Reporters for bioLogical SERS Measurements**; Colin Campbell[1], Patrick Thomson[1], Kate Fisher[1]; [1]University of Edinburgh

9:55 (35) **High Throughput Optofluidic Surface Enhanced Raman Spectroscopy (SERS) Interrogation: Proof of Concept via Lectin Detection of Cancerous Cells**; Marjorie Willner[1], Jonathan Simpson[2], Kay McMillan[2], Michele Zagnoni[2], Duncan Graham[2], Peter Vikesland[1]; [1]Virginia Polytechnic Institute and State University; [2]University of Strathclyde

10:15 (36) **Ultrasensitive Detection with SERS and SEHRS**; Jon Camden[1]; [1]University of Notre Dame

10:35 (37) **Surface-enhanced Raman Scattering (SERS) Spectroscopy for Intracellular Chemical Imaging and Protein Analysis**; Katsumasa Fujita[1]; [1]Osaka University

Monday Morning, *Room 556A*
EXTENDING THE SCOPE OF RAMAN: ROA AND OTHER RECENT ADVANCES
Organizer and Presider: Ewan Blanch

9:15 (38) **Raman Optical Activity of Amide and Disulfide Groups in Peptides and Model Systems**; Vladimir Baumruk[1], Marketa Pazderkova[1, 2], Vaclav Profant[1], Lucie Bednarova[2], Petr Malon[1]; [1]Charles University in Prague, Faculty of Mathematics and Physics; [2]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

9:35 (39) **Vibrational Chiroptical Spectroscopy in Natural Product Chemistry: Have We Achieved Enough?**; Joao Marcos Batista Junior[1]; [1]Federal University of Sao Carlos - UFSCar

9:55 (40) **Insights into the Vibrational Nature of Carbohydrates from Raman Optical Activity**; Shaun Thomas Mutter[1]; [1]University of Manchester / Manchester Institute of Biotechnology

10:15 (41) **Studying the Distribution of Deep Raman Spectroscopy Signals using Liquid Tissue Phantoms with Varying Optical Properties**; Martha Vardaki[1], Benjami Gardner[1], Nicholas Stone[1], Pavel Matousek[2]; [1]School of Physics, University of Exeter; [2]Central Laser Facility, STFC Rutherford Appleton Laboratory

10:35 (42) **Standoff UV Raman Spectroscopy: Spatial Heterodyne Raman Spectrometer for Planetary Applications**; Nirmal Lamsal[1], S. Michael Angel[1], Shiv K. Sharma[2], Tayro Acosta-Maeda[2]; [1]University of South Carolina; [2]University of Hawaii

Monday Morning, *Room 552A*
NOVEL TEACHING METHODS IN ANALYTICAL CHEMISTRY
Organizer and Presider: Jared Baker

9:15 (43) **Flipping the Analytical Chemistry Classroom**; Christopher Harrison[1]; [1]San Diego State University

9:35 (44) **Arduino Powered Instrument Design and Construction in Undergraduate Analytical Chemistry Courses**; Celeste Morris[1]; [1]Northern Kentucky University

9:55 (45) **Multiperspective Views in Teaching Laboratory Techniques**; Kevin Davies[1]; [1]Florida Gulf Coast University

10:15 (46) **Social Media in the Blended Classroom**; Kate Hayden[1]; [1]Birmingham-Southern College, Birmingham AL

10:35 (47) **Perspectives from the Flip: The Active-Learning Experience in Analytical Chemistry**; Jared Baker[1]; [1]Elmira College

TECHNICAL PROGRAM – MONDAY
Orals 9:15 – 10:55 am ♦ Posters 11:00 am – 12:00 pm

Monday Morning, *Room 556B*
ADVANCED TECHNIQUES FOR INFRARED SPECTROSCOPY ON STRUCUTRE-FUNCTION RELATIONS OF PROTEINS
Organizer: Yukihiro Ozaki; Presider: Teizo Kitagawa

9:15 (48) **General Remarks**; Teizo Kitagawa[1]; [1]University of Hyogo

9:25 (49) **Coupling Mechanism in the Reaction of Cytochrome C Oxidase Revealed by Newly Developed Time-Resolved IR Measurements**; Satoru Nakashima[1]; [1]Graduate School of Life Science, University of Hyogo

9:55 (50) **Infrared Spectroscopic Study on the Structure and Dynamics of Sodium Pump Rhodopsin**; Keiichi Inoue[1,2]; [1]Nagoya Institute of Technology; [2]PRESTO, JST

10:15 (51) **Infrared Studies of the Photosynthetic Oxygen Evolving Complex**; Bridgette Barry[1], Udita Brahmachari[1], Zhanjun Gup[1]; [1]Georgia Institute of Technology

10:35 (52) **Novel Time-Resolved IR Spectroscopies to Elucidate the Mechanism of Channelrhodopsin**; Joachim Heberle[1]; [1]FU Berlin

Monday Morning, *Room 553A*
CHARACTERIZATION AND SURFACE SCIENCE OF NANOMATERIALS
Organizer and Presider: Kateryna Artyushkova

9:15 (53) **Finding Needles in Haystacks: Scanning Tunneling Microscopy Reveals the Highly Site-Specific Reactivity of TiO2 Surfaces**; Melissa Hines[1]; [1]Cornell University

9:35 (54) **Atomic Scale Spectrometry and Structure - Correlating Atom Probe Tomography and Transmission Electron Microscopy**; David Diercks[1], Brian Gorman[1]; [1]Colorado School of Mines

9:55 (55) **Single Atom Alloys as a Strategy for Selective Heterogeneous Hydrogenations**; Charles Sykes[1]; [1]Tufts University

10:15 (56) **Epitaxial Graphene: Not so Plane and Simple**; Phillip First[1]; [1]Georgia Institute of Technology

10:35 (57) **Photopatterned Electroless Gold Deposition: Optimizing Film Patterning and Nanoscale Structure for Applications**; Y M Nuwan Bandara[1], Buddini Karawdeniya[1], Julie Whelan[1], Brian Velleco[1], Jason Dwyer[1]; [1]University of Rhode Island

Monday Poster Session
11:00 am – 12:00 pm
Ballroom A

All Monday posters should be put up between 7:30 – 8:30 am and removed by 4:30 pm

Atomic Spectroscopy I Posters

Poster Board #1
(58) **Correlation Analysis between Aging Grade & Crystallite Size and Spectral Characteristics of the Laser-Induced Plasma**; Jidong Lu[1], Meirong Dong[1], Jun LI[1], Xuan Dong[1]; [1]South China University of Technology

Poster Board #2
(59) **Detection of Molecular Emission Bands by LIBS: Application to the Quantitative Analysis of Nitrogen in Solid Materials**; Meirong Dong[1], Jidong Lu[1], Jianhua Yu[1], Bo Zhang[1], Yue Pan[1]; [1]South China University of Technology

Poster Board #3
(60) **Excited State Decay of N2+ at Stratospheric Pressures**; Kumarasiri Konthasinghe[2], Andreas Muller[2], Adam Hopkins[1]; [1]Alakai Defense Systems; [2]University of South Florida

Poster Board #4
(61) **Cold Atmospheric Plasma: An Inside Look Through Optical Diagnostics**; Liesl Krause[1,2], Prasoon Diwakar[1], Ahmed Hassanein[1]; [1]Center for Materials Under Extreme Environment, School of Nuclear Engineering, Purdue University; [2]Department of Electrical and Computer Engineering, College of Engineering, Villanova University

Poster Board #5
(62) **Exploring the Effect of Sample Properties on Spark-Induced Breakdown Spectroscopy**; Michael Marino[1], Payson Dieffenbach[1], Liesl Krause[2], Prasoon Diwakar[1], Ahmed Hassanein[1]; [1]Center for Materials Under Extreme Environment, School of Nuclear Engineering, Purdue University; [2]Department of Electrical and Computer Engineering, College of Engineering, Villanova Universiy

Poster Board #6
(63) **Elemental Analysis of Medicinal Plants from India used for the Treatment of Cardiovascular Heart Diseases by Atomic Absorption Spectroscopy and Nondestructive Instrumental Neutron Activation Analysis**; Bharati Pardeshi[1]; [1]PDEA

Poster Board #7
(64) **Chlorine Isotope Determination by High-Resolution Continuum Source Graphite Furnace Molecular Absorption Spectrometry**; Esperanza García-Ruiz[1], Flavio V. Nakadi[2], Marcia A.M.S. da Veiga[2], Maite Aramendía[1,3], Martín Resano[1]; [1]University of Zaragoza; [2]Universidade de Sao Paulo; [3]Centro Universitario de la Defensa-Academia General Militar de Zaragoza

Poster Board #8
(65) **Significance of Plasma-Ambient Conditions in Emission Features of Laser Ablation Plasmas**; Patrick Skrodzki[1,2], Niral Shah[1], Jason Becker[1,2], Sivanandan Harilal[1], Mark Phillips[1], Brian Brumfield[1],Nicole LaHaye[1]; [1]Pacific Northwest National Laboratory; [2]Purdue University

Poster Board #9
(66) **Develpment of High-Density Microplasma Emission Source using 3-D Molding Process Based on Microsterolithography**; Ken Kakegawa[1], Ryoto Harigane[2], Mari Aida[1], Hidekazu Miyahara[1], Shoji Maruo[2], Akitoshi Okino[1]; [1]Department of Energy Sciences, Tokyo Institute of Technology; [2]Department of Mechanical Engineering, Yokohama National University

Poster Board #10
(67) **Thermomechanical Characterization of Resilin by Combining Contact Resonance Atomic Force Microscope and Nano Thermal Analysis**; Ehsan Rezaei[1], Charles Nguyen[1], Anastasia Desyatova Desyatova[1], Deepak Rudrappa[2], Paul Blum[2], Joseph Turner[1]; [1]Mechanical and Materials Engineering, University of Nebraska-Lincoln; [2]School of Biological Sciences, University of Nebraska-Lincoln

Poster Board #11
(68) **The Use of XYZ Sample Manipulator in Quadrupole Glow Discharge Mass Spectrometer**; Maciej Miśnik[1,2], Piotr Konarski[1], Aleksander Zawada[1,3]; [1]Institute of Tele and Radio Technology, ul. Ratuszowa 11, 03-450 Warszawa; [2]Gdańsk University of Technology, ul. G. Narutowicza 11/12, 80-233 Gdańsk; [3]Military University of Technology, ul. Kaliskiego 2, 01-476 Warszawa

TECHNICAL PROGRAM – MONDAY
Posters 11:00 am – 12:00 pm

Poster Board #12

(69) **The Use of Transition Rate Diagrams to Identify Changes in Discharge Processes when O2 or H2 is Present in a Cu/Ne glow Discharge**; Edward Steers[2], Zdenek Weiss[1], Sohail Mushtaq[2], Volker Hoffmann[4], Viktoria Weinstein[2]; [1]LECO Instrumente Plzeň spol. s r.o.; [2]London Metropolitan University, London; [3]Imperial College London; [4]IFW Dresden

Poster Board #13

(70) **Does Asymmetric Charge Transfer Play an Important Role as the Ionization Mode in Low Power-Low Pressure GD-MS?**; Edward Steers[1], Sohail Mushtaq[1], Glyn Churchill[2], DeAnn Barnhart[2], Volker Hoffmann[3], Karol Putyera[4],Juliet Pickering; [1]London Metropolitan University; [2]Nu Instruments Ltd.; [3]IFW Dresden; [4]Evans Analytical Group

Forensic and Security Posters

Poster Board #14

(71) **Forensic STR Profiling Based Smart Barcode, a Highly Efficient and Cost Effective Human Identification System**; Andleeb Zahra[1,2,3], Bilal Hussain[1], Amer Jamil[4]; [1]Government College University Faisalabad Pakistan; [2]COmsats Institute of Technology Islamabad Pakistan; [3]Koc University, Istanbul , Turkey; [4]University of Agriculture Faisalabad Pakistan

Poster Board #15

(72) **Estimation of the Age of Bloodstains under Different Environmental Conditions with Fourier Transform Infrared Spectroscopy and Multivariate Statistical Analysis**; Zhenyu Lu[1], Brianna Cassidy[1], Stephanie Dejong[1], Katherine Witherspoon[1], Michael Myrick[1], Stephen Morgan[1]; [1]University of South Carolina

Poster Board #16

(73) **An Experimental Study of the Forensic Luminol Test for Detection of Bloodstains**; Brianna Cassidy[1], Zhenyu Lu[1], Kathrine Witherspoon[1], Jennifer Martin[1], Stephanie DeJong[1], Raymond Belliveau[1],Michael Myrick[1], Stephen Morgan[1]; [1]University of South Carolina

Poster Board #17

(74) **Lost in Translation: Bridging Vibrational Spectroscopy Knowledge from Scientists to End Users**; Luisa T.M. Profeta[1], Alan Ford[1], Alen Tomczak[1], Jack Burton[1], Ken Pohl[1]; [1]Alakai Defense Systems

Poster Board #18

(75) **Novel Concept for Forensic Analysis of Biomarkers**; Jan Halamek[1]; [1]Department of Chemistry, University at Albany, SUNY

Poster Board #19

(76) **New and Practical Methods to Characterize Organic Gunshot Residue**; Sydney Brooks[1], Brittany Yeager[1], Suzanne Bell[1]; [1]West Virginia University

Poster Board #20

(77) **The Surprising Effect of Temperature on the Weathering of Gasoline**; Ashley Cochran[1], Heather Birks[1], Tyler Williams[1], Glen P. Jackson[1]; [1]West Virginia University

Poster Board #21

(78) **Raman and Laser Induced Fluorescence Spectroscopy on Ageing Fingerprints**; Lars Landström[1], Christian Lejon[1], Therese Mikaelsson[1], Göran Kidfelt[2], Milja Kanerva[2], Cecilia Vahlberg[2],Kent Rosengren[2], Per Ola Andersson[1]; [1]CBRN Defence and Security, Swedish Defence Research Agency (FOI); [2]Nationellt Forensiskt Center (NFC)

Poster Board #22

(79) **Detection of Trace Evidence Particles by Mid-Infrared Laser Reflectance Imaging**; Raymond Belliveau[1], Stephanie DeJong[1], Lu Zhenyu[1], Brianna Cassidy[1], Stephen Morgan[1], Michael Myrick[1]; [1]University of South Carolina, Department of Chemistry and Biochemistry

Poster Board #23

(80) **A Raman 'Spectroscopic Clock' for Bloodstain Age Determination: The First Week After Deposition**; Kyle C. Doty[1], Gregory McLaughlin[1], Igor K. Lednev[1]; [1]University at Albany

LIBS Posters

Poster Board #24

(81) **Self-Absorption Measurements of Resonant Aluminum Lines**; David Surmick[1], Christian Parigger[1]; [1]University of Tennessee Space Institute

Poster Board #25

(82) **Laser-Induced Plasma Diagnostics with the Hydrogen Balmer beta Line**; Ghaneshwar Gautam[1], Christian Parigger[1]; [1]University of Tennessee Space Institute

Poster Board #26

(83) **Bio-distribution of Magnetic Gold Nanoparticle in Liver through Changes of Ca Channel Pump Detected by LIBS Technique**; Ola Ahmed, Hisham Imam[2], Abdel Rahman Zekri[3]; [1]National Cancer institute, Cairo University, Egypt; [2]National institute of laser enhanced science (NILES), Cairo University, Egypt; [3]National Cancer institute, Cairo University, Egypt

Poster Board #27

(84) **Discrimination of Polymers from Plasma Parameters using Laser Induced Breakdown Spectroscopy**; M Atif; [1]King Saud University

Poster Board #28

(85) **The Role of Gas Dynamics on the Formation of AlO in Laser-Ablation Plumes**; Sivanandan Harilal[1], Brian Brumfield[1], Jeremy Yeak[2], Mark Phillips[1]; [1]Pacific Northwest National Laboratory; [2]PM & AM Research

Poster Board #29

(86) **Multiblock Analysis Applied to LIBS and XRF Data of Geological Materials**; Faten Ammari[1], Léna Bassel[1], Catherine Ferrier[3], Delphine Lacanette-Puyo[4], Rémy Chapoulie[1], Bruno Bousquet[2]; [1]Université Bordeaux Montaigne, IRAMAT-CRP2A, UMR 5060 CNRS; [2]Université de Bordeaux, CELIA, UMR 5107 CNRS; [3]Université de Bordeaux, PACEA, UMR 5199 CNRS; [4]Université de Bordeaux, I2M-TREFLE, UMR 5295 CNRS

Poster Board #30

(87) **Improved Electron Collisional Line Broadening for High Resolution LIBS Modeling in the Plasma Kinetics Code ATOMIC**; Heather Johns[1], David Kilcrease[1], James Colgan[1], Elizabeth Judge[1], James Barefield[1], Samuel Clegg[1]; [1]Los Alamos National Laboratory

Poster Board #31

(88) **Temporally and Spatially-Resolved Absorption Spectroscopy of Atomic Oxygen in an Air Spark**; Brian Brumfield[1], Sivanandan Harilal[1], Mark Phillips[1]; [1]Pacific Northwest National Laboratory

Poster Board #32

(89) **Laser-induced Breakdown Spectra of Rocks at Variable Ablation and Collection Angles**; Elly Breves[1], Kate Lepore[1], M. Darby Dyar[1], Steven C. Bender[2], Robert L. Tokar[2]; [1]Mount Holyoke College; [2]Planetary Science Institute

Poster Board #33

(90) **Application of the Laser-Induced Breakdown Spectroscopy Technique in Steel and Metal Industry**; Vincenzo Palleschi[1,2], Emanuela Grifoni[1], Stefano Legnaioli[1,2], Stefano Pagnotta[1], Giulia Lorenzetti[1]; [1]Applied and Laser Spectroscopy Laboratory, ICCOM-CNR, Pisa, Italy; [2]National Interuniversity Consortium of Materials Science and Technology (INSTM)

TECHNICAL PROGRAM – MONDAY
Posters 11:00 am – 12:00 pm

Poster Board #34

(91) **Determination of Elemental Composition of Shale Rocks by Laser Induced Breakdown Spectroscopy (LIBS)**; Jinesh Jain[1], Alexander Bol'shakov[2], Hervé Sanghapi[1], Christina Lopano[1], Dustin McIntyre[1], Richard Russo[2]; [1]National Energy Technology Laboratory; [2]Applied Spectra, Inc.

Poster Board #35

(92) **Signal Enhancement in Double-pulse LIBS of Various Metals in Relation to their Physical and Thermal Properties: A Statistical Analysis**; Patrick Skrodzki[1], Jason Becker[1], Prasoon Diwakar[1], Ahmed Hassanein[1]; [1]Center for Materials Under eXtreme Environment, School of Nuclear Engineering Purdue University

Poster Board #36

(93) **The Role of Material Properties on Emission Spectra in Nano- and Femtosecond Laser-Induced Breakdown Spectroscopy**; Jason Becker[1], Patrick Skrodzki[1], Prasoon Diwakar[1], Ahmed Hassanein[1]; [1]Center for Materials Under eXtreme Environment, School of Nuclear Engineering Purdue University

Materials Characterization Posters

Poster Board #37

(94) **Protonation Effects of Alumina Surface on the First Electronic Transition of Liquid Water Studied by Far-Ultraviolet Spectroscopy**; Takeyoshi Goto[1], Yukihiro Ozaki[1]; [1]Kwansei Gakuin Unversity

Poster Board #38

(95) **Electronic Transitions of Hydrated Amino Acids in the Wavelength Region 145−300 nm Studied by Far-Ultraviolet Spectroscopy**; Takeyoshi Goto[1], Yukihiro Ozaki[1]; [1]Kwansei Gakuin Unversity

Poster Board #39

(96) **Thermal Analysis of Thermally Reversible Gels Made of a Bio-based, Biodegradable Polymer**; Brian Sobieski[1], Liang Gong[1], John Rabolt[1], Isao Noda[1], Bruce Chase[1], Steve Aubuchon[1,2]; [1]University of Delaware; [2]TA Instruments

Poster Board #40

(97) **Temperature Dependence of FUV Spectra for Aqueous Solutions of Alkali Halide to the Freezing-point of Eutectic**; Yusuke Morisawa[1], Yuka Nishikawa[1], Akifumi Ikehata[2]; [1]Kinki University; [2]NFRI, NARO

Poster Board #41

(98) **Computing Molar Extinction Coefficient of Capsaicin Using Absorbance Spectroscopy in the Visible Range**; Abraham Lopez[1], José Javier Báez Rojas[1], Jorge Castro Ramos[1], Karen Esmonde-White[2]; [1]National Institute of Astrophysics Optics and Electronics; [2]University of Michigan, Medical School

Poster Board #42

(99) **Measuring Thermal Properties of Oilseeds using Unilateral Nuclear Magnetic Resonance sensor**; Maria G. A. Carosio[1], André de S. Carvalho[2], Luis F. Cabeça[3], Luiz A. Colnago[1]; [1]EMBRAPA Instrumentation; [2]Institute of Chemistry of São Carlos; [3]Federal Technological University of Parana

Poster Board #43

(100) **Moving Window Two-Dimensional Correlation Spectroscopy of the Early Stage Crystallization of Polyethylene**; Ying Jin, Anthony Kotula[1], Angela Hight Walker[1], Kalman Migler[1], Young Jong Lee[1]; [1]National Institute of Standards and Technology

Poster Board #44

(101) **Spectroscopic Markers for Uranyl Phosphates: A Vibrational Study**; Dale L. Perry[1], Nataliya Kalashnyk[2], Eric Faulques[3], Florian Massuyeau[3]; [1]Lawrence Berkeley National Laboratory, University of California, Berkeley; [2]Institut Matériaux Microéléctronique Nanosciences de Provence (IM2NP), Université d' Aix-Marseille, UMR CNRS 7334; [3]Institut des Matériaux Jean Rouxel, Université de Nantes, UMR CNRS 6502

Poster Board #45

(102) **Elemental Characterization of Glass Tesserae via X-Ray Fluorescence Spectrometry**; Andrew Sparks[1], Mary Kate Donais[1]; [1]Saint Anselm College

Poster Board #46

(103) **First Electronic Transition of Water Molecules in Binary Solutions Studied by Far-Ultraviolet Spectroscopy**; Kodai Kishibe[1], Takeyoshi Goto[1], Hiroto Tanaka[1], Yukihiro Ozaki[1]; [1]Graduate School of Science and Technology, Kwansei Gakuin University

Poster Board #47

(104) **Thermal Behavior and Lamella Structures of Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) Studied by Low-Frequency Raman, Terahertz Spectroscopy, and Small Angle X-ray Scattering**; Dian Marlina[1], Mengfan Wan[1], Koh Yoshida[1], Hiromichi Hoshina[2], Harumi Sato[3], Yukihiro Ozaki[1]; [1]Graduate School of Science and Technology, Kwansei Gakuin University; [2]RIKEN; [3]Graduate School of Human Development and Environment, Kobe University

Nanomaterials Posters

Poster Board #48

(105) **Non-hydrolytic Processing of Transition Metal-Doped TiO2 Nanostructures for Photocatalytic Applications**; Swati Naik[1], Gabriel Caruntu[1]; [1]Central Michigan University

Poster Board #48

(106) **Coupling Single Molecule Spectroscopy and Electrochemistry in Zero-Mode Waveguides**; Lawrence Zaino, Dane Grismer, Donghoon Han, Paul Bohn[1]; [1]University of Notre Dame

Poster Board #50

(107) **Measurement of Spatially Confined Nanoclusters of Porphyrins Using Conductive-Probe Atomic Force Microscope**; Xianglin Zhai[1], Neepa KuruppuArachchige[1], Pedro Derosa[2], Jayne Garno[1]; [1]Louisiana State University; [2]Louisiana Tech University

Poster Board #51

(108) **Turn-On Fluorescence as a Strategy for Monitoring the Catalyzed Reduction of Nitrite by Pd-on-Au Nanoparticles**; Anthony Stender[1], Emilie Ringe[1]; [1]Rice University

Poster Board #52

(109) **Studies of Electronic States of CNT/Rubber Nanocomposites by using Attenuated Total Reflectance Spectroscopy in the Ultraviolet Region**; Yusuke Morisawa[1], Kenta Kobashi[2], Ichiro Tanabe[2], Harumi Sato[3], Takeyoshi Goto[2], Yukihiro Ozaki[2]; [1]Department of Chemistry, School of Science and Engineering, Kinki University; [2]Department of Chemistry, School of Science and Technology, KwanseiGakuin University; [3]Graduate School of Human Development and Environment, Kobe University

Poster Board #53

(110) **Investigation of Electronic States of Nano Carbon/Polymer Nanocomposites by Attenuated Total Reflectance-Ultraviolet Spectroscopy**; Kenta Kobashi[1], Ichiro Tanabe[1], Yusuke Morisawa[2], Harumi Sato[3], Takeyoshi Goto[1], Yukihiro Ozaki[1]; [1]Graduate School of Science and Technology, Kwansei Gakuin Univ; [2]Graduate School of Science and Technology, Kinki Univ; [3]Graduate School of Human Development and Environment, Kobe Univ

Poster Board #54

(111) **Structural and Magnetic Properties of Cobalt Substituted Magnetite/Ferrihydrite Composites**; Dale L. Perry[3], K. I. Camacho[1], N. Pariona[1], Arturo I. Martinez[1], E. Baggio-Saitovitch[2]; [1]Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional Unidad Saltillo; [2]Centro Brasileiro de Pesquisas Físicas, Río de Janeiro; [3]Lawrence Berkeley National Laboratory, University of California, Berkeley

Monday Afternoon, *Room 550A/B*
FUNDAMENTALS AND NOVEL APPLICATIONS OF LA-ICP-MS: II
Organizer: Jorge Pisoneror; Presider: Bodo Hattendorf

1:20 (112) **Evaluation of Different Strategies for Laser-Induced Aerosol Mixing and Filtering in Order to Improve the Capabilities of LA-ICP-MS.**; Jorge Pisonero[1], David Blanco[2], Natalia Beltrán[2], Nerea Bordel[1]; [1]Department of Physics, University of Oviedo; [2]Department of Manufacturing Engineering, University of Oviedo, Campus of Gijón

1:40 (113) **Laser Ablation-ICP-Mass Spectrometry : Sensitive, Rapid and User Friendly Analytical Technique of Trace Metals for Both Geochemical and Biochemical Samples**; Takafumi Hirata[1]; [1]Kyoto University

2:00 (114) **State of the Art in Bio-Imaging by LA-ICP-MS**; Philip Doble[1]; [1]UTS

2:20 (115) **Development of a Laser Ablation−Inductively Coupled Plasma−Mass Spectrometry Cell and Deconvolution Approaches for Fast High Resolution 3D Imaging**; Stijn J. M. Van Malderen[1], Johannes T. van Elteren[2], Frank Vanhaecke[1]; [1]Department of Analytical Chemistry, Ghent University, Belgium; [2]Analytical Chemistry Laboratory, National Institute of Chemistry, Slovenia

2:40 (116) **Femtosecond Laser Ablation-Based Mass Spectrometry: An Ideal Tool for Stoichiometric Analysis of Thin Films on the Nanoscale**; Nicole LaHaye[1,2], Jose Kurian[3], Prasoon Diwakar[2], Lambert Alff[3], Sivanandan Harilal[1]; [1]Pacific Northwest National Laboratory; [2]Purdue University; [3]Technische Universitat Darmstadt

Monday Afternoon, *Room 554A/B*
AWARD SESSION HONORING 2015 ACS SPECTROCHEMICAL AWARD WINNER FRANK BRIGHT
Organizer and Presiders: Frank Bright and Steven Ray

1:20 (117) **To be Frank and Bright— What More Could One Hope for in a Scientific Colleague and Friend?**; Gary M. Hieftje[1], Elise A. Dennis[1], Alexander Gundlach-Graham[2], Steven J. Ray[1]; [1]Indiana University; [2]ETH Zürich

1:40 (118) **Interplay of Chromatography and Spectroscopy with Carbon Nanoparticles**; Luis Colon[1], Zuqin Xue[1], Karina Tirado-González[1], Amaris Borges-Muñoz[1]; [1]University at Buffalo - SUNY

2:00 (119) **Quantum Dots and Upconverting Nanoparticles: Using Paper Platforms for Multiplexed Optical Sensing by Resonance Energy Transfer**; Ulrich Krull[1], M. Omair Noor[1], Feng Zhou[1], Samer Doughan[1], Yi Han[1], Anna Shahmuradyan[1],Uvaraj Uddayasankar[1]; [1]University of Toronto Mississauga

2:20 (120) **Genome-Inspired Aptamers: Affinity Derived from Nature**; Linda McGown[1]; [1]Rensselaer Polytechnic Institute

2:40 (121) **Seeing the Light: Studies of the Ocular Surface**; Frank Bright[1]; [1]SUNY-Buffalo

Monday Afternoon, *Room 555A*
BIOMEDICAL AND FORENSIC APPLICATIONS OF VIBRATIONAL SPECTROSCOPY
Organizers: Igor K. Lednev and Juergen Popp;
Presider: Igor K. Lednev

1:20 (122) **Raman Spectroscopic Approaches - Possible Solutions for Unmet Medical Needs?**; Juergen Popp[1,2]; [1]Leibniz Institute of Photonic Technology; [2]Institute of Physical Chemistry and Abbe Center of Photonics

1:40 (123) **Practical Considerations in using Raman Spectroscopy for Aging of Blood Stains**; Anita Mahadevan-Jansen[1], Kiana Jansen[1], Maggie O'Connor[1], Maurice Aalders, Isaac Pence[1]; [1]Vanderbilt University

2:00 (124) **Unsupervised and Supervised Multivariate Statistical Analysis of a Large Lung Spectral**; Max Diem[1]; [1]Northeastern University

2:20 (125) **Advanced Statistics of Raman Spectroscopic Data for Disease Diagnostics and Forensic Purposes**; Lenka Halamkova[1], Kyle C. Doty[1], Gregory McLaughlin[1], Elena Ryzhikova[1], Oleksandr Kazakov[1], Igor K. Lednev[1]; [1]University at Albany, SUNY

2:40 (126) **Speed Acquisition Improvement in Raman Imaging via Compressive Sensing**; Nicolas Spegazzini[1], Rishikesh Pandey[1], Ishan Barman[2], Ramachandra Rao Dasari[1]; [1]Massachusttes Institute of Technology; [2]Johns Hopkins University

Monday Afternoon, *Room 551B*
ENSURING PUBLIC SAFETY BY CHEMOMETRIC AUTHENTICATION OF FOOD AND BOTANICALS
Organizer and Presider: James Harnly

1:20 (127) **Advanced Chemometric Strategies for Food Authentication**; Federico Marini[1]; [1]University of Rome La Sapienza

1:40 (128) **Instrumental Approaches and Chemometric Analyses for Establishing Authenticity of Botanical Products**; Paula N. Brown[1], Michael Chan[1], Jamie Finley[1], Christina E. Turi[2], Andrew R. Lewis[3]; [1]British Columbia Institute of Technology; [2]University of British Columbia; [3]Simon Fraser University

2:00 (129) **A UV-Vis-PCA Approach to Botanical Identity Confirmation using DNA Validated Botanical Reference Materials**; Jeremy Stewart[1]; [1]Gaia Herbs, Inc

2:20 (130) **Chemometrics in the United States Pharmacopeia**; Lucy L. Botros[1], Jeffrey C. Moore[1], Alan R. Potts[1]; [1]U.S. Pharmacopeial Convention

2:40 (131) **Spectral Fingerprinting: Following the Transition from Raw Botanical to Finished Product**; James Harnly[1]; [1]US Department of Agriculture

TECHNICAL PROGRAM – MONDAY
Orals 1:20 – 3:00 pm

Monday Afternoon, *Room 551A*
EXPLOSIVE DETECTION I
Organizer and Presider: Jimmie Oxley

1:20 (132) **Nanomaterial Sensors for Trace Chemical Detection**; Ling Zang[1]; [1]University of Utah

1:40 (133) **Fluorescence Detection of Explosives: A Study Towards Optimization of an Array of Thin Film Optical Sensors**; William Euler[1], Hui Qi Zhang[1], Mingyu Liu[1], Matthew Mullen[1]; [1]University of Rhode Island

2:00 (134) **Issues in Explosive Detection: Sampling**; Jimmie Oxley[1]; [1]University of Rhode Island

2:20 (135) **HPIMS in Explosive Detection and Forensic Applications**; Ching Wu[1], Anthony Midey[1], Adam Griachen[1], Mark Osgood[1]; [1]Excellims Corporation

2:40 (136) **HMTD Decomposition: A Kinetic Study**; Lucus Steinkamp[1], Lauryn DeGreeff[2], Kevin Johnson[2], Greg Collins[2], Susan Rose-Pehrsson[2]; [1]National Research Council; [2]Nova Research, Inc., U.S. Naval Research Laboratory

Monday Afternoon, *Ballroom E*
STANDARDS, PROTOCOLS AND QUANTITATIVE ANALYSIS
Organizer and Presider: Amy Bauer

1:20 (137) **Quantitative Analysis of Coal Using Laser Induced Breakdown Spectroscopy**; Zhe Wang[1], Zongyu Hou[1, 2], Tingbi Yuan[1,2]; [1]State Key Lab of Power Systems, Department of Thermal Engineering, Tsinghua-BP Clean Energy Center, Tsinghua University; [2]China Guodian Science and Technology Research Institute

2:00 (138) **Choices and Improvements in Baseline Removal in LIBS Spectroscopy**; Melinda (Darby) Dyar[1], Thomas Boucher[2], Stephen Giguere[2], CJ Carey[2], Sridhar Magadevan[2]; [1]Mount Holyoke College; [2]University of Massachusetts at Amherst

2:20 (139) **Analysis of Wear Metals in Engine Oil using LIBS**; Markus Gaelli[1], Amy Bauer[1]; [1]TSI Incorporated

2:40 (140) **Exploring Matrix Effects on Quantitative Analysis of LIBS Data from Rock Powders Doped with Cr, Ni, Mn, Co, Zn, and S**; Kate Lepore[1], Elly Breves[1], M. Darby Dyar[1]; [1]Mount Holyoke College

Monday Afternoon, *Room 552B*
SENSING TECHNIQUES FOR COUNTERFEIT DRUG DETECTION II
Organizer: Anna Luczak; Presider: Ravi Kalyanaraman

1:20 (141) **Process Patent Protection: Protecting Intellectual Property via Natural-Abundance Stable Isotopes**; John Jasper[1], Martin Pavane[2], Dean Eyler[3], Ila Sharma[4], Albert Lee[4]; [1]Nature's Fingerprint / MIT LLC; [2]Cozen O; [3]Gray Plant Mooty; [4]Chemir Analytical Services

1:40 (142) **A Tiered Analytical Approach for Investigating Poor Quality Emergency Contraceptives**; Facundo Fernandez[1], Maria Eugenia Monge[1], Prabha Dwivedi[1], Manshui Zhou[1], David Jenkins[2], Paul Newton[3,4]; [1]Georgia Institute of Technology; [2]Product Quality and Compliance, FHI 360; [3]Lao-Oxford-Mahosot Hospital-Wellcome Trust Research Unit, Microbiology Laboratory, Mahosot Hospital; [4]WorldWide Antimalarial Resistance Network, Churchill Hospital

2:00 (144) **Meeting Authentication Challenges with Spectroscopic Solutions**; Jeffry Denault[1], Robert Beal[1]; [1]Eli Lilly and Company

2:20 (145) **Raman Spectral Fingerprinting for Biologics Counterfeit Drug Detection**; Ravi Kalyanaraman[1], Anna Luczak[1], Jeremy Peters[1], Varsha Ganesh[1]; [1]Bristol-Myers Squibb

Monday Afternoon, *Room 555B*
BIOANALYTICAL SERS I
Organizer and Presider: Roy Goodacre

1:20 (146) **Rationally Designed Mixed-Monolayer Glyconanoparticles for the Detection of Cholera Toxin by SERS**; Duncan Graham[1], Jonathan Simpson[1], Derek Craig[1], Karen Faulds[1]; [1]University of Strathclyde

1:40 (147) **Metabolite Identification by Sheath-Flow SERS**; Zachary Schultz[1], Matthew Bailey[1], Kevin Jacobs[1]; [1]University of Notre Dame

2:00 (148) **Development of SERS for Monitoring Small Molecule Metabolites**; Mark McDermott[1,2], Shereen Elbayomy[1,2], Albert Cao[1,2]; [1]University of Alberta; [2]National Institute for Nanotechnology

2:20 (149) **Stimulated Raman Spectroscopy for SERS of Biological Systems**; Renee Frontiera[1], W. Ruchira Silva[1], Emily L. Keller[1]; [1]University of Minnesota

2:40 (150) **The Use of Surface Enhanced Raman Scattering (SERS) as an Alternative High-Throughput Screening Method for Applications in Industrial Biocatalysis**; Chloe Westley[1], Yun Xu[1], Andrew Carnell[2], Nicholas Turner[1], Royston Goodacre[1]; [1]Department of Chemistry, University of Manchester, Manchester Institute of Biotechnology; [2]Department of Chemistry, University of Liverpool

Monday Afternoon, *Room 556A*
RAMAN MICROSCOPY
Organizers: Katsumasa Fujita and Duncan Graham; Presider: Katsumasa Fujita

1:20 (151) **Structure of Porous PMMA Thin Film Examined with Multifocus Raman Microspectroscopy**; Koichi Iwata[1], Ashok Samuel[2], Soshi Yabumoto[2], Kenichi Kawamura[3]; [1]Gakushuin University; [2]National Chiao Tung University, Taiwan; [3]Tokyo Instruments

1:40 (152) **Linear and Non-Linear Fiber-Based Raman-spectroscopy for Biophotonic Applications**; Juergen Popp[1,2]; [1]Leibniz Institute of Photonic Technology; [2]Institute of Physical Chemistry and Abbe Center of Photonics

2:00 (153) **Label-free Raman mapping of Living Mammalian Cells - A Valuable New Tool for Investigating Complex Cellular Systems**; Katherine Hollywood[1], LornaAshton[2], Katherine Lau[3], Saba Khan[1], Nicholas Lockyer[1], Mark Dunne[1],Karen Cosgrove[1], Alan Dickson[1], Royston Goodacre[1]; [1]University of Manchester, UK; [2]Lancaster University, UK; [3]Renishaw PLC, UK

2:20 (154) **Rapid, Quantitative Spectroscopic Imaging using Coherent Anti-Stokes Raman Scattering**; Marcus Cicerone[1]; [1]National Institute of Standards and Technology

2:40 (155) **Bioorthogonal Stimulated Raman Imaging for Biomedicine**; Wei Min[1], Lu Wei[1]; [1]Columbia University

Monday Afternoon, *Room 552A*
ADVOCATING FOR WOMEN IN SCIENCE
Organizers and Presiders: Ingeborg Iping Petterson and Anna Donnell

1:20 (156) **Learning Risk-Taking as a Young Female Chemist**; Sarah Maurer[1]; [1]Central Connecticut State University

1:40 (157) **Challenges in Managing a Diverse Workforce**; Fred LaPlant[1]; [1]3M

2:00 (158) **Don't Call Us Dropouts (please)! Choosing Nontraditional Career Paths in the Sciences**; Emily Monosson[1]; [1]Independent

2:20 (159) **Adventures Abroad! Pursuing International (European) Academic Positions**; Ingeborg Iping Petterson[1]; [1]Biomedical Physics, University of Exeter

2:40 (160) **How a Frozen Banana Shaped My Career Path**; Heather Brooke[1]; [1]CAMO Software Inc.

Monday Afternoon, *Room 553A*
NON-LINEAR OPTICAL SPECTROSCOPY FOR SURFACE SCIENCE
Organizer and Presider: Patrick Koelsch

1:20 (161) **Probing Ion Lipid Interactions by Vibrational Sum Frequency Spectroscopy**; Paul Cremer[1]; [1]Penn State University

1:40 (162) **Protein Structures and Folding at Interfaces Probed by Chiral Sum Frequency Generation Vibrational Spectroscopy**; Elsa Yan[1]; [1]Yale University

2:00 (163) **Molecular structure at Solid Surfaces: Understanding the Role of Bulk Effects**; Dennis Hore[1]; [1]University of Victoria

2:20 (164) **Direct Small-Molecule Detection in a Primary Antibody Assay using Second > Harmonic Generation**; John Conboy[1]; [1]University of Utah

2:40 (165) **What Makes Aqueous Foams Stable? A Combined Oscillating Bubble and Vibrational Sum-Frequency Spectroscopy Study**; Patrick Koelsch[1], Matthias J. Hofmann[2], Robert Weikl[2], Hubert Motschmann[2]; [1]University of Washington, Department of Bioengineering; [2]University of Regensburg, Institute of Physical and Theoretical Chemistry

Monday Afternoon, *Room 550A/B*
BIOAPPLICATIONS OF ICP-MS
Organizers and Presiders: Maria Montes-Bayón and Jörg Bettmer

3:50 (166) **Characterization of the Metalloproteome of Histoplasma capsulatum and Its Implications Regarding the Pathogenic Response Under Low Zn Stress**; Anna Donnell[1], Alexey Porollo[2], George Deepe[1], Joseph Caruso[1]; [1]University of Cincinnati; [2]Cincinnati Childrens' Hospital

4:10 (167) **The Use of Stable Isotope Labeling in Mass Spectrometry Based Bioanalysis**; Stephan Hann[1,2], Teresa Mairinger[1], Eva Oburger[3], Markus Puschenreiter[3], Gunda Koellensperger[4]; [1]Division of Analytical Chemistry, Department of Chemistry, BOKU Vienna, Austria; [2]Austrian Center of Industrial Biotechnology (ACIB); [3]Institute of Soil Research, BOKU Vienna, Austria; [4]Institute of Analytical Chemistry, University of Vienna, Austria

4:30 (168) **Applications of ICPMS and MC-ICPMS at Chemical Metrology, National Research Council Canada**; Lu Yang[1]; [1]National Research Council Canada

4:50 (169) **ICP-MS for Multiplex Analysis of Copy Number Variations In Tumor Cells**; Maria Montes-Bayon[1], Tamara Iglesias[1], Marta Espina[1,2], L. Maria Sierra[1,2], Elisa Blanco-González[1]; [1]University of Oviedo; [2]Oncology University Institute (IUOPA)

5:10 (170) **Are Matrix Effects in ICP-MS Independent of Analyte Ion Mass (With or Without High Negative Voltage Ion Extraction)?**; Shi Jiao[1], John W. Olesik[1]; [1]Ohio State University

Monday Afternoon, *Room 555A*
VIBRATIONAL SPECTROSCOPY: TOWARD CLINICAL APPLICATIONS
Organizer and Presider: Nicole J. Crane

3:50 (171) **Fiber Enhanced Raman Multi-Gas Spectroscopy for Breath Analysis**; Torsten Frosch[1], Timea Boegoezi[1], Stefan Hanf[1], Tobias Jochum[1], Juergen Popp[1,2,3]; [1]Leibniz Institute of Photonic Technology; [2]Friedrich Schiller University, Institute for Physical Chemistry; [3]Friedrich Schiller University, Abbe Centre of Photonics

4:10 (172) **IR Imaging: Applications in Wound and Transplant Pathology**; Michael Walsh[1], Bennett Davidson[1], Hari Sreedhar[1], Vishal Varma[1], Peter Nguyen[1], Sanjeev Akkina[1],Aliya Husain[2], Suman Setty[1], Andre Kajdacsy-Balla[1], William Ennis[1]; [1]University of Illinois At Chicago; [2]University of Chicago

4:30 (173) **Shining Light Inside Middle Ear: What Raman Spectroscopy Tells Us about Infection?**; Rishikesh Pandey[1], Nicolas Spegazzini[1], Tulio A Valdez[2], Ishan Barman[3], Ramachandra Rao Dasari[1]; [1]MIT; [2]Connecticut Children; [3]Johns Hopkins University

4:50 (174) **Multi-centre Raman Spectral Histopathology of Deparaffinised Oesophageal Tissues.**; Jennifer Dorney[1], Martin Isabelle[2], Gavin Rhys-Lloyd[2], Catherine Kendall[2], Riana Gaifulina[3], Aaran Lewis[3],Geraint Thomas[3], Katherine Lau[4], David Reece[4], Nick Stone[1]; [1]University of Exeter, Exeter; [2]Gloucester Hospital, Gloucester, United KIngdom; [3]University College London; [4]Renishaw PLC UK

5:10 (175) **Addressing Variability of Tissue Raman Spectroscopy for Clinical Diagnostics**; Isaac Pence[1], Anita Mahadevan-Jansen[1]; [1]Vanderbilt University

Monday Afternoon, *Room 551B*
CHEMOMETRIC KEYS FOR THE INTERPRETATIONOF FORENSIC EVIDENCE
Organizer and Presider: Jose R. Almirall

3:50 (176) **Pattern Recognition/Machine Learning Classification Strategies for Forensic Evidence**; Stephen L. Morgan[1], Nathan C. Fuenffinger[1]; [1]University of South Carolina

4:10 (177) **Development and Evaluation of a Searchable Database for the Characterization and Comparison of Forensic Evidence using Spectrochemical Methods**; Tatiana Trejos[1], Claudia Martinez[1], Ruthmara Corzo[1], Kiran Subedi[1], Rhett Williamson[1], Peter Torrione[2], Jong Yoo[3], Jose Almirall[1]; [1]Florida International University; [2]CoVar Applied Technologies; [3]Applied Spectra, Inc

4:30 (178) **A Bayesian Approach to Interpretion of Multi-element Data**; James Curran[1]; [1]University of Auckland

4:50 (179) **Chemometric Approaches for the Analysis of Chemical Attribute Signatures Generated from Forensically Relevant Samples**; Adam B. Hall[1]; [1]Northeastern Univeristy; [2]Boston University School of Medicine; [3]IonSense, Inc.

5:10 (180) **Evaluation of Analytical Figures of Merit for the Analysis of Nitrogen, Phosphorous, and Sulfur Using Laser Induced Breakdown Spectroscopy (LIBS)**; C. Derrick Quarles Jr.[1], Charles Sisson[1], Jhanis J. Gonzalez[1,2], Richard E. Russo[1,2]; [1]Applied Spectra, Inc.; [2]Lawrence Berkeley National Laboratory

TECHNICAL PROGRAM – MONDAY
Orals 1:20 – 3:00 pm and 3:50 – 5:30 pm

Monday Afternoon, *Room 551A*
NUCLEAR FORENSICS
Organizer and Presider: Andrew Duffin

3:50 (181) **Applications of a New Single Stage Accelerator Mass Spectrometer to Trace Detection and Nuclear Forensics**; Albert Fahey[1], Kamron Fazel[1], Kenneth Grabowski[1], Evan Groopman[1]; [1]Naval Research Laboratory

4:10 (182) **X-Ray Microscopy of Nuclear Materials**; Jesse Ward[1], Greg Eiden[1], Andrew Duffin[1]; [1]Pacific Northwest National Laboratory

4:30 (183) **Advances in Analysis of Samples for Nuclear Non-Proliferation at CEA/DIF**; Bruno Bernard-Michel[1], Fabien Pointurier[1], Maxime Bridoux[1], Anne-Laure Fauré[1], Amélie Hubert[1], Olivier Marie[1],Anne-Claire Pottin[1]; [1]CEA-DIF, Bruyères le Châtel

4:50 (184) **Discrimination of Uranium ore Concentrates from Several Countries by Chemometric Data Analysis**; Josette El Haddad[1], Aissa Harhira[1], Alain Blouin[1], Mohamad Sabsabi[1], Marvin Zaluski[2], Chunsheng Yang[2],Christopher Drummond[2], Slobodan Jovanovic[3], Tanya Hinton[3], Ali El-Jaby[3]; [1]National Research Council Canada - Energy, Mining and Environment; [2]National Research Council Canada - Information and Communications Technologies; [3]Canadian Nuclear Safety Commission

5:10 (185) **DC Arc Spectroscopy – Plasma Characterization for Direct Solid Analysis of Nuclear Materials**; Benjamin T. Manard[1], John Matonic[1], Robert Jump[1], Dennis Montoya[1], Alonso Castro[1], Ning Xu[1]; [1]Los Alamos National Laboratory

Monday Afternoon, *Room 556B*
NEAR IR
Organizer and Presider: Franklin E. (Woody) Barton

3:50 (186) **NIR With Problem Data Sets**; Franklin Barton[1], James de Haseth[1]; [1]Light Light Solutions Instruments, Inc.

4:10 (187) **A New Look at the Derivative Quotient Method in Regression**; David Hopkins[1], Karl Norris[2]; [1]NIR Consultant, Battle Creek, MI; [2]NIR Consultant, Beltsville, MD

4:30 (188) **Ultra-Compact Smart Spectrometers For Food, Agriculture, and Pharmaceutical Applications**; Nada OBrien[1], Christopher Pederson[1], Peng Zou[1]; [1]JDSU Corporation

4:50 (189) **A Novel Configuration for Near-Infrared Analysis of LPG Composition and Quality Control in a Refinery Setting**; Susan Foulk[1], Shashi Mistry[2], Terry Todd[1], Nate Peters[2], Dian Wang[2]; [1]Guided Wave, Inc.; [2]Suncor Energy

5:10 (190) **Field Analysis of Fuel using a Portable Near-Infrared Spectrometer**; Wayne Smith[1], Carl Brouillette[1], Chetan Shende[1], Stuart Farquharson[1]; [1]Real-Time Analyzers, Inc.

Monday Afternoon, *Ballroom E*
LIBS FOR PHARMACEUTICAL AND BIOLOGICAL DIAGNOSTICS
Organizer and Presider: Lydia Breckenridge

3:50 (191) **Recent Progress and Current Challenges in Using LIBS for Bacteriological Identification**; Steven Rehse[1], Dylan Malenfant[1], Derek Gillies[1], Vlora Riberdy[1], Anthony Piazza[1]; [1]University of Windsor

4:30 (192) **Laser-Induced Breakdown Spectroscopy for the Evaluation of Residual Catalysts in Pharmaceuticals**; Lydia Breckenridge[1]; [1]Bristol-Myers Squibb

4:50 (193) **Identification of Meat Species by using Laser Induced Breakdown Spectroscopy**; Gonca Bilge[1], Banu Sezer[1], Hasan Murat Velioğlu[2], Kemal Efe Eseller[3], Halil Berberoğlu[4], İsmail Hakkı Boyacı[1]; [1]Hacettepe University, Department of Food Engineering; [2]Namık Kemal University, Department of Agricultural Biotechnology; [3]Atılım University, Department of Electrical & Electronics Engineering; [4]Gazi University, Department of Physics

5:10 (194) **Study of Plasma and Identification of Hazardous Elements in the Polystyrene using Laser Induced Breakdown Spectroscopy**; W. Aslam Farooq[1]; [1]King Saud University

Monday Afternoon, *Room 552B*
PHARMACEUTICAL APPLICATIONS OF LOW WAVENUMBER SPECTROSCOPY
Organizer and Presider: James Carriere

3:50 (195) **Application of Low Frequency Raman During the Crystallization Process**; John Wasylyk[1], Ming Huang[1], Robert Wethman[1]; [1]Bristol-Myers Squibb Co.

4:10 (196) **The Contribution of the Low-Frequency Raman Spectroscopy to the Structural Description of Disordered Molecular Systems and Their Transformations: Application to Pharmaceuticals**; Alain Hedoux[1], Laurent Paccou[1], Yannick Guinet[1]; [1]University Lille 1, UMET - UMR CNRS 8207

4:30 (197) **Chemical Imaging of Crystalline Components in Pharmaceutical Dosage Forms by Using Low Frequency Raman Spectroscopy**; Toshiro Fukami[1], Motoki Inoue[1], Hiroshi Hisada[1], Tatsuo Koide[2]; [1]Meiji Pharmaceutical University; [2]National Institute of Health Sciences

4:50 (198) **Calibration of a Terahertz Analyzer for Predicting Solid Fraction in Roller-Compacted Ribbons and Tablets in a Small-Scale Piloting Study to Facilitate Pharmaceutical Formulation Development**; Mark Sullivan[1], Elaine Harrop Stone[2], Monwara Hoque[2], Xiao Hua Zhou[1], Richard McKay[1]; [1]Advantest America Inc; [2]Merlin Powder Characterisation Ltd

5:10 (199) **Low Wavenumber Raman Spectroscopy Applications in API Phase Discovery and Characterization**; Courtney Maguire[1], Andrew Brunskill[1]; [1]Merck Research Laboratories

Monday Afternoon, *Room 555B*
HOT TOPIC DISCUSSION SESSION – TERS RESOLUTION
Organizers: Duncan Graham, Pavel Matousek, and Ian Lewis;
Presider: Duncan Graham

3:50 (200) **Recent Advances in Tip-Enhanced Raman Spectroscopy**; Richard Van Duyne[1]; [1]Northwestern University

4:10 (201) **Resolution and Enhancement in TERS Microscopy**; Satoshi Kawata[1], Atsushi Taguchi[1]; [1]Osaka University

4:30 (202) **Molecular Structure Changes on the Nanometre Scale Investigated and Induced by TERS**; Volker Deckert[1,2]; [1]University of Jena; [2]Leibnitz Institute of Photonic Technology

4:50 **Discussion**

TECHNICAL PROGRAM – MONDAY
Orals 1:20 – 3:00 pm and 3:50 – 5:30 pm

Monday Afternoon, *Room 556A*
PHARMACEUTICAL RAMAN
Organizers: Ian Lewis, Duncan Graham, and Pavel Matousek;
Presider: Don Pivonka

3:50 (203) **Application of Vibrational Spectroscopy to Further the Understanding of Drug Product Stability, Dissolution, and Exposure**; Don Pivonka[1], William Rocco[1], Dilip Modi[1]; [1]Incyte Inc.

4:10 (204) **Quantification of Residual Crystallinity in Pharmaceutical Formulations using Transmission Raman Spectroscopy**; Mark Mabry[1]; Julia Griffen[1], Matthew Bloomfield[2], Andrew Owen[1], Darren Andrews[1], Pavel Matousek[3]; [1]Cobalt Light Systems, Ltd; [2]Cobalt Light Systems, Inc; [3]Central Laser Facility, STFC Rutherford Appleton Laboratory

4:30 (205) **A Directly Correlated Raman and uHPLC-MS Content Uniformity Method for Dry Powder Inhalers Developed through DoE, Chemometrics and Mathematical Modeling**; Lauren Seabrooks[1], Nicole Canfield[1], Justin Pennington[1]; [1]Merck

4:50 (206) **Screening of Antibiotics Using Portable Spectrometers**; Jason Rodriguez[1], Latevi Lawson[1], Hirsch Srivastava[1], Megha Mohan[1]; [1]FDA

5:10 (207) **Prediction of Bead Coating Thickness using Raman Quantitative Model**; Hanzhou Feng[1], James Drennen[1], Carl Anderson[1,2]; [1]Duquesne University, Graduate School of Pharmaceutical Sciences; [2]Duquesne University

Monday Afternoon, *Room 552A*
CAREERS AND DIVERSITY IN ANALYTICAL SCIENCE DISCUSSION PANEL
Organizers and Presiders: Ingeborg Iping Petterson and Anna Donnell

3:50 (208) **Wanderlust and the Traveling (Female) Scientist**; Sarah Maurer[1]; [1]Central Connecticut State University

4:10 (209) **Are You the Only Professional Woman in the Organization?**; Ellen Miseo[1]; [1]Hamamatsu Corp.

4:30 (210) **A Nontraditional Career Path**; Emily Monosson[1]; [1]Independent/Ronin Institute

4:50 (211) **Discussion Panel**; Fred LaPlant[1]; [1]3M

5:10 (212) **Diversity in the STEM fields: Increasing Participation and Visibility of Women and Other Underrepresented Minority Groups in Research and Science-Related Careers**; Colin Ingram[1]; [1]Andor Technology

Monday Afternoon, *Room 553A*
***IN-SITU* SURFACE SCIENCE**
Organizer: Andrei Kolmakov; Presider: Kateryna Artyushkova

3:50 (213) **Characterizing Working Catalysts with Correlated Electron and Photon Probes**; Eric Stach[1]; [1]Brookhaven National Laboratory

4:30 (214) ***In situ* Probing of Environmental Liquid Surfaces and Interfaces using Microfluidics: Toward Multimodal and Mesoscale Imaging**; Xiao-Ying Yu[1], Zihua Zhu[2]; [1]Fundamental and Computer Sciences Directory; [2]W. R. Environmental Molecular Science Laboratory

4:50 (215) **Surface of Oxide-Based Catalysts during Catalysis Tracked with Ambient Pressure XPS and Its Correlation with Catalytic Performances**; Franklin (Feng) Tao[1], Shiran Zhang[1], Luan Nguyen[1], Junjun Shan[1]; [1]University of Kansas

TECHNICAL PROGRAM – TUESDAY
Plenary Lectures, *Ballroom B/C*
Presider: Alexandra Ros

8:00 am – Coblentz Society Craver Award
(216) **Vibrational Spectroscopic Imaging of Living Systems: Emerging Platform for Biology and Medicine**; Ji-Xin Cheng[1]; [1]Purdue University

8:30 am – FACSS Charles Mann Award for Applied Raman Spectroscopy
(217) **UV Resonance Raman Spectroscopic Studies of Protein Structure and Dynamics**; Sanford Asher[1], David Punihaole[1], Elizabeth M. Dahlburg[1], Ryan S. Jakubek[1], Zhenmin Hong[1]; [1]University of Pittsburgh

Orals 9:15 – 10:55 am

Tuesday Morning, *Room 550A/B*
ICP-MS IN THE ANALYSIS OF NANOMATERIALS
Organizers: Maria Montes-Bayón and Jörg Bettmer;
Presider: Maria Montes-Bayón

9:15 (218) **icpTOF: Advantages of Sensitive Simultaneous Detection for Analysis of Nanomaterials**; Olga Borovinskaya[1], Martin Tanner[1]; [1]TOFWERK AG

9:35 (219) **Analytical Insights into Human Risk Assessments of Noble Metal Nanomaterials**; Petra Krystek[1]; [1]VU University Amsterdam

9:55 (220) **Single Particle ICP-MS in a Multitechnique Approach to Elucidate the Fate of Silver Nanoparticles in Burnt Patients**; Marco Roman[1,4], Chiara Rigo[1], Vincenzo Vindigni[2], Hiram Castillo-Michel[3], Warren R.L. Cairns[4]; [1]University Ca; [2]Burns Center, University Hospital of Padua; [3]European Synchrotron Radiation Facility (ESRF), Grenoble; [4]Institute for the Dynamics of Environmental Processes (IDPA-CNR), Venice

10:15 (221) **HPLC-ICP-MS for the Determination of Gold Nanoparticles in Biological Tissues**; Jörg Bettmer[1], Juan Soto-Alvaredo[1], Carlos López-Chaves[2], Maria Montes-Bayón[1], Cristina Sanchez-González[2], Juan Llopis-González[2]; [1]University of Oviedo; [2]University of Granada

10:35 (222) **Cloud Point Extraction for Silver Nanoparticle and Ion Quantification**; Nicole Hanks[1], Joseph Caruso[1], Peng Zhang[1]; [1]University of Cincinnati

Tuesday Morning, *Room 554A/B*
CRAVER AWARD SESSION HONORING JI-XIN CHENG
Organizers: Ji-Xin Cheng and James Rydzak;
Presider: James Rydzak

9:15 (223) **Developing Single Particle Orientation and Rotational Tracking for Understanding Endocytosis and Intracellular Transport**; Ning Fang[1], Kuangcai Chen[2], Ashley Augspurger[2]; [1]Georgia State University; [2]Iowa State University

9:35 (224) **High Speed Molecular Imaging by Phosphorescence Lifetime Multiphoton Microscopy**; Scott Howard[1]; [1]University of Notre Dame

9:55 (225) **Ultrafast Nanoscopy of Energy and Charge Transport**; Libai Huang[1]; [1]Purdue University

10:15 (226) **Gigapixel Fluorescence Histology for Rapid 'No-Cut' Surgical Pathology**; J. Quincy Brown[1]; [1]Tulane University

10:35 (227) **TERS Characterization of Membrane Receptors**; Zachary Schultz[1], Hao Wang[1]; [1]University of Notre Dame

Tuesday Morning, *Room 555A*
METABOLOMICS AND PERSONALIZED MEDICINE
Organizer and Presider: Roy Goodacre

9:15 (228) **Pharmacometabolomics Enabling Tools for Systems Pharmacology and Precision Medicine**; Rima Kaddurah-Daouk[1,2]; [1]Duke University Medical Center; [2]On behalf of the Pharmacometabolomics Research Network

9:35 (229) **Stable Isotope Resolved Metabolomics (SIRM) on Fresh Human Tissues as a Preclinical Drug Testing Platform**; Andrew Lane[1], Teresa Fan[1], Alexander Belshoff[2], Richard Higashi[1], Jeremiah Martin[1], Michael Bousamra[2]; [1]University of Kentucky; [2]University of Louisville

9:55 (230) **Personalized Medicine in Human Space Flight**; Michael A Schmidt[1]; [1]Sovaris Aerospace, LLC

10:15 (231) **Metabolomic Applications in Nutritional Research**; Lorraine Brennan[1]; [1]UCD Institute of Food and Health

10:35 (232) **NMR as an Important Analytical Tool for Identifying Drug Metabolites in Support of Drug Discovery**; Yingzi Wang[1], Xiaoliang Zhuo[1], John Leet[1], Stella Huang[1], Joseph Cantone[1], Dieter Drexler[1], Kim Johnson[1], Benjamin Johnson[1], Michael Reily[1], Adrienne Tymiak[1]; [1]Bristol-Myers Squibb

Tuesday Morning, *Room 551B*
CHEMOMETRIC TOOLS TO DISCOVER THE NEXT MAGIC BULLET VIA BIOLOGICAL SPECTROSCOPY
Organizer and Presider: Barry K. Lavine

9:15 (233) **Pattern Recognition Studies of Serum N-Linked Glycans obtained by MALDI-IMS-MS Profiling**; Barry Lavine[1], Maissa Gaye[2], David Clemmer[2], Tao Ding[1], H Shion[3], W. Chen[3],A. Hussein[3], Y. Hu[4], S. Zhou[4], Yehia Mechref[4]; [1]Department of Chemistry, Oklahoma State University; [2]Department of Chemistry, Indiana University; [3]Waters Corporation, Pharmaceutical Life Sciences; [4]Department of Chemistry & Biochemistry, Texas Tech University

9:35 (234) **Medical Applications of Multivariate Statistical Process Control**; Lionel Blanchet[1,2], Jasper Engel[3], Frederik-Jan van Schooten[1]; [1]Department of Toxicology, Maastricht University Medical Center, the Netherlands; [2]Top Institute Food and Nutrition (TIFN), Wageningen, the Netherlands; [3]NERC Metabolomics Facility, School of Biosciences, Birmingham University

9:55 (235) **Sparse Deconvolution of High-Density Super-Resolution Images**; Cyril Ruckebusch[1], Romain Bernex[1], Siewert Hugelier[1], Olivier Devos[2], [1], Johan de Rooi[2],Paul Ailers[2]; [1]LASIR CNRS Université de Lille, France; [2]Department of Biostatistics, Erasmus Medical Center, Rotterdam, The Netherlands

10:15 (236) **Multivariate Curve Resolution of Mass Spectrometry Imaging (MSI) of Biological Tissues**; Roma Tauler[1], Carne Bedia[1], Joaquim Jaumot[1]; [1]IDAEA-CSIC

10:35 (237) **Investigations on the Analysis Workflow for Biomedical Application of Raman Spectroscopy**; Thomas Bocklitz[1], Jürgen Popp[1, 2]; [1]University of Jena, Institute of Physical Chemistry; [2]Institue of Photonic Technology

TECHNICAL PROGRAM – TUESDAY
Orals 9:15 – 10:55 am

Tuesday Morning, *Room 552B*
GC-MS BASED DETECTION OF EMERGING FLAME RETARDANTS IN THE ENVIRONMENT
Organizers: Carrie McDonough and Rainer Lohmann;
Presider: Rainer Lohmann

9:15 (238) **Detection of Truly Dissolved and Gaseous Flame Retardants in the Lower Great Lakes Region using Polyethylene Passive Samplers**; Carrie McDonough[1], Rainer Lohmann[1]; [1]Graduate School of Oceanography, University of Rhode Island

9:35 (239) **A Great Lakes Perspective on Flame Retardants: Lessons from the Integrated Atmsopheric Deposiiton Network.**; Marta Venier[1], Amina Salamova[1], Todd Nettesheim[2], Ron Hites[1]; [1]Indiana University; [2]Environmental Protection Agency Great Lakes National Program office; [4]Indiana University

9:55 (240) **Emerging Flame Retardants in North American Aquatic Ecosystems**; Da Chen[1], Rebecca Sutton[2], Jeremy Moore[3], Doug Adams[4], Yan Wu[1], Hillary Marler[1],Hillary Marler[1]; [1]Southern Illinois University; [2]San Francisco Estuary Institute; [3]US Fish and Wildlife Service; [4]Cape Canaveral Scientific, Inc.

10:15 (241) **Strategies and Techniques for Identifying Unknown Compounds in Environmental Samples**; Eric J Reiner[1,3], Karl J Jobst[1, 3], Miren Pena-Abaurrea[1], Anne L Myers[1], Li Shen[2], Alina Muscalu[2], Ralph Ruffolo[2], Xavier Ortiz[2], Paul A Helm[2]; [1]University of Toronto; [2]Ontario Ministy of the Environment and Climate Change; [3]McMaster University

Tuesday Morning, *Room 551A*
EXPLOSIVE DETECTION II: TRACE, ON-SITE AND *IN-SITU*
Organizer and Presider: Suzanne Bell

9:15 (242) **Detection of TNT and RDX Based on Gold Nanoparticles Molecular Imprinted Matrix by SPR and SERS**; Geneviève Granger[1], Nathalia Bukar[1], Jean-François Masson[1], Andreea R. Schmitzer[1]; [1]Département de Chimie, Université de Montréal, Montréal, Canada

9:35 (243) **Generation and Quantitation of Parts per Quadrillion Levels of TNT and RDX**; Braden Giordano[1], Benjamin Andrews[2], Adam Lubrano[2]; [1]U.S. Naval Research Laboratory; [2]Nova Research, Inc.

9:55 (244) **Analysis and Delivery of Vapor from Binary Explosive Mixtures for Instrumental and Canine Detection**; Susan Rose-Pehrsson[1,2], Lauryn DeGreeff[1], Frank Lucus Steinkamp[3], Braden Giordano[1], Christopher Katilie[1,2]; [1]U.S. Naval Research Laboratory; [2]Nova Research, Inc.; [3]National Research Council

10:15 (245) **Trace Explosive Detection using Zinc Oxide Nanowire Catalysts**; Zachary Caron[1], Otto Gregory[1]; [1]University of Rhode Island, Department of Chemical Engineering

10:35 (246) ***In-situ* Detection of Energetic Materials Based on Surface Plasmon Spectroscopies**; Thibault Brulé[1], Geneviève Granger[1], Natalia Bukar[1], Marc Vidal[1], Jean François Masson[1]; [1]Département de Chimie, Université de Montréal

Tuesday Morning, *Room 556B*
NANOSCALE IR I
Organizer and Presider: Jing Yang

9:15 (247) **AFM-IR Applications in Bio-Molecules Production**; Rolando Rebois[1], Ariane Deniset-Besseau[1], Delphine Onidas[1], Alexandre Dazzi[1]; [1]Laboratoire de Chimie Physique - Université Paris-Sud

9:35 (248) **AFM-IR Spectroscopy and Imaging of Polymer Nanofibers and Thin Films at the Nanoscale**; John Rabolt[1], Liang Gong[1], Isao Noda[1,3], Bruce Chase[1], C. J. McBrin[1], Curtis Marcott[1,2]; [1]Department of Materials Science and Engineering, University of Delaware; [2]LightLightSoluions; [3]Department of Materials Science and Engineering, University of Delaware

9:55 (249) **Correlated Nano-Chemical and Nano-Mechanical Imaging of Protein Nanoribbons Involved in Dental Enamel Formation**; Martin Wagner[1], Karina Carneiro[2], Stefan Habelitz[2], Thomas Mueller[1]; [1]Bruker Nano Surfaces; [2]University of California, Preventive and Restorative Dental Sciences

10:15 (250) **Introducing nano-FTIR – Imaging and Spectroscopy at 10 nm Spatial Resolution**; Tobias Gokus[1], Andreas Huber[1], Florian Huth[1]; [1]Neaspec GmbH

10:35 (251) **Characterization of a Polyethylene–Polyamide Multilayer Film using Nanoscale Infrared Spectroscopy and Imaging**; Mauritz Kelchtermans[1], Michael Lo[2], Eoghan Dillon[2], Kevin Kjoller[2], Craig Prater[2], Curtis Marcott[3]; [1]ExxonMobil Chemical Europe, Belgium; [2]Anasys Instruments; [3]Light Light Solutions

Tuesday Morning, *Ballroom E*
NEW HARDWARE AND NOVEL METHODS IN LIBS
Organizer and Presider: Vassilia Zorba

9:15 (252) **Single Particle LIBS Analysis in Optical Traps. Imaging, Multielemental Analysis, and Detection Power**; Javier Laserna[1]; [1]Universidad de Malaga

9:55 (253) **Pathways Towards High-Resolution Chemical Analysis and Imaging with Femtosecond LIBS**; Vassilia Zorba[1]; [1]Lawrence Berkeley National Laboratory

10:15 (254) **New Hybrid Calibration-Free/Artificial Neural Networks Approach for Quantitative Analysis**; Vincenzo Palleschi[1]; [1]National Research Council

10:35 (255) **New Methodology for Quantitative Laser-Induced Breakdown Spectroscopy Based on CSigma graphs. Application to Fused Glass Samples**; Carlos Aragon[1,2], Jose Antonio Aguilera[1, 2]; [1]Departamento de Fisica, Universidad Publica de Navarra; [2]Institute for Advanced Materials, Public University of Navarre

Tuesday Morning, *Room 553A*
CONTINUOUS/FLOW PAT
Organizer and Presider: Nancy L. Jestel

9:15 (256) **Development of a Process Analytical Solution for Real-Time Monitoring of Continuous Flow Reactors**; Brian Marquardt[1], Thomas Dearing[2], Michael Roberto[3], Olav Bleie[4]; [1]University of Washington; [2]MarqMetrix Inc; [3]Infometrix; [4]Univ. of Bergen, Norway

9:35 (257) **Recent Advances in Automatic Continuous Online Monitoring of Polymerization reactions (ACOMP)**; Wayne Reed[2], Michael F. Drenski[1]; [1]Advanced Polymer Monitoring Technologies, Inc.; [2]Tulane University

9:55 (258) **Development of NIR Methodology for Process Monitoring and Control using an Offline Calibration Approach**; Evan Hetrick[1], Zhenqi Shi[1], Lukas Barnes[1], David Myers[1], Bryan Castle[1], Salvador Garcia Munoz[1],Ian Leavesley[1]; [1]Eli Lilly and Company

10:15 (259) ***In situ* ATR-FTIR: A Technological Shift in Continuous Processing**; Dom Hebrault[1]; [1]Dom Hebrault

10:35 (260) **Getting More Out of Process Measurements with Diode Array Spectrometers: Instrumental and Analysis Approaches**; Robert Lascola[1], Patrick O'Rourke[1], Elizabeth Evans[1], Edward Kyser[1]; [1]Savannah River National Laboratory

TECHNICAL PROGRAM – TUESDAY
Orals 9:15 – 10:55 am ♦ Posters 11:00 am – 12:00 pm

Tuesday Morning, *Room 555B*
EMERGING RAMAN TECHNIQUES AND APPLICATIONS I
Organizers and Presiders: Ian Lewis, Ducan Graham and Pavel Matousek

9:15 (261) **Semiconductor-enhanced Raman Scattering: Towards Applications in Highly Robust SERS Sensing**; Yukihiro Ozaki[1], Wei Ji[1], Yue Wang[2], Ichiro Tanabe[1], Bing Zhao[2]; [1]Department of Chemistry, School of Science and Technology, Kwansei Gakuin University; [2]State Key Laboratory of Supramolecular Structure and Materials, Jilin University

9:35 (262) **Coherent Raman Spectroscopy with Optical Frequency Combs**; Takuro Ideguchi[1,2], Simon Holzner[2], Birgitta Bernhardt[2], Guy Guelachvili[3], Theodor Hänsch[2,4], Nathalie Picqué[2,3,4]; [1]The University of Tokyo; [2]Max-Planck-Institut für Quantenoptik; [3]Institut des Sciences Moléculaires d'Orsay, CNRS; [4]Ludwig-Maximilians-Universität München

9:55 (263) **Functionalised Nanoparticles for the Detection of Explosives and Small Molecule by SERS**; Karen Faulds[1], Rachel Norman[1], Duncan Graham[1], Neil Shand[2]; [1]University of Strathclyde; [2]Defence Science and Technology Laboratory

FACSS Student Award

10:15 (264) **Raman Spectroscopy of Single Electrospun Nanofibers**; Marie Richard-Lacroix[1], Christian Pellerin[1]; [1]University of Montreal

10:35 (265) **Spectroscopy on Mars - Searching for Signs of Life**; Ian Hutchinson[1], Richard Ingley[1], Howell Edwards[1], Nick Waltham[2]; [1]University of Leicester; [2]Rutherford Appleton Laboratories

Tuesday Morning, *Room 556A*
BIOANALYTICAL APPLICATIONS OF PLASMONICS
Organizer: Jean-Francois Masson; Presider: Amanda Haes

9:15 (266) **Nanoplasmonic Analysis of Norovirus on Structured Lipid Membranes**; Andreas Dahlin[1]; [1]Chalmers University of Technology

9:35 (267) **Head-to-Head Comparison of the Performance of SERS and ELISA Diagnostic Tests for Infectious Disease**; Marc Porter[1], Lars Laurentius[1], Nicholas Owens[1], Alexis Crawford[1], Jennifer Granger[1]; [1]University of Utah

9:55 (268) **Single Nanoparticle SPRI Microscopy and Plasmonic Nanocone Arrays For Biosensing**; Robert M. Corn[1], Adam Maley[1], Millie Fung[1]; [1]Dept. of Chemistry, University of California-Irvine

10:15 (269) **Microdialysis SPR: Sensing in Whole Blood**; Jean-Francois Masson[1]; [1]Département de Chimie, Université de Montréal, Montréal, Canada

10:35 (270) **Poly(n-isopropylacrylamide): Growth Kinetics in Grafting from and Thickness Change upon Temperature Induced Brush Collapse in Water**; Gustav Emilsson[1], Kunli Xiong[1], Andreas Dahlin[1]; [1]Dept. of Applied Physics, Chalmers University of Technology

Tuesday Poster Session
11:00 am – 12:00 pm
Exhibit Hall C/D

All Tuesday posters should be put up between 7:30 – 8:30 am and removed by 4:30 pm

Atomic Spectroscopy II Posters

Poster Board #1
(271) **Development of SRM 3232 Kelp for Dietary Supplement Measurements**; Lee Yu[1]; [1]National Institute of Standards and Technology

Poster Board #2
(272) **Identification of Stroke Metalloprotein Biomarkers and Metal Profile in Human Blood Plasma**; Keaton Nahan[1], Julio Landero[1], Opeolu Adeoye[2], Joseph Caruso[1]; [1]University of Cincinnati, McMicken College of the Arts and Sciences; [2]University of Cincinnati, Medical Center

Poster Board #3
(273) **Determination of Calcium, Magnesium, and Aluminum in Pine from the Southern Appalachians**; David Butcher[1], Alyssa Bailey[1]; [1]Western Carolina University

Poster Board #4
(274) **Calculation of Ion Beam Formation behind the Skimmer Cone of an ICP-MS**; Ross Spencer[1]; [1]Brigham Young University

Poster Board #5
(275) **Determination of Residual Unbound Cr(III) and Cr(VI) in a Cr(III)-EDTA API by HPLC-ICP-MS**; Qiang Tu[1], Tiebang Wang[1], Xiaoyi Gong[1]; [1]Merck & Co., Inc.

Poster Board #6
(276) **Challenges in Trace Element Analysis of Cobalt Precursors**; Lisa Milstein Mey-Ami[1], Phil Clancy[1], Fuhe Li[1], Hugh Gotts[1]; [1]Air Liquide Balazs Nanoanalysis

Poster Board #7
(277) **Elemental Quantification of Carbon via Production of Polyatomic Ions in Plasma Assisted Reaction Chemical Ionization (PARCI)**; Peter Josef Haferl[1], Haopeng Wang[1], Kaveh Jorabchi[1]; [1]Georgetown University

Poster Board #8
(278) **Absorption Spectroscopy of 238U in Laser-Induced Plasma**; Jason Becker[1], Brian Brumfield[1], Nicole LaHay[1], Patrick Skrodzki[1], Mark Phillips[1], Sivanandan Harilal[1]; [1]PNNL

Poster Board #9
(279) **Development and Validation of a New Method to Measure Activity of the Na+, K+ ATPase Using ICP-MS QQQ**; Cory Stiner[1], Julio Landero[1], Judith Heiny[1]; [1]University of Cincinnati

Poster Board #10
(280) **A Green and Fast Approach to Arsenic Speciation**; Maria C. Hespanhol da Silva[1,3], Julio A. Landero[2], Joseph A. Caruso[2]; [1]Universidade Federal de Viçosa; [2]University of Cincinnati; [3]Conselho Nacional de Desenvolvimento Científico e Tecnológico

Poster Board #11
(281) **Effect of Laser Wavelength and Ambient Pressure on Late-Time Bulk Particle Emission**; Niral Shah[1], Patrick Skrodzki[1], Brian Brumfield[1], Nicole LaHaye[1], Sivanandan Harilal[1], Mark Phillips[1]; [1]Pacific Northwest National Laboratory

Poster Board #12
(282) **Method Development and Validation for the Analysis of Polyacrylic Lithography Reagents by ICPMS**; Phil Clancy[1], Hugh Gotts[1], Scott Anderson[1]; [1]Air Liquide-Balazs NanoAnalytical

Chemometrics Posters

Poster Board #13
(283) **Combining Statistics and Chemometrics for Guidance of Continuous Improvement Efforts**; Mark Henson[1]; [1]Shire Pharmaceuticals

TECHNICAL PROGRAM – TUESDAY
Posters 11:00 am – 12:00 pm

Poster Board #14

(284) **Withdrawn**

Poster Board #15

(285) **Multivariate Analysis of Absolute and Complex Number Microwave Spectra Measured on Pharmaceutical Formulations**; Olof Svensson[1], Halldis Thoroddsen[2], Álvaro Díaz-Bolado[1], Anders Sparén[1], Mats Josefson[1]; [1]AstraZeneca R&D Mölndal, Mölndal, Sweden; [2]Chalmers University of Technology, Göteborg, Sweden

Poster Board #16

(286) **Fluorescence Excitation Spectroscopy and Imaging Multivariate Optical Computing for the Characterization of Natural Phytoplankton Populations**; Shawna Tazik[1], Joseph Swanstrom[1], Cameron M. Rekully[1], Stefan T. Faulkner[1], Nicholas S. Viole[1], Timothy J. Shaw[1],Tammi L. Richardson[2], Michael L. Myrick[1]; [1]University of South Carolina, Department of Chemistry and Biochemistry; [2]University of South Carolina, Marine Science Program and Department of Biological Sciences

Poster Board #17

(287) **A Convex Optimization Approach to Calibration Transfer**; Thomas Boucher[1], Melinda Dyar[2], CJ Carey[1], Stephen Giguere[1], Sridhar Mahadevan[1]; [1]University of Massachusetts Amherst; [2]Mount Holyoke College

Poster Board #18

(288) **A Framework for Fully Customized Baseline Removal**; Stephen Giguere[1], M. Darby Dyar[2], CJ Carey[1], Thomas Boucher[1], Sridhar Mahadevan[1]; [1]College of Information and Computer Sciences, University of Massachusetts, Amherst; [2]Department of Astronomy, Mount Holyoke College

Poster Board #19

(289) **Characterizing Calibration Data Sets by Fusion of Dissimilarity Merits Including Outlier Detection**; Brett Brownfield[1], John Kalivas[1]; [1]Idaho State University

Poster Board #20

(290) **Investigation of Cyclodextrin Complexes with PAHs using Steady-State Fluorescence and Parallel Factor Analysis**; Joseph Chiarelli, Jonathan Kenny; [1]Tufts University

Poster Board #21

(291) **MATSA: A User-Friendly Software Program for Magnetic Audio Tape Spectral Analysis**; Nathan C. Fuenffinger[1], Brianna M. Cassidy[1], Zhenyu Lu[1], Michael L. Myrick[1], Eric M. Breitung[2], Stephen L. Morgan[1]; [1]University of South Carolina; [2]Library of Congress

Poster Board #22

(292) **An Effective Approach to Building a Calibration Matrix for a Multi-Component Mixture**; Huggins Z. Msimanga[1], Mihyang Song[2], Newsha Tavakoli[3], Truong Thach Ho Lam[4]; [1]Kennesaw State University; [2]Mercer Univeristy College of Pharmacy; [3]Georgia Institute of Technology; [4]Philadelphia College of Osteopathic Medicine

Poster Board #23

(293) **Clustering in Spectroscopy - How Important is the Review Process?**; Michael Boruta[1]; [1]ACD/Labs

LIBS Posters

Poster Board #24

(294) **Comparison of Metal Concentrations in Soil with LIBS, XRF, and ICP-MS**; Jay Clausen[1]; [1]US Army Corps of Engineers ERDC-CRREL

Poster Board #25

(295) **Optimization of Liquid Jet System for Laser-Induced Breakdown Spectroscopy Analysis**; Pavel Porizka[2], Katarina Skocovska[1], Jan Novotny[2], David Prochazka[2], Karel Novotny[2,3], Jozef Kaiser[2]; [1]Faculty of Mechanical Engineering, Brno University of Technology; [2]CEITEC BUT - Central European Institute of Technology, Brno University of Technology; [3]CEITEC MU - Central European Institute of Technology, Masaryk University

Poster Board #26

(296) **Multivariate Classification and Quantification of Sedimentary Rocks Analyzed using Stand-Off Laser-Induced Breakdown Spectroscopy System**; Pavel Porizka[1], Jan Novotny[1], Gabriela Vitkova[1], David Prochazka[1], Jakub Klus[1], Michal Brada[1],Ales Hrdlicka[1,2], Karel Novotny[1, 2], Jozef Kaiser[1, 2]; [1]CEITEC BUT - Central European Institute of Technology , Brno University of Technology; [2]CEITEC MU - Central European Institute of Technology, Masaryk University,

Poster Board #27

(297) **The Effects of Laser Pulse Energy, Spot Size, and Wavelength on Laser Produced Plasmas in Transverse Magnetic Fields**; Payson Dieffenbach[1], Michael Marino[1], Prasoon Diwakar[1], Ahmed Hassanein[1]; [1]Center for Materials Under Extreme Environment, School of Nuclear Engineering, Purdue University

Poster Board #28

(298) **Analyzing Ice with LIBS**; Jay Clausen[1], Richard Hark[2], Alexander Bol'shakov[3], John Plummer[4]; [1]USACE ERDC CRREL; [2]Juanita College; [3]Applied Spectra Inc.; [4]JR Plumer Associates LLC

Poster Board #29

(299) **Spectroscopic Analysis of Cerium, Cesium and Strontium (Nuclear Surrogates) using Laser Induced Breakdown Spectroscopy (LIBS)**; Charles Ghany[1,2], Hervé Sanghapi[1, 2], Chet Bhatta[1,2], Bader Alfaraj[1,2], Fang Yueh[2,3], Jagdish Singh[2,3]; [1]Mississippi State University; [2]Institute for Clean Energy Technology; [3]JPS Advanced Technology R&D, LLC, Starkville

Poster Board #30

(300) **Comparative Study of Elemental Nutrients in Organic and Conventional Vegetables by Laser Induced Breakdown Spectroscopy (LIBS).**; Chet Bhatt[1,2,3], Charles Ghany[1, 2, 3], Bader Alfarraj[1,2,3], Fang Yueh[1,2], Jagdish Singh[1,2,3]; [1]Mississippi State University; [2]Institute of Clean Energy Technology (ICET); [3]Department of Physics and Astronomy, MSU

Poster Board #31

(301) **Overview of Some Theoretical Modeling of LIBS Emission Spectra**; David Kilcrease[1], Heather Johns[1], James Colgan[1], Beth Judge[2], James Barefield II[2], Roger Wiens[3],Sam Clegg[4]; [1]Theoretical Division, Los Alamos National Laboratory; [2]Chemical Diagnostics and Engineering, Los Alamos National Laboratory; [3]Space and Remote Sensing Division, Los Alamos National Laboratory; [4]Physical Chemistry and Applied Spectroscopy, Los Alamos National Laboratory

Poster Board #32

(302) **A Study of Wheat Flour Tortillas using Laser Induced Breakdown Spectroscopy (LIBS)**; Charles Ghany[1,2], Hervé Sanghapi[1, 2], Chet Bhatta[1,2], Bader Alfaraj[1,2], Fang Yueh[2,3], Jagdish Singh[2,3]; [1]Mississippi State University; [2]Institute for Clean Energy Technology; [3]JPS Advanced Technology R&D, LLC, Starkville

TECHNICAL PROGRAM – TUESDAY

Posters 11:00 am – 12:00 pm ♦ What's Hot Vendor Presentations 11:40 am – 1:10 pm ♦ Orals 1:20 – 3:00 pm

Poster Board #33

(303) **Laser Ablation Molecular Isotopic Spectrometry of Rare Isotopes**; A.A. Bol'shakov[1], X.L. Mao[2], J.J. Gonzalez[1,2], R.E. Russo[1,2]; [1]Applied Spectra Inc; [2]Lawrence Berkeley National Laboratory

Poster Board #34

(304) **Evaluation of Optical Depths of Sr Emission Lines in Laser Induced Breakdown Spectroscopy (LIBS)**; Bader Alfarraj, Herve Sanghapi, Charles Ghany, Chet Bhatt, Fang Yueh, Singh Jagdish; [1]ICET-MSU

Poster Board #35

(305) **Femtosecond Laser Ablation: A Molecular Dynamics Study**; Alexander Miloshevsky[1], Mark Phillips[2], Gennady Miloshevsky[1], Sivanandan Harilal[2]; [1]Purdue University; [2]Pacific Northwest National Laboratory

Poster Board #36

(306) **Simultaneous Measurement of Conserved Scalars in Flames using LIBS**; Wendong Wu[1], Richard Axelbaum[1]; [1]Washington University in St.Louis

Poster Board #37

(307) **Adaptive Multi-Sensor Data Fusion Model for *in-situ* Mars Exploration**; Tajana Schneiderman[1], Pablo Sobron[2]; [1]The Ohio State University; [2]The SETI Institute

RAMAN Posters

Poster Board #38

(308) **Application of Low and Mid Frequency Raman for Characterization of Amorphous-Crystalline Indomethacin.**; Michaella Raglione Raglione[1], John Wasylyk[2], Peter Larkin[3]; [1]The University of Delaware; [2]Bristol Myers Squibb; [3]Cytec

Poster Board #39

(309) **High Throughput Integrated Raman Probe with Elongated Core Collection Fiber-optic**; Robert Chimenti[1]; [1]Innovative Photonic Solutions

Poster Board #40

(310) **Improved Material Identification in the Field using a Long Wavelength Handheld Raman Spectrometer**; Claire Dentinger[1], Claude Robotham[1], Eric Roy[1]; [1]Rigaku Raman Tehcnologies

Poster Board #41

(311) **Calorimetry-Derived Vectors to Resolve Pure Raman Spectral Components of Phospholipid Vesicle Phase Transitions**; Jay Kitt[1], Joel Harris[1]; [1]University of Utah

Poster Board #42

(312) **Advances in Kaiser Raman Analyzers for *in situ* Studies of Small Volume Liquid-phase Reactors**; Ian Lewis[1], Sean Gilliam[1], Lisa Ganster[1]; [1]Kaiser Optical

Poster Board #43

(313) **State of the Art Microanalysis using Raman Microscopy**; Peng Wang[1], Thomas Tague[1], Sergey Shilov[1]; [1]Bruker Optics Inc

Poster Board #44

(314) **High-Speed Compressive Raman and Fluorescence Imaging of Pharmaceutical Composites**; Owen Rehrauer[1], Bharat Mankani[1], Greg Buzzard[1], Brad Lucier[1], Dor Ben-Amotz[1]; [1]Purdue University

Poster Board #45

(315) **Impact of Radiation Environment on the Performance of Analytical Instrumentation for Planetary Missions**; Arthur Smalley[1], Ian Hutchinson[1], Richard Ingley[1], Melissa McHugh[1]; [1]University of Leicester

Poster Board #46

(316) **Transmission Raman Spectroscopy using a Spatial Heterodyne Raman Spectrometer**; K. Alicia Strange (Fessler)[1], Kelly Paul[1], S. Michael Angel[1]; [1]The University of South Carolina

Poster Board #47

(317) **Raman Analysis of Ancient Carbonaceous Matter of Relevance to Martian Geology**; Richard Ingley[1], Cédric Malherbe[2], Ian Hutchinson[1], John Parnell[4]; [1]University of Leicester; [2]University of Liège; [3]University of Leicester; [4]University of Aberdeen

Poster Board #48

(318) **Wide-Field, Hyperspectral Raman Spectroscopy Using a Fiber Array Spectral Translator Coupled with a Spatial Heterodyne Spectrometer**; Nathaniel Gomer[1], Matthew Nelson[1], S. Michael Angel[2]; [1]ChemImage Sensor Systems; [2]University of South Carolina

Poster Board #49

(319) **How Low Can You Go? Modelling a Raman Spectrometer to Determine how Instrument Parameters Affect Lower Sensitivity Limits**; Liam Harris[1], Ian Hutchinson[1], Richard Ingley[1], Howell Edwards[1]; [1]University of Leicester

Poster Board #50

(320) **Optimising the Performance of a Stand-Off Raman Spectroscopy Instrument For Planetary Exploration Applications**; Melissa McHugh[1], Ian B. Hutchinson[1], Richard Ingley[1], Nick Nelms[2], Howell G.M. Edwards[1]; [1]University of Leicester; [2]European Space Research and Technology Centre, European Space Agency

Poster Board #51

(321) **Synthesis and Characterisation of Novel SERS Active Phosphate Capped Gold Nanoparticles**; Peter White[1], Wassie Mersha[1], Mark Baron[1]; [1]University of Lincoln

Poster Board #52

(322) **The Analysis of Blue Solvent Dyes by SERS using Treated Silver Nanoparticles**; Peter White[1], Thomas Purbrick[1], Mark Baron[1]; [1]University of Lincoln

11:40 am – 1:10 pm
WHAT'S HOT VENDOR PRESENTATIONS, *Exhibit Hall C/D*
Presider: Brian Dable, *Arete Associates*
Complimenary lunch is available in the exhibit hall for all conferees

11:40	**Princeton** "LightField — The Future of Scientific Imaging and Spectroscopy Software"
11:50	**Ondax** "New Low-frequency THz-Raman® Probe for *in-situ* Measurements"
12:00	**B&W Tek** "The Latest in Portable Raman Instrumentation"
12:10	**Horiba** "Raman Spectroscopy and Imaging of 2D Phonons"
12:20	**Ocean Optics** "Flame: Blazing a New Path in NIR Spectroscopy"
12:30	**Innovative Photonic Solutions** "High Throughput Integrated Raman Probes"
12:40	**Renishaw** "Innovative Raman imaging"
12:50	**Kaiser Optical Systems "**Illuminating Your Chemistry with Raman"
1:00	**BioTools** "A BioTools Portable Raman Microscope: An R&D 100 Market Disrupter"

Tuesday Afternoon, *Room 550A/B*
INNOVATIVE ATMOSPHERIC-PRESSURE PLASMA IONIZATION SOURCES
Organizer and Presider: Jacob Shelley

1:20	(323) **Ambient Ionization and a Decade of DART**; Robert Cody[1]; [1]JEOL USA, Inc.
1:40	(324) **Laser Induced Plasma for Ambient Ionization**; Jens Riedel[1]; [1]BAM Federal Institute for Materials Research and Testing

TECHNICAL PROGRAM – TUESDAY
Orals 1:20 – 3:00 pm

2:00 (325) **Expanding Analytical Frontiers of the Solution-Cathode Glow Discharge**; Andrew Schwartz[1], Kelsey Williams[2], Jacob Shelley[2], Steven Ray[1], Gary Hieftje[1]; [1]Indiana University, Department of Chemistry; [2]Department of Chemistry and Biochemistry, Kent State University

2:20 (326) **Laser Ablation Sample Transfer for Tissue Proteomics and Genomics**; Kermit Murray[1], Fabrizio Donnarumma[1]; [1]Louisiana State University

2:40 (327) **Correlation-based Technique to Facilitate Detection, Identification, and Differentiation of Many Analytes in Direct Mass Spectrometry Approaches**; Jacob Shelley[1], Yi You[1], Sunil Badal[1], Allyson Beechy[1]; [1]Department of Chemistry and Biochemistry, Kent State University

Tuesday Afternoon, *Room 554A/B*
FACSS CHARLES MANN AWARD SESSION HONORING SANFORD ASHER
Organizer: Richard Van Duyne; Presiders: Richard Van Duyne and Bhavya Sharma

1:20 (328) **Probing Low Frequency Vibrational Excitations and Their Effect on Electron and Proton Transport in proteins**; Paul Champion[1]; [1]Northeastern University

1:40 (329) **Plasmonically Enhanced Raman Spectra of Cells and Body Fluids: SERS Applications in Diagnostics and Forensics**; Lawrence Ziegler[1]; [1]Boston University

2:00 (330) **Predictability and Sensitivity of ROA Spectroscopy for Structure Elucidation of Protein Therapeutics**; Rina Dukor[1]; [1]BioTools Inc

2:20 (331) **Enhanced Vibrational Optical Activity: Making Small Big**; Laurence Nafie[1]; [1]Syracuse University

2:40 (332) **Raman Spectroscopy of Amyloid Fibrils**; Igor Lednev[1], Valentin Sereda[1]; [1]University at Albany, SUNY

Tuesday Afternoon, *Room 551B*
CHEMOMETRICS IN PHARMACEUTICAL INDUSTRY
Organizer and Presider: Guoxiang Chen

1:20 (333) **PAT and Multivariate Condition Monitoring for Drug Product Continuous Process**; Yang (Angela) Liu[1]; [1]Pfizer Worldwide Research & Development

1:40 (334) **Validation of Bioanalytical Methods: DoE Methodology**; Roujian Zhang[1];Qiang Qin[1], Benhur Ogaby[1], Binbing Yu[1], Lingmin Zeng[1], [1]MedImmune

2:00 (335) **Screening Soy Hydrolysates for the Production of a Recombinant Therapeutic Protein in Commercial Cell Line by Combined Approach of NIR and Chemometrics**; Guiyang Li[1], Zai-qing Wen[1], Guoxiang Chen[2]; [1]Amgen Inc; [2]MedImmune, LLC

2:20 (336) **Utilizing CoA and Spectroscopic Data To Aid Model Maintenance of Real Time Release Methods**; Dongsheng Bu[1], Yan Zhang[1], Dimuthu Jayawickrama[1], Gary McGeorge[1]; [1]Bristol-Myers Squibb

2:40 (337) **Development and Validation of API Characterization Methods via On-line Raman Measurements for Real-Time Release Testing**; John-David McElderry[1], Chunsheng Cai[1], Justin Pritchard[1], Frank Qi[1], Kelly Swinney[1]; [1]Vertex Pharmaceuticals

Tuesday Afternoon, *Room 552B*
LC-MS BASED DETECTION OF PERFLUORINATED CONTAMINANTS IN THE ENVIRONMENT
Organizer: Rainer Lohmann; Presider: Carrie McDonough

1:20 (338) **The Role of Polyfluoroalkyl Substances in Understanding Perfluoroalkyl Acid Contamination at Aqueous Film-Forming Foam Impacted Sites**; Christopher Higgins[1], Simon Roberts[1]; [1]Colorado School of Mines

1:40 (339) **Comparison of Online and Offline Solid Phase Extraction Methods for Analysis of Perfluoroalkyl Acids in Water using Liquid Chromatography Tandem Mass Spectrometry**; Xianming Zhang[1], Andrea Weber[1], Cindy Hu[1], Wenlu Zhao[2], Minggang Cai[2], Pete August[2],Rainer Lohmann[2], Chad Vecitis[1], Elsie Sunderland[1]; [1]School of Engineering and Applied Sciences, Harvard University; [2]Graduate School of Oceanography, University of Rhode Island

2:00 (340) **Analytical Challenges on Newly Identified Commercial Fluorosurfactants and Extractable Organofluorine in Human**; Leo Yeung[1], Scott Mabury[1]; [1]University of Toronto - Department of Chemistry

2:20 (341) **Perfluorophosphinates and Other Perfluorinated Acids in Northern Pike and Double-Crested Cormorants**; Amila De Silva[1]; [1]Environment Canada

2:40 (342) **Pilot Whales as an Indicator of Temporal Patterns in PFASs in North Atlantic Seawater**; Elsie Sunderland[1], Bjarni Mikkelsen[2], Maria Dam[3], Rosanna Bossi[4]; [1]Harvard University; [2]The Faroese Museum of Natural History; [3]Environment Agency, Faroe Islands; [4]Aarhus University, Faculty of Science and Technology

Tuesday Afternoon, *Room 551A*
MASS SPECTROMETRY IN FORENSICS
Organizer and Presider: Guido Verbeck

1:20 (343) **Development of a Portable, Ion Trap, Mass Spectrometer with Multi-Interface Support for Analyte Sampling**; Yang Cui[1], Eric Bergles[1], Mike Chai[1], Charlie Zhang[1], William Yang[1]; [1]BaySpec, Inc.

1:40 (344) **You Can't Tell a Book by Its Cover: Analytical Adventures in Anthropodermic Bibliopegy**; Daniel Kirby[1], Anna N. Dhody[2], Beth Lander[2], Richard R. Hark[3,4]; [1]Peabody Museum of Archaeology and Ethnology; [2]The College of Physicians of Philadelphia; [3]Brown University, John Hay Library; [4]Juniata College, Department of Chemistry

2:00 (345) **GC-MS and GC-IR Studies on Substituted Cathinones: Bath Salt-type Aminoketone Designer Drugs**; Randall Clark[1], Jack DeRuiter[1], Younis Abiedalla[1], Karim Abdel-Hay[1]; [1]Auburn University

2:20 (346) **Probabilistic Detection of Firearms Discharge Residue on Skin Using Ion Mobility Spectrometry and Neural Networks**; Suzanne Bell[1]; [1]West Virginia University

2:40 (347) **A Case Study in the Determination of Geographical Origin for Dalbergia, a CITES Listed Wood Species**; James Jordan[1], Michael Doughten[2], Tyler Coplen[2], Haiping Qi[2], Ed Espinoza[3]; [1]National Geospatial-Intelligence Agency; [2]U.S. Geological Survey; [3]U.S. Fish & Wildlife Forensics Laboratory

Tuesday Afternoon, *Room 556B*
NANOSCALE IR II
Organizer and Presider: Jing Yang

1:20 (348) **Measuring Correlated Composition and Optical Properties at the Nanoscale with the PTIR Technique: Application to Perovskites Solar Cells**; Andrea Centrone[1]; [1]NIST, Center for Nanoscale Science and Technology

1:40 (349) **Assessing the Chemical, Mechanical and Structural Properties of Shale at Nanoscale**; Jing Yang[1], Andrew Pomerantz[1]; [1]Schlumberger-Doll Research Center, Schlumberger

2:00 (350) **IP-Enhanced Infrared Photoexpansion Nanospectroscopy in Air and Aqueous Solutions**; Mikhail Belkin[1], Mingzhou Jin[1], Feng Lu[1]; [1]The University of Texas at Austin

TECHNICAL PROGRAM – TUESDAY
Orals 1:20 – 3:00 pm and 3:50 – 5:30 pm

2:20 (351) **High Speed Infrared Nanospectroscopy with Sub-Monolayer Sensitivity**; Craig Prater[1], Eoghan Dillon[1], Qichi Hu[1], Honghua Yang[1], Curtis Marcott[3], Feng Lu[2],Mingzhou Jin[2], Mikhail Belkin[2], Kevin Kjoller[1]; [1]Anasys Instruments; [2]The University of Texas at Austin; [3]Light Light Solutions

2:40 (352) **Resonance Tracking in Resonance Enhanced Infrared Nanoscopy**; Georg Ramer[1], Anna Balbekova[1], Andreas Schwaighofer[1], Bernhard Lendl[1]; [1]Vienna University of Technology, Institute of Chemical Technologies and Analytics

Tuesday Afternoon, *Room 552A*
ELECTRO- AND LIQUID PHASE-SEPARATION TECHNIQUES
Organizer and Presider: Blanca H. Lapizco-Encinas

1:20 (353) **3D Carbon-electrode Dielectrophoresis in Sample Preparation**; Rodrigo Martinez-Duarte[1]; [1]Clemson University

1:40 (354) **Experimental Evidence of Deterministic Absolute Negative Mobility for Organelles and Colloids**; Alexandra Ros[1], Jinghui Luo[1], Katherine Muratore[2], Edgar Arriaga[2]; [1]Arizona State University; [2]University of Minnesota

2:00 (355) **DNA Fractionation using Surface Dielectrophoresis**; Ghislain Tchantchou[1], Jeremy Buhain[1], Sagnik Basuray[1]; [1]New Jersey Institute of Technology

2:20 (356) **Ultrafast Immunoassays by Coupling Dielectrophoretic Biomarker Enrichment on Nano-Slit Device with Electrochemical Detection**; Nathan Swami[1], Walter Varhue[1], Bankim Sanghavi[1], Kuo-Tang Liao[2], Chia-Fu Chou[2]; [1]Electrical Engineering, University of Virginia; [2]Institute of Physics, Academia Sinica, Taiwan

2:40 (357) **Particle Separation Employing Dielectrophoresis**; Blanca Lapizco-Encinas[1]; [1]Rochester Institute of Technology

Tuesday Afternoon, *Ballroom E*
HANDHELD LIBS
Organizer and Presider: Steve Buckley

1:20 (358) **Portable LIBS from Research to Reality**; Francois Doucet[1], Lutfu Ozcan[1]; [1]ELEMISSION Inc.

1:40 (359) **Handheld LIBS for Metal Alloy Analysis**; Phillip Tan[1], Greg Petersen[1], Jacob Scheckman[1]; [1]TSI Incorporated

2:00 (360) **A Novel Handheld LIBS Analyzer and Its Applications**; Sean Wang[1], Jing Li[1], Katherine Bakeev[1], Qun Li[1]; [1]B&W Tek, Inc.

2:20 (361) **Advances in Handheld LIBS Instrumentation for Soil and Geochemical Monitoring**; Brendan Connors[1], Morgan Jennings[1], Justin Spott[1], David Day[1]; [1]SciAps, Inc.

2:40 (362) **Metals Analysis - When to Use Portable XRF, LIBS, or OES, a presentation by Oxford Instruments**; David Clifford[1]; [1]Oxford Instruments

Tuesday Afternoon, *Room 553A*
ADVANCES IN APPLICATIONS OF HANDHELD/PORTABLE SPECTROMETERS
Organizer and Presider: Jason Rodriguez

1:20 (363) **Ultra-miniaturized Hyperspectral Imager**; William Yang[1]; [1]BaySpec, Inc.

1:40 (364) **Developing Screening Methods for Drug Compounds Using Portable Ion Mobility Spectrometry**; Connie Ruzicka[1]; [1]US Food and Drug Administration

2:00 (365) **Portable/Handheld Infrared Spectrometers becoming a Reality for the Food Industry**; Luis Rodriguez-Saona[1]; [1]The Ohio State University

2:20 (366) **The Versatility of Portable Raman in Process Development**; Thomas Padlo[1], Katherine Bakeev[1], Philip Zhou[1]; [1]B&W Tek, Inc.

2:40 (367) **Progress in Portable Visible Spectrometry**; Alexander Scheeline[1]; [1]SpectroClick

Tuesday Afternoon, *Room 555B*
EMERGING RAMAN TECHNIQUES AND APPLICATIONS II
Organizers and Presiders: Ian Lewis, Duncan Graham, and Pavel Matusek

1:20 (368) **Raman spectroscopy for Enantioselective Analysis of Chiral Systems**; Johannes Kiefer[1]; [1]Universitaet Bremen

1:40 (369) **Surface Enhanced Raman Optical Activity as a New Chirally-Sensitive Nanoprobe**; Ewan Blanch[1,2], Saeideh Ostovar pour[1, 2], Lisa Rocks[3], Karen Faulds[3], Duncan Graham[3], Vaclav Parchansky[4],Petr Bour[4]; [1]RMIT University; [2]University of Manchester; [3]University of Strathclyde; [4]Charles University

2:00 (370) **Raman Spectroscopy Detects Invasive Brain Cancer Cells in Humans**; Kevin Petrecca[1]; [1]McGill University

2:20 (371) **Deep UV Raman and TERS Microscopy**; Satoshi Kawata[1]; [1]Osaka University

2:40 (372) **Selective-sampling Raman Micro-Spectroscopy for Tissue Diagnosis**; Ioan Notingher[1]; [1]University of Nottingham

Tuesday Afternoon, *Room 555A*
RAMAN IMAGING/MICROSCOPY II
Organizers: Ian Lewis, Duncan Graham, and Pavel Matousek; Presider: Katsumasa Fujita

1:20 (373) **Three-Dimensional Raman Imaging of Ion-Exchanged Waveguides**; David Tuschel[1]; [1]HORIBA Scientific

1:40 (374) ***In Situ* Analysis of Materials under Mechanical Stress: A Novel Instrument for Simultaneous Nanoindentation and Raman Spectroscopy**; Chris Michaels[1], Yvonne Gerbig[1], Robert Cook[1]; [1]NIST

2:00 (375) **Confocal Raman Microscopy Investigation of Solute Accumulation into Individual C18 Particles**; David Bryce[1], Jay Kitt[1], Joel Harris[1]; [1]University of Utah

2:20 (376) **AFM and Raman Mapping of Neural Stem Cells Before and After Differentiation**; Radu Alex Boitor[1], Faris Sinjab[1], Ioan Notingher[1]; [1]The University of Nottingham

2:40 (377) **Coherent Anti-Stokes Raman Scattering Correlation Spectroscopy and Imaging**; Karen Antonio[1], Zachary Schultz[1]; [1]University of Notre Dame

Tuesday Afternoon, *Room 556A*
NANOSTRUCTURED MATERIALS FOR PLASMONICS I
Organizer: Jean-Francois Masson; Presider: Zachary Schultz

1:20 (378) **New Hybrid Plasmonic Mode and Applications to Bimodal SPRI / SERS Interrogation Sensing System**; Michael Canva[1,2]; [1]LCF, Laboratoire Charles Fabry - Institut d; [2]LN2, Laboratoire Nanotechnologies Nanosystèmes - U. de Sherbrooke / CNRS

1:40 (379) **Optics, Plasmonics and SharpEdgeOnics in Novel Nanoarchitectures**; Michael J. Naughton[1]; [1]Boston College

2:00 (380) **Plasmonic Gold Nanohole Arrays for Surface-Enhanced Raman Scattering Biosensing**; Nianqiang (Nick) Wu[1], Peng Zheng[1], Xuefei Gao[1]; [1]West Virginia University

2:20 (381) **Mapping the Extracellular Space using Ion-Selective Core-Shell Luminescent Nanoparticles**; Denis Boudreau[1,2], Jérémie Asselin[1, 2], Philippe Legros[1,2], Mazeyar Pavinzadeh Gashti[1], Rihab Bouchareb[3], Jesse Greener[1],Patrick Mathieu[3]; [1]Department of Chemistry, Université Laval; [2]Center for optics, photonics and lasers, Université Laval; [3]Quebec Heart and Lung Institute, Université Laval

2:40 (382) Withdrawn

TECHNICAL PROGRAM – TUESDAY
Orals 3:50 – 5:30 pm

Tuesday Afternoon, *Room 550A/B*
ATMOSPHERIC PRESSURE PLASMAS & LIQUID CATHODE GLOW DISCHARGES
Organizer and Presider: Steven Ray

3:50 (383) **Particle-Image-Velocimetry Analysis of Aerosol from a Solution-Cathode-Glow-Discharge**; Allen White[1], Andrew Schwartz[2], Steven Ray[2], Gary Hieftje[2]; [1]Indiana University, Rose-Hulman Institute of Technology; [2]Indiana University, Department of Chemistry

4:10 (384) **Measurements of Solvated Electrons at a Plasma-Liquid Interface via Optical Absorption Spectroscopy**; Paul Rumbach[1], David Bartels[1], R. Mohan Sankaran[2], David Go[1]; [1]University of Notre Dame; [2]Case Western Reserve University

4:30 (385) **Design Modifications to a Solution Cathode Glow Discharge and Examples of Industrial Application**; Stuart Schroeder[1]; [1]Alberta Innovates Technology Futures

4:50 (386) **Discharges with Liquid Electrode: Properties and Mechanisms**; Peter Bruggeman[1]; [1]University of Minnesota

5:10 (387) **Highly Sensitive Elemental Analysis for Cd by Solution-Anode Glow Discharge Atomic Emission Spectrometry**; Zhenli Zhu[1]; [1]China University of Geosciences (Wuhan)

Tuesday Afternoon, *Room 554A/B*
CHEMOMETRICS FOR SPECTROSCOPIC/SPECTROMETRIC DATA
Organizer: Thomas Bocklitz; Presider: Jürgen Popp

3:50 (388) **Data Pre-Processing and Data Processing for Multivariate Spectral Analyses**; Max Diem[1]; [1]Northeastern University

4:10 (389) **Single Cell Raman Imaging: Problems and Pitfalls When Comparing Images for Quantitative and Qualitative Purposes.**; Martin A. B. Hedegaard[1]; [1]University of Southern Denmark, Department of Chemical Engineering, Biotechnology and Environmental Technology

4:30 (390) **Sample and Model Selection for Local Modeling Utilizing Data Fusion Ranking Techniques**; Rachel Emerson[1,2], John Kalivas[1]; [1]Idaho State University; [2]Idaho National Laboratory

4:50 (391) **Issues in Hierarchical Modeling of Complex Chemical Data**; Steven Brown[1]; [1]University of Delaware

5:10 (392) **Feasibility of an End-of-Shift Monitor for the Determination of α-Quartz in Mine Dusts**; Peter Griffiths[1], Andrew Weakley[2], Arthur Miller[3], Emanuele Cauda[4]; [1]Griffiths Consulting LLC; [2]University of California, Davis; [3]National Institute of Occupational Safety and Health, Spokane; [4]National Institute of Occupational Safety and Health, Pittsburgh

Tuesday Afternoon, *Room 555A*
DIABETES AND ITS COMPLICATIONS
Organizer and Presider: Michael Walsh

3:50 (393) **Using NMR Spectroscopy to Gain Novel Insights for Diabetes Drug Design**; Wolfgang Peti[1,2,3]; [1]Brown University School of Medicine; [2]Brown University; [3]University of Copenhagen

4:10 (394) **Raman Spectroscopy Based Sensing of Alternative Glycemic Markers: Quo vadis?**; Rishikesh Pandey[1], Nicolas Spegazzini[1], Niyom Lue[1], Jeon Woong Kang[1], Gary Horowitz[2], Ishan Barman[3],Ramachandra Dasari[1]; [1]Massachusttes Institute of Technology; [2]Harvard Medical School; [3]Johns Hopkins University

4:30 (395) **Raman-based Blood Glucose Concentration Prediction by Structural Calibration**; Nicolas Spegazzini[1], Rishikesh Pandey[1], Jeon Woong Kang[1], Ishan Barman[2], Ramachandra Rao Dasari[1]; [1]Massachusttes Institute of Technology; [2]Johns Hopkins University

4:50 (396) **Early Diagnosis of End Stage Renal Disease Due to Diabetes using IR Imaging**; Vishal Varma[1,2], Andre Kajdacsy-Balla[1, 4], Sanjeev Akkina[3,4], Suman Setty[1.4], Michael Walsh[1,2,4]; [1]Department of Pathology, University of Illinois at Chicago; [2]Department of Bioengineering, University of Illinois at Chicago; [3]Department of Medicine, University of Illinois at Chicago; [4]University of Illinois Cancer Center

5:10 (397) **Multivariate Analysis as a Tool to Extract Characteristic Bands Associated with Diabetic Retina Tissue using Synchrotron Infrared Spectromicroscopy**; Ebrahim Aboualizadeh[1], Christine Sorenson[2], Reyhaneh Sepehr[3], Mahsa Ranji[3], Nader Sheibani[4], Carol Hirschmugl[1]; [1]University of Wisconsin-Milwaukee, Department of Physics; [2]Department of Pediatrics, University of Wisconsin School of Medicine and Public Health; [3]Biophotonics Laboratory, University of Wisconsin Milwaukee, Department of Electrical Engineering and Computer Science; [4]Department of Ophthalmology and Visual Sciences, University of Wisconsin School of Medicine and Public Health

Tuesday Afternoon, *Room 551A*
AMBIENT IONIZATION AND NON-CHROMATOGRAPHIC APPROACHES IN FORENSICS AND HOMELAND SECURITY
Organizer and Presider: Adam B. Hall

3:50 (398) **Ambient Ionization in the Security Industry: Atmospheric Pressure Photoionization (APPI) for Explosives Trace Detectors (ETDs)**; Jack Syage[1], Karl Hanold[1], Andrey Vilkov[1]; [1]Morpho Detection, LLC

4:10 (399) **Characterizing and Databasing Drugs and Drug Analogs to Stay Ahead of Clandestine Designer Drug Laboratories**; Kristina Williams[1], Guido Verbeck[1]; [1]University of North Texas

4:30 (400) **Mobilized Open Air Ionization: Detection of Explosives and Dangerous Supplements with a Compact DART-MS**; Frederick Li[2], Joseph Lapointe[1], Joseph Tice[1], Adam Hall[3], Brian Musselman[1]; [1]IonSense, Inc. Saugus, MA; [2]Boston University School of Medicine: Biomedical Forensic Sciences Program, Boston, MA; [3]Northeastern University: The Barnett Institute of Chemical and Biological Analysis and the Department of Chemistry and Chemical Biology, Boston, MA

4:50 (401) **MALDI-MS as a Tool for the Characterization of Inks for Forensic Document Analysis**; Rhett Williamson[1], José Almirall[1]; [1]Florida International University

5:10 (402) **Direct Sample Analysis Using Electrospray Ionization High Performance Ion Mobility-Mass Spectrometry**; Adam Graichen[1], Robert Jackson[1], Jianglin Wu[1], Ching Wu[1], Mark Osgood[1]; [1]Excellims Corporation

TECHNICAL PROGRAM – TUESDAY
Orals 3:50 – 5:30 pm

Tuesday Afternoon, *Room 556B*
NANOSCALE IR III
Organizer and Presider: Jing Yang

3:50 (403) **Nanoscale Chemical Imaging of Phase-Separated Polymer Systems and Organic-Inorganic Films**; Mark Rickard[1], Gregory Meyers[1], Carl Reinhardt[1], Jamie Stanley[1]; [1]The Dow Chemical Company

4:10 (404) **NanoMineralogy of Extraterrestrial Samples Using AFM-tip Enhanced Infrared Spectroscopy**; Gerardo Dominguez[1], Alex McLeod[2], Zack Gainsforth[3], Priscilla Kelly[2], Fritz Keilmann[4], Andrew Westphal[3],Mark Thiemens[2], Dimitri Basov[2]; [1]California State University, San Marcos; [2]University of California, San Diego; [3]University of California, Berkeley; [4]Ludwig-Maximilians-Universität and Center for Nanoscience

4:30 (405) **Looking Inside Single Cells and Tissue using Nanoscale Infrared Spectroscopy**; Curtis Marcott[1], Eoghan Dillon[2], Qichi Hu[2], Kevin Kjoller[2]; [1]Light Light Soluitons; [2]Anasys Instruments

4:50 (406) **AFM-IR Studies of Individual Electrospun Nanofibers: Structural Analysis and Mapping of Poly[(R)-3-hydroxybutyrate-co-(R)-3-hydroxyhexanoate] (PHBHx) Fibers**; Liang Gong[1], D. Bruce Chase[1], Isao Noda[1,2], C.J. McBrin[1], John Rabolt[1]; [1]Department of Materials Science and Engineering, University of Delaware; [2]Meredian Bioplastics

5:10 (407) **Photothermal AFM-IR of Bacteria – Polyurethane Bilayers: Impact of Local Sample – Cantilever Damping on Quantitative IR Measurements**; Daniel Barlow[1], Justin Biffinger[1], Allison Cockrell[3], Michael Lo[2], Kevin Kjoller[2], Debra Cook[2],Woo Kyung Lee[1], Pehr Pehrrson[1], Wendy Goodson[4], John Russell[1]; [1]Chemistry Division, Naval Research Lab; [2]Anasys Instruments; [3]Nova Research, Inc.; [4]Nanostructured & Biological Materials Branch, Materials & Manufacturing Directorate, Air Force Research Laboratory

Tuesday Afternoon, *Room 552A*
MINIATURIZATION
Organizer and Presider: Carlos D. Garcia

3:50 (408) **Miniaturized Raman Spectrometers for Space Applications: the Detectability of Biomarkers in Geological Matrices Relevant to Mars Exploration**; Cedric Malherbe[1], Melissa Mchugh[1], Ian B. Hutchinson[1], Richard Ingley[1], Howell G. M. Edwards[1]; [1]University of Leicester, Department of Physics and Astronomy

4:10 (409) **Sampling and Preconcentration of Volatile Organic Compounds Using Capillary Microectraction of Volatiles (CMV)**; Natasha Kreitals[1], Anamary Tarifa[1], Dnisha Hamblin[1], Jose Almirall[1]; [1]Florida International University

4:30 (410) **Sample Delivery of Biphasic Droplets Containing Protein Crystals For Serial Femtosecond Crystallography With An X-Ray Free Electron Laser**; Austin Echelmeier[1], Garrett Nelson[1], Bahige G. Abdallah[1], Uwe Weierstall[1], John C. H. Spence[1], Petra Fromme[1],Alexandra Ros[1]; [1]Arizona State University

4:50 (411) **Electrokinetic Biomarker Enrichment in Physiological Media by Coupling Dielectrophoresis with Ion Conductivity Gradients in Nanoslits**; Nathan Swami[1], Ali Rohani[1], Walter Varhue[1], Kuo-Tang Liao[2], Chia-Fu Chou[2]; [1]Electrical Engineering, University of Virginia; [2]Institute of Physics, Academia Sinica, Taiwan

5:10 (412) **Using Pyrolyzed Paper for Electrochemical Detection in Microfluidic Paper-Based Analytical Devices**; Carlos Garcia[2], Elizabeth Evans[1], Jason Giuliani[1], Gema Duran[3], Angel Rios[3], Tomas Benavidez[1]; [1]UT San Antonio; [2]Clemson University; [3]University of Castilla-La Mancha

Tuesday Afternoon, *Ballroom E*
LIBS FOR ENVIRONMENTAL AND FOOD MONITORING
Organizer and Presider: Madhavi Martin

3:50 (413) **Using LIBS to Determine Ground Water Quality Changes Due to Subsurface Activities**; Dustin McIntyre[1], Christian Goueguel[2, 3], Cantwell Carson[3], Herve Sanghapi[3], Jinesh Jain[2]; [1]USDOE NETL; [2]AECOM/URS; [3]ORISE

4:10 (414) **Analysis of Bakery and Dairy Products by Laser Induced Breakdown Spectroscopy**; Kemal Eseller[1], Gonca Bilge[2], İsmail Boyaci[2]; [1]Atilim University; [2]Hacettepe University

4:30 (415) **LIBS Analysis of Plant Samples – Advantages and Limitations**; Jozef Kaiser[1], Jan Novotný[1], David Prochazka[1], Pavel Pořízka[1], Aleš Hrdlička[1], Karel Novotný[1]; [1]Brno University of Technology, CEITEC - Central European Institute of Technology

4:50 (416) **Laser-Induced Breakdown Spectroscopy: Application to Nuclear Waste Management**; Jagdish Singh[2], Fang Yu Yueh[1]; [1]Institute for Clean Energy Technology, Mississippi State University; [2]JPS Advanced Technology R&D LLC,

5:10 (417) **LIBS to the Extreme: High-dose Radiochemical Analyses where ICP Methods Cannot Follow**; Rodger Martin[1], Tom Hylton[1]; [1]Oak Ridge National Laboratory

Tuesday Afternoon, *Room 553A*
SAS PAT TECHNICAL SECTION: PAT IN THE PHARMACEUTICAL INDUSTRIES I
Organizer: Brandye Smith-Goettler; Presider: James Rydzak

3:30 **SAS PAT Technical Section Business Meeting**

3:50 (418) **Transmission Raman Analysis of Bilayered Tablets**; Gary McGeorge[1], Yan Zhang[1]; [1]Bristol-Myers Squibb

4:10 (419) **PAT Methods Development for the Pharmaceutical Industry**; Carl Anderson[1]; [1]Duquesne University

4:30 (420) **A NIR In-Process Control Method for Determination of API Concentration in Tablets Manufactured by a Continuous Process**; Frank Qi[1]; [1]Vertex

4:50 (421) **Monitoring Drying Performance of Pharmaceutical API by Raman Spectroscopy and Mass Spectrometry**; Ming Huang[1], Daniel Hsieh[1], Robert Wethman[1], John Wasylyk[1]; [1]Bristol-Myers Squibb Co.

5:10 (422) **To Find Needles in Haystacks, Use a Metal Detector; Pharmaceutical Materials Analysis by Nonlinear Optical Stokes Ellipsometry**; Garth Simpson[1], Paul Schmitt[1], Niraj Trasi[1], Lynne Taylor[1]; [1]Purdue University

Tuesday Afternoon, *Room 555B*
FORENSIC APPLICATONS OF RAMAN SPECTROSCOPY
Organizer and Presider: Igor K. Lednev

3:50 (423) **Chip based Raman Analytics of Body Fluids**; Juergen Popp[1,2]; [1]Leibniz Institute of Photonic Technology; [2]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena

4:10 (424) **Developing Deep UV Raman Standoff Spectrometer for Trace Explosives**; Sanford Asher[1], Sergei Bykov[1], Katie Gares[1], Kyle Hufziger[1]; [1]University of Pittsburgh

4:30 (425) **An Application of SERS in Forensics: Hair Dyes**; Dmitry Kurouski[1], Richard Van Duyne[1]; [1]Northwestern University

4:50 (426) **Discrimination of Animal and Human Blood Using Raman Spectroscopy and Chemometrics**; Kyle C. Doty[1], Gregory McLaughlin[1], Igor K. Lednev[1]; [1]University at Albany, SUNY

5:10 (427) **Forensic Analyses by Morphologically Directed Raman Spectroscopy**; Brooke Kammrath[1], Andrew Koutrakos[1, 2], Josemar Castillo[3], Joe Wolfgang[3], Deborah Huck-Jones[4]; [1]Henry C. Lee College of Criminal Justice and Forensic Sciences, Dept of Forensic Science, University of New Haven; [2]University of Verona; [3]Malvern Instruments Inc.; [4]Malvern Instruments Ltd

Tuesday Afternoon, *Room 551B*
ANALYTICAL CHEMISTS EASING WORLD POVERTY
Organizer and Presider: Rebecca Airmet

3:50 (428) **Low-cost Bioanalytical Instrumentation for the Developing World**; Alex Nemiroski[1], Dionysios C. Christodouleas[1], Ashok A. Kumar[1], Jonathan W. Hennek[1], George M. Whitesides[1]; [1]Harvard University

4:10 (429) **Arsenic in Drinking Water: Promoting Awareness through Remediation and Measurement Projects for Students**; Julian Tyson[1], Ray Kronquist[2]; [1]University of Massachusetts; [2]Chemists without Borders

4:50 (430) **Three Tales from Vietnam**; Alexander Scheeline[1]; [1]SpectroClick

5:10 (431) **Catalyzing Analytical Chemistry and Natural Products Drug Discovery Around the World**; Nina Dudnik[1]; [1]Seeding Labs

Tuesday Afternoon, *Room 556A*
NANOSTRUCTURED MATERIALS FOR PLASMONICS II
Organizerz; Jean-Francois Masson; Presider: Emilie Ringe

3:50 (432) **Opitical and Sensing Properties of Coupled Nanoplate-Nanosphere Structures Formed with Regio-Selective Control**; Francis Zamborini[1], Prashant Jain[2], Aiqin Fang[1], Sarah White[2]; [1]University of Louisville; [2]University of Illinois

4:10 (433) **Identifying Uranium Speciation in Environmental Samples using Raman and SERS**; Amanda Haes[1], Grace Lu[1], Tori Forbes[1]; [1]University of Iowa

4:30 (434) **Structure and Plasmons of Single Bimetallic Nanorods during Reaction**; Jing Zhao[1], Sravan Thota[1], Shutang Chen[1], Yadong Zhou[2], Shengli Zou[2]; [1]University of Connecticut; [2]University of Central Florida

4:50 (435) **Tunable 3D Plasmonic Cavity as an Ultrasensitive SERS Platform**; François Lagugné-Labarthet[1], Mohammadali Tabatabaei[1], Mohamadreza Najiminaini[1], Jeffrey Carson[1]; [1]Western University

5:10 (436) **Scanning Angle Raman Spectroscopy Measurements of Thin Films and Buried Polymer Interfaces**; Emily Smith[1,2], Jonathan Bobbitt[1, 2], Craig Damin[1,2]; [1]Ames Laboratory; [2]Iowa State University

TECHNICAL PROGRAM – WEDNESDAY
Plenary Lectures, *Ballroom B/C*
Presider: Alexandra Ros

8:00 am – SAS's Lester W. Strock Award.
(437) **Liquid Sampling-Atmospheric Pressure Glow Discharge Microplasmas: Evolving Towards Versatility, Practicality, and Transportability**; R. Kenneth Marcus[1]; [1]Clemson University

8:30 am – Applied Spectroscopy William F. Meggers Award.
(438) **Mid-infrared Diffuse Reflection on Ultrafast Time Scales**; Eric Brauns[1]; [1]University of Idaho

Orals 9:15 – 10:55 am

Wednesday Morning, *Room 552A*
MICROFLUIDICS AND ELECTROPHORESIS FOR BIOANALYTICAL APPLICATIONS
Organizer: Adam Woolley; Presider: Vishal Sahore

9:15 (439) **Electroosmotic Sampling and Microfluidic Determination of Extracellular Thiols in Brain Tissue Cultures**; Stephen Weber[1], Juanfang Wu[1], Jessie Jiang[1], James Landers[2], Erin Redman[3], J.P. Alarie[3],J. Michael Ramsey[3]; [1]University of Pittsburgh; [2]University of Virginia; [3]University of North Carolina

9:35 (440) **Fabrics as Platforms for Electrophoretic Separations**; Shashi Murthy[1], Tanya Narahari[1], Dhananjaya Dendukuri[2]; [1]Northeastern University; [2]Achira Labs

9:55 (441) **Nanogels for Reversibly Patterned Electrophoretic Separations**; Lisa Holland[1], Brandon Durney[1], Tyler Davis[1], Srikanth Gattu[1]; [1]Chemistry Department, West Virginia University

10:15 (442) **Pressure-Actuated Microfluidic Devices for Pre-Term Birth Biomarker Analysis**; Vishal Sahore[1], Suresh Kumar[1], Adam Woolley[1]; [1]Brigham Young University

10:35 (443) **DNA Separation by Sequence**; Linda McGown[1], Jia Zhao[1], Steven Cramer[1], Cecily Wilbanks[1], Shekhar Garde[1], Xueru Tepke[1]; [1]Rensselaer Polytechnic Institute

Wednesday Morning, *Room 550A/B*
FUNDAMENTALS AND NOVEL APPLICATIONS OF GLOW DISCHARGE SPECTROSCOPY I
Organizers: Jorge Pisonero and Parick Chapon;
Presider: Patrick Chapon

9:15 (444) **Time Regimes in Pulsed RF-GD-TOFMS: Properties and Effects on the In-Depth Profile Analysis of Thin Layers**; Nerea Bordel[1], Jorge Pisonero[1], Cristina González-Gago[1], Alfredo Sanz-Medel[1]; [1]University of Oviedo

9:35 (445) **Quantitative Reconstruction of the GDOES Sputter Depth Profile of a Monomolecular Layer Structure of Thiourea on Copper**; JiangYong Wang[1], Yi Liu[1], Wei Jian[1], Siegfried Hofmann[2], Ken Shimizu[3]; [1]Department of Physics, Shantou University; [2]Max Planck Institute for Intelligent Systems; [3]University Chemical Laboratory, Keio University

9:55 (446) **Application of RF Glow Discharge Optical Emission Spectroscopy for Quantitative Depth Profile Analysis of Chemically Strengthened Glass**; Anna Nached[1], Georgiy Guryanov[1], Jamie Vargeson[1]; [1]Science and Technology Division, Corning Incorporated

10:15 (447) **Advances in Glow Discharge Mass Spectrometry for Elemental Analysis for Low Level Detection**; Ekbal Patel[1]; [1]Mass Spectrometry Instruments Ltd

10:35 (448) **Consequences of Heterogeneous Surface Composition in Depth-Resolved Glow Discharge Spectrometry**; Andrew P. Storey[1], Steven Ray[1], Maxim Voronov[2], Volker Hoffmann[2], Wolfgang Buscher[3], Carsten Engelhard[4],Gary Hieftje[1]; [1]Indiana University; [2]IFW Dresden; [3]University of Muenster; [4]University of Siegen

Wednesday Morning, *Room 554A/B*
LESTER STROCK AWARD SYMPOSIUM HONORING R. KENNETH MARCUS
Organizer and Presider: Joe Caruso

9:15 (449) **Shine Little Glow-Ken, Glimmer, Glimmer**; Joseph Caruso[1]; [1]University of Cincinnati

9:35 (450) **Ferritin: A Clinical Biomarker and a Protein Cage for Nanoparticles**; Maria Montes-Bayon[1], Tobias Konz[1], F. Javier Alonso[1], Alfredo Sanz-Medel[1]; [1]University of Oviedo

9:55 (451) **The Liquid Sampling – Atmospheric Pressure Glow Discharge: A Miniaturized Plasma for Giant Problems in Nuclear Forensics**; Benjamin T. Manard[1], Ning Xu[1], Alonso Castro[1], R. Kenneth Marcus[2]; [1]Los Alamos National Laboratory; [2]Clemson University

10:15 (452) **Ken Marcus, Champion of the Glow Discharge or Glow Discharge and Distance-of-Flight Mass Spectrometry: A Match Made in Heaven**; Steven Ray[1], Elise Dennis[2], Christie Enke[2,3], Gary Hieftje[2], David Koppenaal[4]; [1]State University of New York at Buffalo; [2]Indiana University; [3]University of New Mexico; [4]PNNL

10:35 (453) **Ken Marcus and the Glow on the Horizon**; Gary M. Hieftje[1], Andrew J. Schwartz[1], Steven J. Ray[1]; [1]Indiana University

Wednesday Morning, *Room 555A*
SUPER-RESOLUTION MICROSCOPY AND IMAGING
Organizer and Presider: Rohith Reddy

9:15 (454) **Super-Resolution Imaging Using Multi-photon and Multi-photon-like Fluorescence Microscopy Techniques**; George Patterson[1], Maria Ingaramo[1], Andrew York[1]; [1]National Institutes of Health

9:35 (455) **Super-Resolution through Minimalist Representation of Chemical Imaging in Infected Single Red Blood Cell Components using Multiplex Hyperspectral Confocal Raman Imaging**; Nicolas Spegazzini[1], Rishikesh Pandey[1], Ishan Barman[2], Ramachandra Rao Dasari[2]; [1]Massachusttes Institute of Technology; [2]Johns Hopkins University

9:55 (456) **Absorption Spectroscopy and Imaging from the Visible through Mid-IR with 20 nm Resolution Using AFM Probes**; Andrea Centrone[1]; [1]NIST, Center for Nanoscale Science and Technology

10:15 (457) **Fiber Bundle Arrays for Wide-Field, Dynamic SERS Nanoscopy**; Eric Languirand[1], Brian Cullum[1]; [1]University of Maryland, Baltimore County

10:35 (458) ***In situ* ATR-FTIR Spectroscopy and Imaging to Monitor the Purification Process of Antibodies**; Maxime Boulet-Audet[1], Bernadette Byrne[1], Sergei Kazarian[1]; [1]Imperial College London

TECHNICAL PROGRAM – WEDNESDAY
Orals 9:15 – 10:55 am

Wednesday Morning, *Room 551A*
CHEMOMETRICS/DATA ANALYSIS FOR FORENSICS
Organizer and Presider: Stephen L. Morgan

9:15 (459) **Advanced Pattern Recognition Applied to Forensic Evidence**; Nicholas Petraco[1]; [1]John Jay College, City University of New York

9:35 (460) **A Bayesian Approach to Forensic Evidence Interpretation; Converting Analytical Data to Significance Using a Continuous Verbal Scale**; Jose Almirall[1], James Curran[2]; [1]Florida International University; [2]University of Auckland

9:55 (461) **Statistical Method for Comparison of Mass Spectra: Applications for the Identification of Controlled Substances**; Ruth Waddell Smith[1], Melissa A. Bodnar-Willard[2], Victoria L. McGuffin[2]; [1]Forensic Science Program, Michigan State University; [2]Department of Chemistry, Michigan State University

10:15 (462) **Fusion of UV-visible Absorbance and Fluorescence Data for Forensic Discrimination of Dyed Textile Fibers**; Nathan C. Fuenffinger[1], Stephen L. Morgan[1]; [1]University of South Carolina; [2]University of South Carolina

10:35 (463) **Infrared Imaging and Multivariate Curve Resolution Applied to the Forensic Examination of Automotive Paints**; Barry Lavine[1], Matthew Allen[1], Koichi Nishikida[2], Mark Sandercock[0]; [1]Department of Chemistry, Oklahoma State University; [2]Materials Science Center, University of Wisconsin; [3]Forensic Laboratory, Royal Canadian Mounted Police, Canada

Wednesday Morning, *Room 556B*
NEW DEVELOPMENTS IN QCL TECHNOLOGY
Organizer and Presider: Bernhard Lendl

9:15 (464) **High Sensitivity Gas and Liquid Analysis Using Tunable Mid-Infrared Lasers**; Don Kuehl[1], Richard Sharp[1], Eugene Ma[1], Jinhong Kim[1], Charles Marshall[1]; [1]RedShift Systems Corp.

9:35 (465) **Toward Monolithic Integration of a Quantum Cascade Laser Array and an Echelle Grating Multiplexer for Widely-Tunable mid-IR Sources**; Mathieu Carras[1], Clément Gilles[1, 2], Luis Orbe[3], Guillermo Caprintero[3], Gregory Maisons[1]; [1]mirSense, France; [2]III-V Lab, France; [3]Universidad Carlos III de Madrid, Spain

9:55 (466) **Integrated Ring Laser Systems for Spectroscopy based on Quantum Cascade Structures**; Schrenk Werner[1], Rolf Szedlak[1, 2], Daniela Ristanic[1], Benedikt Schwarz[1], Peter Reininger[1], Andreas Harrer[1],Hermann Detz[1], Donald C. MacFarland[1], Aaron M. Andrews[1], Gottfried Strasser[1]; [1]Technische Universität Wien, Center for Micro- and Nanostructures and Institute for Solid State Electronics

10:15 (467) **Monolithic Quantum Cascade Lasers And Their Applications**; Christian Pfluegl[1]; [1]Eos Photonics, Inc.

10:35 (468) **Broadly-tunable Monolithic THz Quantum Cascade Laser Sources**; Mikhail Belkin[1]; [1]The University of Texas at Austin

Wednesday Morning, *Ballroom E*
STANDOFF LIBS
Organizer and Presider: Matthieu Baudelet

9:15 (469) **Standoff LIBS. Concepts and Scenes**; Javier Laserna[1]; [1]Universidad de Malaga

9:55 (470) **Application of Distance Correction to ChemCam LIBS Measurements**; Alissa Mezzacappa[1], Noureddine Melikechi[1], Agnes Cousin[2], Roger Wiens[3], Jeremie Lasue[2], Samuel Clegg[3], Robert Tokar[4], Steven Bender[4], Nina Lanza[3], Sylvestre Maurice[2]; [1]Optical Science Center for Applied Research, Delaware State University; [2]Institut de Recherche en Astophysique et Planetologie (IRAP), Universite' Paul Sabatier, France; [3]Los Alamos National Laboratory; [4]Planetary Science Institute

10:15 (471) **Stand-off LIBS using Laser Filamentation: Fundamental Characterization for Quantitative Analysis**; Matthieu Baudelet[1,2], Matthew Weidman[1], Mark Ramme[1], Khan Lim[1], Magali Durand[1], Martin Richardson[1]; [1]Townes Laser Institute, University of Central Florida; [2]National Center for Forensic Science, University of Central Florida

10:35 (472) **Femtosecond Filament-Laser Ablation Molecular Isotopic Spectrometry**; George Chan[1], Huaming Hou[1], Xianglei Mao[1], Vassilia Zorba[1], Richard Russo[1]; [1]Lawrence Berkeley National Laboratory

Wednesday Morning, *Room 552B*
MASS SPECTROMETRIC TECHNIQUES IN ENVIRONMENTAL ANALYSIS
Organizer and Presider: Kaveh Jorabchi

9:15 (473) **Mass Spectrometry of Airborne Nanoparticles**; Murray Johnston[1]; [1]University of Delaware

9:35 (474) **Rapid Measurement of Nanoparticle and Microparticle Size Distribution and Number Concentration by Inductively Coupled Plasma Mass Spectrometry**; Austin Wilson[1], Chuanqiang Sun[1], John W. Olesik[1]; [1]Ohio State University

9:55 (475) **A New Approach for Halogen Isotope Measurements with Focus of Compound-Specific Isotope Ratio Analysis**; Matthias Gehre[1], Julian Renpenning[1], Kristina Hitzfeld[1], Tetyana Gilevska[1]; [1]Helmholtz Centre for Environmental Research -UFZ

10:15 (476) **Exploring Charge-Transfer Ionization Pathways with the Flowing Atmospheric-Pressure Afterglow (FAPA) Ambient Ionization Source to Expand the Range of Detectable Analytes**; Sunil Badal[1], Shawn Michalak[2], George Chan[3], Jacob Shelley[1]; [1]Department of Chemistry and Biochemistry, Kent State University; [2]Stark State College; [3]Lawrence Berkeley National Laboratory

10:35 (477) **High-Sensitivity Organohalogen Detection and Quantification by PARCI-MS**; Kaveh Jorabchi[1]; [1]Georgetown University

Wednesday Morning, *Room 553A*
SAS PAT TECHNICAL SECTION: PAT IN THE BIOPHARMACEUTICAL INDUSTRIES II
Organizers: Saly Romero-Torres and Brandye Smith-Goettler; Presider: James Rydzak

9:15 (478) **Development of Raman Spectroscopy as a Rapid Identification Method for Raw Materials**; Tony Wang[1], David Meriage[1]; [1]Amgen

9:35 (479) **Micro-Raman Spectroscopy used as a PAT Tool and for Real Time Monitoring of Protein Stability during Freeze Drying**; Tatiana Starciuc[1,2], Laurent Paccou[1, 2], Yannick Guinet[1,2], Alain Hedoux[1,2]; [1]University of Lille 1 Sciences en Technology; [2]University Lille 1, UMET - UMR CNRS 8207

9:55 (480) ***In situ*** **Raman Spectroscopic Monitoring of Multiple Biochemical Species during Microbial Fermentation Process Development**; Karin Balss[1], Sean Gilliam[3], Angelica Spinelli[1], Wojciech Czaja[2]; [1]Janssen Pharmaceuticals; [2]Depuy Synthes; [3]Kaiser Optical Systems

10:15 (481) **PAT Raman Data Acquisition in Biopharmaceutical Development and Manufacturing Environments using Siemens SIPAT Framework**; Stefani Takahashi[1], John Paul Smelko[1], Brandon Berry[1], Robert Song[1]; [1]Biogen

10:35 (482) **CQA Focused Process Analytical Technology for Biologics Manufacturing**; Douglas Richardson[1], Zi Chen[1], Maria Khouzam[1], Daisy Richardson[1], John Higgins[1], David Pollard[1]; [1]Merck

Wednesday Morning, *Room 555B*
BIOANALYTICAL SERS II
Organizer and Presider: Roy Goodacre

9:15 (483) **Gold Nanostars: A Multi-Modality Nanoplatform For Diagnostic and Therapeutic Applications**; Tuan Vo-Dinh[1], Hsin-Neng Wang[1], Yang Liu[1], Andrew Fales[1]; [1]Duke University

9:35 (484) **Gold Superstructures for SERS-based Bioimaging**; Srikanth Singamaneni[1]; [1]Washington University in St. Louis

9:55 (485) **SERS Imaging of Gold Nanoparticles in Biological, Paper, and Granular Matricies**; Peter Vikesland[1], Rebecca Lahr[1], Matthew Chan[1]; [1]Virginia Polytechnic Institute and State University

10:15 (486) **Selective Detection of 100 B. Anthracis Ames Spores in 20 Minutes using a Portable SERS Assay**; Stuart Farquharson[1], Chetan Shende[1], Wayne Smith[1], Carl Brouillette[1], Jay Sperry[3], Todd Sickler[2],Amber Prugh[2], Jason Guicheteau[2]; [1]Real-Time Analyzers, Inc.; [2]US Army; [3]University of Rhode ISland

10:35 (487) **Raman Spectroscopy and SERS Investigations of Rhizosphere and Medically Relevant Bacterial Communities**; Sneha Polisetti[1], Nameera Baig[3], Jennifer Morrell-Falvey[2], Joshua Shrout[4], Mitchel Doktycz[2], Paul Bohn[1,3]; [1]Department of Chemical & Biomolecular Engineering, University of Notre Dame; [2]BioSciences Division, Oak Ridge National Laboratory; [3]Department of Chemistry, University of Notre Dame; [4]Department of Civil and Environmental Engineering & Earth Sciences, University of Notre Dame

Wednesday Morning, *Room 556A*
BIOANALYTICAL APPLICATIONS OF PLASMONICS II
Organizer and Presider: Jean-Francois Masson

9:15 (488) **Plasmon-enhanced Spectroelectrochemistry – An Advanced Tool for Biosensing**; Christa Brosseau[1], Lili Zhao[1], Reem Karaballi[1], Jonathan Blackburn[2]; [1]Saint Mary; [2]University of Cape Town, Cape Town, South Africa

9:35 (489) **Direct Detection of MicroRNA based on Plasmon Hybridization of Nanoparticle Dimers**; Jennifer Chen[1]; [1]York University

9:55 (490) **Filtration of Antigen-Assembled Gold Nanoparticles for SERS Detection**; Jeremy Driskell[1], Arielle Lopez[1], Francis Lovato[1]; [1]Illinois State University

10:15 (491) **Integration of Electrophoretic Capture and Surface Plasmon Resonance Sensing in a Microfluidic Channel**; Karl Booksh[1], Ornella Sathoud[1], Joe Smith[1], Casey Kneale[1], Missy Postelwaite[1], Kimberly Hibsman[1]; [1]University of Delaware

10:35 (492) **Real-time Monitoring Bacterial Growth under Different Flow Rates with Surface Plasmon Resonance Imaging**; Pegah N. Abadian[1], Edgar Goluch[1]; [1]Northeastern University

Wednesday Poster Session
11:00 am – 12:00 pm
Exhibit Hall C/D

All Wednesday posters should be put up between 7:30 – 8:30 am and removed by 3:50 pm

Biomedical and Bioanalytical Posters

Poster Board #1

(493) **Surface Plasmon Resonance and Fluorescence: A Novel Approach for Characterization of Biomolecules Interactions**; Jérémie Labrecque-Carbonneau[1], Jean-François Masson[1]; [1]University of Montreal

Poster Board #2

(494) **Histopathological Characterization of Biological Tissues using High-Resolution Infrared Spectroscopic Imaging**; Jayakrupakar Nallala[1], Gavin Lloyd[2], Neil Shepherd[3], Nicholas Stone[4]; [1]Bio-physics, School of Physics, University of Exeter; [2]Biophotonics Research Unit, Gloucestershire Royal Hospitals; [3]Department of Pathology, Gloucestershire Hospitals; [4]Bio-physics, School of Physics, University of Exeter

Poster Board #3

(495) **Predicting Vascularized Composite Allograft Outcome during Modulated Immunosuppression using Multimodal Imaging**; Nicole Crane[1,2,3], Rajiv Luthra[1, 3], Georg Furtmuller[4], Eric Elster[2], Gerald Brandacher[4], W. P. Andrew Lee[4]; [1]Naval Medical Research Center; [2]Uniformed Services University of Health Sciences; [3]Henry M. Jackson Foundation for the Advancement of Military Medicine; [4]Johns Hopkins University

Poster Board #4

(496) **From Fiber Spectrometers to Fiber Sensors**; Viacheslav Artyushenko[1]; [1]art photonics GmbH

Poster Board #5

(497) **Spectroscopic Investigation of the Effects of Bioavailable Ions on Apatite Mineral Composition and Kinetics**; Mary Tecklenburg[1], Md. Shah Alam[1], Honey Madupalli[1], Andrew Derry[1], James Lamblin[1], Megan Ling[1]; [1]Central Michigan University

Poster Board #6

(498) **Purification and Biochemical Characterization of Highly Active Manganese Peroxidase from Mutant Trametes Versicolor IBL-04 under Solid State Culture**; Muhammad Ramzan[1,2], Muhammad Asgher[1], Raymond Legge[3], Yan Feng[2]; [1]Department of Chemistry & Biochemistry, University of Agriculture Faisalabad, Pakistan; [2]Key State Laboratory of Microbial Metabolism, Shanghai Jiao Tong University, China; [3]Department of Chemical Engineering, University of Waterloo, Canada

Poster Board #7

(499) **Evaluation of Lipophilic Versus Hydrophilic Delivery of Flufenamic Acid in *ex vivo* Human Skin by Confocal Raman Microscopy**; Yelena Pyatski[1], Carol Flach[1], Qihong Zhang[1], Richard Mendelsohn[1]; [1]Rutgers University

TECHNICAL PROGRAM – WEDNESDAY
Posters 11:00 am – 12:00 pm

Poster Board #8

(500) **New Routes for Tissue Pathology using Quantum Cascade Laser Based Imaging Microscopes**; Vishal Varma[1], Hari Sreedhar[1], Peter Nguyen[1], Andrew Graham[2], Francesca Gambacorta[2], Kyle Meinke[1],Oluwatobi Adelaja[1], Aliya Husain[3], Grace Guzman[1], Michael Walsh[1]; [1]University of Illinois at Chicago; [2]University of Illinois at Urbana-Champaign; [3]University of Chicago

Poster Board #9

(501) **Metabolomic Characterization of Leishmania Major and Leishmania Donovani by 1H and 1H-13C HSQC NMR.**; Paulo Falco Cobra[1,2,3], John Markley[3], Otavio Thiemann[4], Luiz Colnago[2]; [1]Instituto de Quimica de Sao Carlos - Universidade de Sao Paulo; [2]EMBRAPA Instrumentacao; [3]Biochemistry Department - University of Wisconsin - Madison; [4]Instituto de Fisica de Sao Carlos - Universidade de Sao Paulo

Poster Board #10

(502) **A pH Reporter Molecule for Measurements and 3D Imaging in Turbid Media**; Kevin Davies[1]; [1]Florida Gulf Coast University

Poster Board #11

(503) **Imaging and Feature Selection using GA-FDA Algorithm for the Classification of HSI Biomedical Images**; Rupali Mankar[1], Vishal Verma[2], Michael Walsh[2], Bueso-Ramos Carlos[3], David Mayerich[1]; [1]University of Houston; [2]Department of Pathology, University of Illinois at Chicago; [3]Division of Pathology/Lab Medicine, The University of Texas MD Anderson Cancer Center, Houston, TX

Poster Board #12

(504) **Deconstruction of Inclusion Bodies and Refolding of Bioactive Protein Using Archaeal Chaperones**; Maruda Shanmugasundaram[1], Nadya Pavlova[2, 3], Andrey Pavlov[4], Jin Y. Wang[5], James E. Galen[5], Alexei Slesarev[4],Antonio del Castillo-Olivares[5], Frank T. Robb[2, 3], Igor K. Lednev[1]; [1]Department of Chemistry, University at Albany, State University of New York, Albany, NY; [2]Department of Microbiology and Immunology, University of Maryland, MD; [3]Institute of Marine and Environmental Technology, University of Maryland, MD, USA; [4]Fidelity Systems, Inc., Gaithersburg, MD; [5]Center for Vaccine Development, University of Maryland, Department of Biology, Montgomery College

Poster Board #13

(505) **Analysis and Evaluation of the UV Radiation as a Disinfectant**; José Gabriel Aguilar Soto[1], Jorge Castro Ramos[2], Humberto Miguel Sansebastián Aguilar[3], Diana Antonieta Sen Salinas[4]; [1]National Institute of Astrophysics, Optics and Electronics (INAOE); [2]National Institute of Astrophysics, Optics and Electronics (INAOE); [3]H&M Biomedical Technology International; [4]Center for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV)

Poster Board #14

(506) **Diffuse Reflectance Spectroscopy and Automatic ABCDE Law Applied in Melanocytic Naevi**; Jorge Castro-Ramos[1], Adriana May-Salazar[2], Gabriel Aguilar-Soto[1], Diana Sen-Salazar[1], Francisco Gutierrez-Gonzalez[3], Reimer Romero-Hernandez[1],Karen Esmonde-White[4]; [1]Instituto Nacional de Astrofisica Optica y Electronica; [2]Instituto Mexicano del Seguro Social; [3]Centro para la prevención del cancer; [4]University of Michigan

Environmental/Oceanographic Posters

Poster Board #15

(507) **Underwater Standoff Fluorescence Instrument for the Detection of Oil in the Seabed, Water Column and Under Ice**; Job Bello[1], Christina Gasbarro[1], Anton Smirnov[1]; [1]EIC Laboratories, Inc.

Poster Board #16

(508) **Effect of CO2-laden Brine Temperature, Pressure and Salinity on the Temperature, Electron Density and Morphology of Laser-Induced Underwater Plasma, and Implications for Groundwater Monitoring in Geological CO2 Sequestration**; Christian Goueguel[1], Dustin McIntyre[1], Jinesh Jain[2], Cantwell Carson[1], Herve Sanghapi[3]; [1]USDOE, National Energy Technology Laboratory; [2]AECOM; [3]Institute for Clean Energy Technology

Poster Board #17

(509) **Ocean Floor Exploration using Multi-Sensor Active Spectroscopy: a Payload Concept**; Pablo Sobron[1,2]; [1]SETI Institute; [2]MalaUva Labs

Poster Board #18

(510) **Infrared Spectroscopic Assessment of Biomass for Bioethanol Generation**; Ramyasri Ailavajhala[1], Mugdha Padalkar[1], Uday Palukuru[1], Arash Hanifi[1], Rashid Kaveh[1], Benoit Van Aken[1],Nancy Pleshko[1]; [1]Temple University

Poster Board #19

(511) **Demonstration of Scalable Analytical Methods for the Screening of Algae Bloom Contaminated Surface Waters by UHPLC-TOFMS Equipped with a Novel and Automated Analyte Search Algorithm**; Stephen White[1], Nicole Lenca[2], Frank Kero[1], Jason Weisenseel[1], Benjamin Southwell[3], Bogdan Bogdanov[1],Craig Young[1], Judy Westrick[2]; [1]PerkinElmer, Oak Brook Technology Center; [2]Wayne State University; [3]Lake Superior State University

Poster Board #20

(512) **The Photoacoustic Effect from Moving Sources**; Wenyu Bai[1], Gerald Diebold[1]; [1]Department of Chemistry, Brown University

Poster Board #21

(513) **Polyethylene: A Novel Approach for Passively Sampling Fluorotelomer Alcohols**; Erik Dixon-Anderson[1], Rainer Lohmann[1]; [1]University of Rhode Island Graduate School of Oceanography

Poster Board #22

(514) **Oligomerizational Behaviour of Nitrophenol under Simulated Atmospheric Conditions**; Hafiz Muhammad Danish Sultan[2], Farhat Yasmeen[1], Muzafar Abbas[1]; [1]University of Engineering and Technology, Lahore; [2]University College of Pharmacy, University of Punjab, Lahore

Poster Board #23

(515) **Investigation of Fluorescence Yield Variability in Emiliania huxleyi**; Stefan Faulkner[1], Cameron Rekully[1], Shawna Tazik[1], Joe Swanstrom[1], Timothy Shaw[1], Tammi Richardson[2],Michael Myrick[1]; [1]University of South Carolina Department of Chemistry and Biochemistry; [2]University of South Carolina Department of Biological Sciences

Poster Board #24

(516) **Design of Optical Interference Filters for Taxonomic Classification of Phytoplankton**; Cameron Rekully[1], Shawna Tazik[1], Stefan Faulkner[1], Timothy Shaw[1], Tammi Richardson[1], Michael Myrick[1]; [1]University of South Carolina

Poster Board #25

(517) **Decrease in Cadmium Levels in Canadian Western Amber Durum from 1995 to 2013**; Anja Richter[1]; [1]Canadian Grain Commission

Molecular: IR/Near IR Posters

Poster Board #26

(518) **Step-Scan, Rapid Scan, and Interleaved Time-Resolved FTIR Spectroscopy: Signal-To-Noise Comparison**; Sergey Shilov[1], Michael Joerger[1], Thomas Tague[1]; [1]Bruker

TECHNICAL PROGRAM – WEDNESDAY
Posters 11:00 am – 12:00 pm

Poster Board #27

(519) **Non-Destructive Analysis of Surface Coatings using the Agilent 4300 Handheld FTIR analyzer**; Dipak Mainali[1], Leung Tang[1]; [1]Agilent Technologies

Poster Board #28

(520) **Near Infrared Spectral Evaluation of Tissue Engineered Cartilage Correlates to Gene Expression of constructs**; Farzad Yousefi[1], Ramyasri Ailavajhala[1], Uday Palukuru[1], Syeda Yusra Nahri[1], Nancy Pleshko[1]; [1]Department of Bioengineering, Temple University, PA

Poster Board #29

(521) **Differential Excitation Spectroscopy: A New Technique**; Boyd Hunter[1], Jason Cox[1], Paul Harrison[1], Bill Walters[1], Michael Miller[2]; [1]Kestrel Corporation; [2]Southwest Research Institute

Poster Board #30

(522) **Vibrational Spectroscopy of an Imidazolium Ionic Liquid Confined in a Metal Organic Framework**; Johannes Kiefer[1], Manish Singh[2], James Anderson[2], Nilesh Dhumal[3], Hyung Kim[3]; [1]Universitaet Bremen; [2]University of Aberdeen; [3]Carnegie Mellon University Pittsburgh

Poster Board #31

(523) ***In-situ* Spectroscopic Study on Small Molecules Diffusion in Anion Exchange Membranes**; Ying Jin[1], Xiaohui Liu[1], Wenxu Zhang[1], E. Bryan Coughlin[1]; [1]Polymer Science and Engineering, University of Massachusetts Amherst

Poster Board #33

(525) **Removal of Bone Marrow Contributions for Evaluation of Bone Water by Near Infrared (NIR) Spectroscopy**; Hee Jin Yang[1], Mugdha Padalkar[1], Michael Ispiryan[2], Chamith Rajapakse[2], Nancy Pleshko[1]; [1]Temple University; [2]University of Pennsylvania

Poster Board #34

(526) **Design and Performance of a New Diamond Attenuated Total Reflection-Video Microscopy Accessory**; David Schiering[1]; [1]Czitek

Poster Board #35

(527) **Application of Near-Infrared Transflection and Transmission, and Hand-Held Raman Spectroscopy in Analysis of Ketoprofen in Pharmaceutical Gel**; Keith Freel[1], Ahmed Shawky[2,4], Ahmed Ibrahim[2,4], Eman Elzanfaly[3], Maissa Salem[2], Ahmed El Gindy[2],Stephen Hoag[4]; [1]Metrohm USA, Inc.; [2]Analytical Chemistry Department, Faculty of Pharmacy, Misr International University, Egypt; [3]Analytical Chemistry Department, Faculty of Pharmacy, Cairo University, Egypt; [4]School of Pharmacy, University of Maryland, MD

Poster Board #36

(528) **Dynamics of an Internal Protonated Water Cluster: an Isotope Exchange Study of Photosynthetic Oxygen Evolution**; Udita Brahmachari[1], Bridgette Barry[1]; [1]Georgia Institute of Technology

Poster Board #37

(529) **Cryogenic Vibrational Spectroscopy Traps an Internal Protonated Water Cluster in Photosystem II**; Zhanjun Guo[1], Bridgette Barry[1]; [1]Georgia Institute of Technology

Poster Board #38

(530) **Monitoring the Disruption and Reformation of Stratum Corneum Lipids Packing Order *in vivo* with ATR IR**; Guangru Mao[1], M. Catherine Mack[1], Hao Ouyang[1]; [1]Johnson & Johnson Consumer Inc.

Poster Board #39

(531) **Infrared Imaging for Identification of Tissue Damage in Pathology**; Bennett Davidson[1,3], Michael Walsh[3], William Ennis[2], Timothy Koh[3], Andre Kajdacsy-Balla[3], Sagar Nadimpali[1]; [1]Department of Bioengineering, College of Engineering and Medicine, University of Illinois at Chicago; [2]Department of Surgery and Section of Wound Healing and Tissue Repair, College of Medicine, University of Illinois at Chicago; [3]Department of Pathology and Spectral Pathology Lab, College of Medicine, University of Illinois at Chicago

Raman Posters

Poster Board #40

(532) **Probing Triplet-Triplet Energy Transfer Efficiency in Artificial Photosynthetic Pigments using Resonance Raman Spectroscopy**; Elizabeth Kish[1], Katherine WongCarter[2], Smitha Pillai[2], Gerdenis Kodis[2], Dalvin D. Mendez-Hernandez, Junming Ho, Ana L. Moore[2,3], Thomas Moore[2], Devens Gust[2], Bruno Robert[1]; [1]Department of Life Sciences, CEA Saclay, France; [2]Department of Chemistry and Biochemistry, Arizona State University; [3]Department of Chemistry, Yale University

Poster Board #41

(533) **Effects of Molecular Absorption Cross-Section on Raman System Throughput**; Justin Cooper[1], Adam Hopkins[2]; [1]Alakai Defense Systems; [2]Alakai Defense Systems

Poster Board #42

(534) **In-line Quality Control of Cross-linking for Photovoltaic Encapsulants via Raman Spectroscopy**; Mark Kemper[1], Christina Hirschl[2], Martin Kraft[2], Bradford Behr[1]; [1]Tornado Spectral Systems; [2]CTR Carinthian Tech Research AG

Poster Board #43

(535) **Transmission Raman Spectroscopy an Alternate Tool to Traditional HPLC to Determine the Content Uniformity of Solid Dosage Forms**; Michelle Raikes[1], Reggie Saraceno[1], Prince Korah[1], Julia Griffen[2]; [1]Boehringer Ingelheim Pharmaceuticals; [2]Cobalt Light Systems Ltd

Poster Board #44

(536) **Multi-wavelength Dispersive Raman Spectrometer and Microscope for Non-destructive Pharmaceutical Ingredient Analysis**; Jack Qian[1]; [1]BaySpec Inc.

Poster Board #45

(537) **Raman Monitoring of the Carbonization Process of Metal–Organic Frameworks**; Szetsen Lee[1], Yu-Ting Gong[1], Bing-Han Li[1], Chia-Her Lin[1]; [1]Chung Yuan Christian University

Poster Board #46

(538) **Characterization of Graphene and Other Two-Dimensional Materials by Raman Spectroscopy**; Pierre Negri[1], Tim Prusnick[1], Ian Haywood, Olga Milikofu[3], Tim Batten[2]; [1]Renishaw Inc.; [2]Renishaw Plc.; [3]Renishaw K.K.

Poster Board #47

(539) **Coherent Raman Microscopic Study during the Stretching of a Homologous PE Blend**; Ying Jin[1], Ian Ryu[1], Chad Snyder[1], Young Jong Lee[1]; [1]National Institute of Standards and Technology

Poster Board #48

(540) **Assessing Composition and Morphometry Properties of Ostrich Cartilage as Possible Tissue Engineering Scaffolds**; C. Erika Ramírez[1], Jorge L. Flores[1], Verónica M. Rodríaguez Betancourtt[1], JI Delgado-Saucedo[1], Héctor Pérez Ladrón de Guevara[3], Miguel Guzmán[2],Adán T. Paíno[1], Karen Esmonde-White[4]; [1]Universidad de Guadalajara - CUCEI; [2]Higher Technological Institute of Irapuato - ITESI; [3]Universidad de Guadalajara - CULAGOS; [4]University of Michigan - Medical School

Poster Board #49

(541) **Automated Chemical ID of Particles using Raman Spectroscopy**; Vincent Larat[1], Eunah Lee[1], Bernd Bleisteiner[1], David Tuschel[1], Simon Fitzgerald[1]; [1]HORIBA Scientific

Poster Board #50

(542) **Classification of High and Low Glycated Hemoglobin in Diabetic Patients with Raman Spectroscopy and PCA-SVM**; Villa Manriquez José Fabián[1], Castro Ramos Jorge [2], Gutierrez Delgado Francisco[3]; [1]Instituto Nacional de Astrofisica Optica y Electronica; [2]Instituto Nacional de Astrofisica Optica y Electronica; [3]Centro de Estudios y Prevención del Cancer a.c.

Poster Board #51

(543) **Comparing Raman Mapping of Colon Tissue with Immunohistochemistry for Tissue Classification**; Aaran Lewis[1], Riana Gaifulina[1], Jennifer Dorney[2], Martin Isabelle[3], Manuel Rodriguez-Justo[1], Naomi Guppy[1], Nick Stone[2], Catherine Kendall[3], Katherine Lau[4], Geraint Thomas[1]; [1]University College London; [2]University of Exeter; [3]Gloucestershire Hospitals NHS Foundation Trust; [4]Renishaw PLC

Poster Board #52

(544) **Identification of Polymeric Microfibers in Fish Stomach and Great Lakes Waters using Raman Spectroscopy**; Karen Esmonde-White[1], Rachel Cable[,2], Melissa Duhaime[2]; [1]University of Michigan Medical School; [2]University of Michigan

Poster Board #53

(545) **Comparison of Machine Learning Methods to Identify Bacteria using Raman Spectroscopy**; Cynthia Hanson, Elizabeth Vargis[1]; [1]Utah State University

Poster Board #54

(546) **Measuring Copolymer Chemical Heterogeneity by Combining SEC with Offline Raman Spectroscopy**; Aaron Urbas[1], Andre Striegel[1], Leena Pitkanen[1]; [1]National Institute of Standards and Technology

11:40 am – 1:10 pm
WHAT'S HOT VENDOR PRESENTATIONS, *Exhibit Hall C/D*
Presider: Brian Dable, *Arete Associates*
Complimenary lunch is available in the exhibit hall for all conferees

11:40 **Ibsen** "New Miniature Spectrometers for the DUV"
11:50 **Hanna**
12:00 **Daylight Solutions**
12:10 **Applied Spectra**
12:20 **PD-LD** "The Many Colors of Raman"
12:30 **Metrohm** "Get to Know Metrohm: Spectroscopy Solutions"
12:40 **Tornado** "HTVS-Based Raman Spectroscopy: A Tool for Enhanced Process Understanding"
12:50 **Thermo** "Application updates of TruScan handheld Raman"
1:00 **Eigenvector**

Wednesday Afternoon, *Room 552A*
MICROFLUIDIC ELECTROPHORESIS MODES FOR MASS SPECTROMETRIC ANALYSIS
Organizer and Presider: Bryan Fonslow

1:20 (547) **A Robust Method for Capillary Isoelectric Focusing Coupled with Mass Spectrometry**; David Chen[1], Shuai Sherry Zhao[1]; [1]University of British Columbia

1:40 (548) **High Peak Capacity Separations of Proteins and Peptides Using Two Dimensional Micro Free Flow Electrophoresis**; Michael Bowser[1], Matthew Geiger[1], Alexander Johnson[1], Nicholas Frost[1]; [1]University of Minnesota, Department of Chemistry

2:00 (549) **Multiplexed Separations for Biomarker Discovery in Metabolomics: Urinary Markers of Smoke-Exposure in Firefighters**; Philip Britz-McKibbin[1]; [1]Department of Chemistry & Chemical Biology, McMaster University, Hamilton, ON, Canada

2:20 (550) **Coupling CE with MALDI Imaging MS and ESI MS for Enhanced Analysis of Signaling Molecules**; Lingjun Li[1], Xuefei Zhong[1], Shan Jiang[1], Zichuan Zhang[1]; [1]University of Wisconsin

2:40 (551) **Analysis of Proteins, Protein Complexes and Proteomes under Native and Denaturing Conditions using Sheathless Capillary Electrophoresis Coupled with Mass Spectrometry**; Alexander R. Ivanov[1], Rosa Viner[2], Marcia R. Santos[2], Arseniy M. Belov[1], David R. Bush[1], Chitra K. Ratnayake[3], Barry L. Karger[1]; [1]Northeastern University, Barnett Institute of Chemical and Biological Analysis, Boston, MA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Sciex, Brea, CA

Wednesday Afternoon, *Room 550A/B*
A LIFETIME OF SPECTROSCOPY: CELEBRATING WORK OF EDWARD STEERS
Organizer: Petr Smid; Presider: Peter Robinson

1:20 (552) **From the VG 9000 to Nu Astrum – How Magnetic Sector GDMS was Made a Commercial Reality**; John Cantle[1]; [1]Nu Instruments

1:40 (553) **Pushing the Boundaries in Glow-Discharge Spectrometry— a Tribute to Edward Steers**; Gary M. Hieftje[1], Andrew P. Storey[1], Jacob T. Shelley[2], Steven J. Ray[1]; [1]Indiana University; [2]Kent State University

2:00 (554) **Measurement of Oxygen in Solid Samples using Analytical Glow Discharges with Optical or Mass Spectrometric Detection**; Volker Hoffmann[1], Edward Steers[2], Sohail Mushtaq[2], Juliet Pickering[3], Cristina Gonzalez Gago[4], Petr Smid[4],Thomas Hofmann[4], Cornel Venzago[, 4], Wolfgang Gruner[1]; [1]IFW Dresden; [2]London Metropolitan University; [3]Imperial College, London; [4]AQura GmbH

2:20 (555) **Investigations towards Matrix Independent Calibrations in Glow Discharge Mass Spectrometry**; Petr Smid[1], Cristina Gonzalez-Gago[2], Volker Hoffmann[3], Cornel Venzago[1], Thomas Hofmann[1]; [1]AQura GmbH; [2]University of Oviedo; [3]IFW Dresden

2:40 (556) **One Thing Leads to Another: Sixty Years of Spectroscopy Research**; Edward Steers[1]; [1]London Metropolitan University

Wednesday Afternoon, *Room 554A/B*
MEGGERS AWARD SYMPOSIUM HONORING ERIC BRAUNS
Organizer and Presider: Peter Griffiths

1:20 (557) **To Subtract or Not to Subtract, that is the Question….. in Interpretation of Soil Organic Matter Spectra**; Francisco Calderon[1], Andrew Margenot[2], Sanjai Parikh[2]; [1]USDA-ARS, Akron, Colorado; [2]Department of Land, Air and Water Resources, University of California Davis

1:40 (558) **Modeling the Time-Resolved Diffuse Reflectance**; Arnold Kim[1]; [1]University of California, Merced

2:00 (559) **QCL-Standoff MIR Reflectance Spectroscopy Measurements of Hazardous Chemicals and Biological Threats**; Samuel P. Hernández-Rivera[1], Leonardo C. Pacheco-Londoño[1], Amira Padilla-Jimenez[1], Nataly J. Galan-Freylr[1], Carlos Rios[1,2], John R. Castro-Suarez[1]; [1]Department of Chemistry, University of Puerto Rico-Mayaguez

2:20 (560) **Quantitative Infrared Directional/Hemispherical Reflectance Measurements**; Thomas Blake[1], Carolyn Brauer[1], Yin-Fong Su[1], Russell Tonkyn[1], Tanya Myers[1], Brenda Kunkel[1], Bruce Bernacki[1], Timothy Johnson[1]; [1]Pacific Northwest National Laboratory

2:40 (561) **Detection Limits for Blood on Fabrics via IR Diffuse Reflection**; Michael Myrick[1], Stephanie DeJong[1], Ray Belliveau[1], Stephen Morgan[1], Brianna Cassidy[1], Zhenyu Lu[1]; [1]University of South Carolina

Wednesday Afternoon, *Room 555A*
PATHOGENS
Organizer: Bradford Clay; Presider: Karen Esmonde-White

1:20 (562) **Evaluation of Phage Susceptibility in Acinetobacter baumannii**; Meron Ghebremedhin[1,4], Nicole Crane[1, 2, 4], James Regeimbal[1,2], Anna Jacobs[3], Brendan Corey[3]; [1]Naval Medical Research Center; [2]Uniformed Services University of Health Sciences; [3]Walter Reed Army Institute of Research; [4]Henry M. Jackson Foundation for the Advancement of Military Medicine

1:40 (563) **Direct Bacterial Analysis by Ambient Ionization Mass Spectrometry**; Pu Wei[1], Christopher Pulliam[1], Soumabha Bag[1], Alan K. Jamusch[1], Saerom Kim[1], Rafal M. Pielak[2], R. Graham Cooks[1]; [1]Purdue University; [2]L'Oréal California Research Center, San Francisco, CA

2:00 (564) **An Analytical Approach to Designing Clinical MALDI-TOF Mass Spectrometer Instrumentation**; James VanGordon[1]; [1]bioMerieux, Inc.

2:20 (565) **Surface Enhanced Raman Spectroscopy of Bacteria-Infected Wound Effluent of Combat Related Injuries**; Nicole Crane[1,2,3], Shubha Yesupriya[1], Meron Ghebremedhin[1,3]; [1]Naval Medical Research Center; [2]Uniformed Services University of Health Sciences; [3]Henry M. Jackson Foundation for the Advancement of Military Medicine

2:40 (566) **Monitoring Bacterial Biofilm Growth and Removal using a Quartz Crystal Microbalance**; Hunter Sismaet[1], Pegah Abadian[1], Edgar Goluch[1]; [1]Northeastern University

Wednesday Afternoon, *Room 556B*
QUANTUM CASCADE LASERS: APPLICATIONS
Organizer and Presider: Bernhard Lendl

1:20 (567) **Resonance Enhanced AFM-IR Induced by Quantum Cascade Laser**; Alexandre Dazzi[1], Jérémie Mathurin[1], Johanna Saunier[2], Najet Yagoubi[2], Ariane Deniset-Besseau[1], Kevin Kjoller[3]; [1]Laboratoire de Chimie Physique - Université Paris-Sud; [2]Matériaux pour la santé, Faculté de Pharmacie, Chatenay-Malabry; [3]Anasys Instruments

1:40 (568) **Linear and Nonlinear Vibrational Mid-Infrared Photothermal Spectroscopy with a Compact Fiber Laser Probe**; Atcha Totachawattana[1,3], Shyamsunder Erramilli[2,3,4], Michelle Sander[1,3,4]; [1]Electrical and Computer Engineering, Boston University; [2]Physics and Biomedical Engineering, Boston University; [3]BU Photonics Center; [4]Materials Science and Engineering, Boston University

2:00 (569) **Laser Direct IR Imaging - A New Paradigm for Mid-IR Spectroscopic Imaging**; Charles Hoke[1], Yuri Beregovski[1], Andrew Ghetler[1], Yang Han[1], Christopher Moon[1], Richard Tella[1]; [1]Agilent Technologies, Inc.

2:20 (570) **Fast Time-resolved IR Measurements using EC-QCL**; Michael George[1]; [1]University of Nottingham

2:40 (571) **EC-QC Laser Spectroscopy for mid-IR Transmission Measurements of Proteins in Aqueous Solution**; Bernhard Lendl[1], Andreas Schwaighofer[1], Mirta R. Alcaraz[1]; [1]Technische Universität Wien

Wednesday Afternoon, *Ballroom E*
LIBS FOR FORENSIC AND HOMELAND SECURITY
Organizer and Presider: Jose R. Almirall

1:20 (572) **Contribution and Impact of Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) and Laser Induced Breakdown Spectroscopy (LIBS) Tandem system to Forensic Evidence Analysis**; Jhanis J. Gonzalez[1,2], C. Derrick Quarles Jr.[2], Dayana D. Oropeza[1], Charles Sisson[2], Xianglei Mao[1], Vassilia Zorba[1], Rick Russo[1,2]; [1]Lawrence Berkeley National Laboratory; [2]Applied Spectra, Inc.

1:40 (573) **The Discrimination of Printing Inks using Laser Induced Breakdown Spectroscopy for Forensic Applications**; Ruthmara Corzo[1], Jose Almirall[1]; [1]Florida International University

2:00 (574) **Quantitative Evaluation of Spectral Interference in LIBS**; Jessica Chappell[1,3], Brandon Seesahai[2], Martin Richardson[2], Michael Sigman[1,3], Matthieu Baudelet[1,3]; [1]National Center for Forensic Science, University of Central Florida; [2]Townes Laser Institute, CREOL-The College of Optics and Photonics, University of Central Florida; [3]Chemistry Department, University of Central Florida

2:20 (575) **Evaluation of a Handheld LIBS Instrument for First Responder and Forensic Applications**; Richard R. Hark[1,2,3], David Day[1, 2, 3], Anthony H. Downey[2,3], Adam Miller[2], John Plumer[2]; [1]SciAps, Inc.; [2]Synergos Global Security, LLC; [3]Juniata College, Department of Chemistry

2:40 (576) **Quantitative Elemental Composition Measurements of Plant Materials using LIBS**; Amy Bauer[1], Markus Gaelli[1], Steven Buckley[1], Robert Robinsky[1]; [1]TSI, Incorporated

Wednesday Afternoon, *Room 552B*
AMBIENT IONIZATION METHODS: DEVELOPMENTS AND APPLICATIONS
Organizers: Demian Ifa and Rebecca Jockusch; Presider: Demian Ifa

1:20 (577) **Enhanced Analysis of Adherent Human Cells and Molecular Imaging of Microbial Growth by Laser Ablation Electrospray Ionization Mass Spectrometry**; Akos Vertes[1], Hang Li[1], Pranav Balan[1], Linwen Zhang[1]; [1]George Washington University

1:40 (578) **Applications of Chemometrics to Ambient Ionization MS Analysis**; Valentina Pirro[1], Alan K. Jarmusch[1], Christina R. Ferreira[1], R. Graham Cooks[1]; [1]Chemistry Department, Purdue University

2:00 (579) **Mass Spectrometry Imaging of Secondary Metabolites Directly on Fungal Cultures**; Nicholas Oberlies[1]; [1]University of North Carolina at Greensboro

2:20 (580) **The Bioaccumulation of a Toxic Ionic Liquid in Zebrafish (Danio rerio) Analyzed by DESI-MS Imaging**; Consuelo Perez[1], Alessandra Tata[1], Michel L. DeCampos[3], Chun Peng[2], Demian R. Ifa[1]; [1]Department of Chemistry, York University, Toronto, Ontario, Canada; [2]Department of Biology, York University, Toronto, Ontario, Canada; [3]UNICAMP, Campinas, São Paulo, Brazil

2:40 (581) **Direct Analysis of Copper and Molybdenum in Water by Microwave Plasma Torch Coupled with the Linear Ion Trap Mass Spectrometry**; Tao Jiang[1], Xiaohong Xiong[1], Wenhao Qi[1], Meilin Yang[1], Qiuju Liu[1], Lanfang Yi[1],Zhiqiang Zhu[1], Huanwen Chen[1]; [1]Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China Institute of Technology

TECHNICAL PROGRAM – WEDNESDAY
Orals 1:20 – 3:00 pm and 3:50 – 5:30 pm

Wednesday Afternoon, *Room 553A*
***IN SITU* ANALYSIS OF INDUSTRIAL PROCESSES AND REACTIONS DURING R&D**
Organizers: Xiaoyun (Shawn) Chen and Mark Richard;
Presider: Xiaoyun (Shawn) Chen

1:20 (582) **Product Development Challenges in Specialty Chemicals**; Steven Scheifers[1]; [1]Stepan Company

1:40 (583) **Optimally Dividing Available Samples into Calibration and Validation Sets**; Bryan Bowie[1]; [1]ExxonMobil Research & Engineering

2:00 (584) **Raman Spectroscopy for Lab Scale in situ Applications**; Xianghuai Wang[1], John Roberts[1], Kevin Wier[1], Dimitris Katsoulis[1]; [1]Dow Corning Corporation

2:20 (585) **Moving Vibrational Spectroscopy from Chemical Process Monitoring to Bio-Process Monitoring**; Jim Cronin[1]; [1]DuPont

2:40 (586) **PAT Application in Lubricant Industry**; Henry Xiao[1]; [1]Infineum

Wednesday Afternoon, *Room 555B*
SPATIALLY OFFSET RAMAN SPECTROSCOPY
Organizer and Presider: Pavel Matousek

1:20 (587) **Biomedical Applications of SESORS: Through Bone and Blood Vessels**; Bhavya Sharma[1], Richard Van Duyne[1]; [1]Northwestern University

1:40 (588) **Development of SORS for Nonchemical Subsurface Analysis**; Nick Stone[1], Ben Gardner[1], Pavel Matousek[2]; [1]University of Exeter, UK; [2]Central Laser Facility, STFC Rutherford Appleton Laboratory

2:00 (589) **Development of Micro-SORS for Subsurface Analysis of Thin Layers in Art and other Areas**; Claudia Conti[1], Chiara Colombo[1], Marco Realini[1], Pavel Matousek[2]; [1]Consiglio Nazionale delle Ricerche, Istituto per la Conservazione e la Valorizzazione dei Beni Culturali (ICVBC), Italy; [2]Central Laser Facility, STFC Rutherford Appleton Laboratory

2:20 (590) ***In vivo* Raman Spectroscopy for Assessing Tissues in Chronic Wounds**; Karen Esmonde-White[1], Crystal Holmes[1], Michael Morris[2]; [1]University of Michigan Medical School; [2]University of Michigan

2:40 (591) **Implementation of SORS for Three-dimensional Breast Margin Assessment**; Anita Mahadevan-Jansen[1], T Quyen Nguyen[2], Jennifer Giltnane[1], Brittany Caldwell[1], Melinda Sanders[1], Mark Kelley[1]; [1]Vanderbilt University; [2]Northwestern University

Wednesday Afternoon, *Room 551B*
CHEMISTRY IN ART AND ARCHAEOLOGY
Organizer and Presider: Mary Kate Donais

1:20 (592) **Investigating the Technology and Provenance of Bloomery Iron using Slag Chemistry: Methodological Challenges and Archaeological Potential**; Michael Charlton[1]; [1]UCL Institute of Archaeology

1:40 (593) **Classification and Geographic Origin of Garnets using Laser-Induced Breakdown Spectroscopy (LIBS)**; Richard R. Hark[1], Peter A. Defnet[1], Michael Wise[2], Russell S. Harmon[3]; [1]Department of Chemistry, Juniata College; [2]Department of Mineral Sciences, National Museum of Natural History, Smithsonian Institution; [3]Department of Marine, Earth and Atmospheric Sciences, North Carolina State University

2:00 (594) **Characterisation of Binders Used in Aboriginal and European Painted Artefacts Using Pyrolysis Gas Chromatography Mass Spectrometry**; Rachel Popelka-Filcoff[1], Tiffany Reeves[1], Fabien Pottier[2], Claire Lenehan[1]; [1]Flinders University; [2]Museum National

2:20 (595) **Archaeometry and Human Life Ways**; David George[1]; [1]Saint Anselm College

2:40 (596) **Understanding the Materials and Techniques of Early Photographs through Non-Invasive Analysis and Reconstructions**; Silvia A. Centeno[1], Anna Vila[2], Emmanuelle Marquis[3], Yimeng Chen[3], Julia Kohanek[3], Yan Dong[3],Alejandro Schrott[4], Lisa Barro[5], Nora W. Kennedy[5]; [1]The Metropolitan Museum of Art, Department of Scientific Research.; [2]Statens Museum for Kunst, Center for Art Technological Studies and Conservation,; [3]Department of Materials Science and Engineering, University of Michigan; [4]IBM Research, Thomas J. Watson Center, NY; [5]The Metropolitan Museum of Art, Department of Photograph Coservation

Wednesday Afternoon, *Room 556A*
NEW PLASMONIC MATERIALS AND TECHNIQUES
Organizer and Presider: Jean-Francois Masson

1:20 (597) **Plasmonic Sensing at the Single Particle Level**; Emilie Ringe[1]; [1]Rice University

1:40 (598) **Mapping Electric Fields Induced By Plasmons with Vibrational Stark Shifts**; Zachary Schultz[1], Daniel Kwasnieski[1], Hao Wang[1], James Marr[1]; [1]University of Notre Dame

2:00 (599) **Reaching Beyond All-Metallic Plasmonics with Optoplasmonic Metallo-Dielectric Hybrid Materials**; Bjoern Reinhard[1]; [1]Boston University

2:40 (601) **One-Pot Synthesis of Silver Nanoparticles with an Ultra-Thin Silica Shell and Their Integration into SERS and LSPR Substrates**; Daniel Willett[1], George Chumanov[1]; [1]Clemson University

2:20 (600) **Tuning Surface Plasmon Resonances on Gold Nanostars**; Laura Fabris[1], Theodoros Tsoulos[1], Roney Thomas[1,3], Swarnapali Indrasekara[1,2]; [1]Rutgers University; [2]Rice University; [3]Wesleyan University

Wednesday Afternoon, *Room 554A/B*
RSC/ACS SYMPOSIUM – ANALYSIS WITH PHOTONS – LASER & SYNCHROTRON SPECTROSCOPY SCIENCE AND APPLICATIONS II
Organizers: Rebecca Brodie and David Koppenaal;
Presider: Rebecca Brodie and Doug Duckworth

3:50 (602) **Synchrotron Infrared Nano-Spectroscopy (SINS) of Fungal Cell Wall Composition**; Kathleen Gough[1], Catherine Findlay[1], Robert Johns[2], Hans Bechtel[2], Michael Martin[2], Susan Kaminskyj[3],Tanya Dahms[4]; [1]University of Manitoba; [2]Advanced Light Source Berkeley Lab; [3]University of Saskatchewan; [4]University of Regina

4:10 (603) **Synchrotron Based Broadband IR Microspectroscopy and Spectromicrotomography**; Caol Hirschmugl[1]; [1]UW-Milwaukee

4:30 (604) **Vibrational Spectroscopy: Disease Diagnostics and Beyond**; Hugh J. Byrne[1]; [1]Dublin Institute of Technology

4:50 (605) **Infrared Spectral Imaging of Live Cells though Water**; Peter Gardner[1], James Doherty[1], Michael Pilling[1], Zhe Zhang[1], Graeme Clemens[1], Alex Henderson[1], Gianfelice Cinque[2]; [1]Manchester Institute of Biotechnology, University of Manchester; [2]Diamond Light Source, Diamond House

5:10 (606) **Single Cell Analysis for Biological and Biomedical Applications Using Mid-IR Synchrotron Light and Laser Sources**; Ganesh D Sockalingum[1], Valérie Untereiner[1], Abigail V Rutter[2], Marie Guilbert[1], Nick R Forsyth[2], Christophe Sandt[4],Paul Dumas[4], Katia Wehbe[3], Gianfelice Cinque[3], Josep Sule-Suso[1]; [1]University of Reims Champagne -Ardenne, FR; [2]University of Keele, UK; [3]Diamond Synchrotron, UK; [4]Soleil Synchrotron, FR

Wednesday Afternoon, *Room 552A*
BIOPOLYMERS IN ELECTRIC FIELDS
Organizer: Jason R. Dwyer; Presider: Ed Goluch

3:50 (607) **Single Molecule Detection with Nanometer-Scale Pores**; John Kasianowicz[1], Joseph Robertson[1], Arvind Balijepalli[1], Sina Bavari[2], Rekha Panchal[2], Jingyue Ju[3],Minchien Chen[3], Shiv Kumar[3], Carl Fuller[3], Joseph Reiner[4]; [1]NIST, Physical Measurement Laboratory, Gaithersburg, MD; [2]US Army Medical Research Institute for Infectious Diseases, Ft. Detrick, MD; [3]Dept. of Chemical Engineering, Columbia University, New York, NY; [4]Department of Physics, Virginia Commonwealth University, Richmond, VA

4:10 (608) **Engineered Protein Nanopores for Challenging Tasks in Molecular Diagnosis**; Liviu Movileanu[1]; [1]Syracuse University

4:30 (609) **Molecular-Level Design of Nanoscale Tools for Enhanced Single-Molecule Sensing**; Julie Whelan[1], Nuwan Bandara[1], Buddini Karawdeniya[1], Jason Dwyer[1]; [1]University of Rhode Island

4:50 (610) **Solid-state Single-Molecule Detection of DNA in Nanochannels**; John Oliver[1]; [1]Nabsys Inc

5:10 (611) **Deformation of Bacterial Morphology in Sub-Micrometer Constrictions under Applied Pressure**; Nil Tandogan[1], Edgar D. Goluch[1]; [1]Northeastern University

Wednesday Afternoon, *Room 550A/B*
FUNDAMENTALS AND NOVEL APPLICATIONS OF GLOW DISCHARGE SPECTROSCOPY II
Organizers: Jorge Pisonero and Patrick Chapon;
Presider: Jorge Pisonero

3:50 (612) **A Study of Strategic Calibrations and Analyte Calculations**; Kim Marshall[1]; [1]Leco Corporation

4:10 (613) **Applied Applications for GD OES in First Solar's Material Analysis Department**; Kristin Robison[1]; [1]First Solar

4:30 (614) **Comparison of Two Analytical Techniques GD-MS and SIMS Applied in Depth Profile Analysis**; Piotr Konarski[1]; [1]Institute of Tele and Radio Technology

4:50 (615) **The More You Look, the More You Find! – the Role of Penning and Charge Transfer Processes in Analytical Glow Discharges**; Edward Steers[1], Sohail Mushtaq[1], Volker Hoffmann[2], Juliet Pickering[3], Petr Smid[1,4], Zdenek Weiss[4]; [1]London Metropolitan University; [2]Leibniz Institute for Solid State and Material Research Dresden; [3]Imperial College, London; [4]LECO

5:10 (616) **Glow Discharge Optical Emission (GD-OES) Application for Thin Film Analysis of Metal Powders**; Arne Bengtson[1], Mats Randelius[1]; [1]Swerea KIMAB AB

Wednesday Afternoon, *Room 555A*
TRANSLATION AND COMMERCIALIZATION OF ANALYTICAL TECHNOLOGIES
Organizer and Presider: Karen Esmonde-White

3:50 (617) **The Education of a Former Academic or Women Who Gave Me the Business**; Alexander Scheeline[1]; [1]SpectroClick

4:10 (618) **Ideas to Finance Your Spectroscopy Innovation**; Roshan Shettty[1]; [1]Anasys Instruments

4:30 (619) **Finding a Niche Market in Busy Spectroscopy Field**; Rina Dukor[1]; [1]BioTools, Inc.

4:50 (620) **When a Great Medical Device Isn't Great for the Company**; Bradford Clay[1]; [1]bioMerieux, Inc.

5:10 **Speaker Roundtable**

Wednesday Afternoon, *Room 556B*
DIFFICULT DATA SETS
Organizer and Presider: Woody Barton

3:50 (621) **Improving Multivariate Calibration Results for Optical Spectrometers**; Michael F Roberto[1], Randy Pell[1], L. Scott Ramos[1], Brian G. Rohrback[1]; [1]Infometrix, Inc.

4:10 (622) **SERS Detection of Foodborne Pathogens at 10 cfu/g Food in Less than 5 Hours**; Chetan Shende[1], Katie Dana[1], Jay Sperry[2], Stuart Farquharson[1]; [1]Real-Time Analyzers, Inc.; [2]University of Rhode Island

4:30 (623) **Data Transfer Between a FT-NIR Laboratory and a Miniaturized Hand-held NIR Spectrometer**; Heinz Siesler[1], Uwe Hoffmann[2], Frank Pfeifer[1]; [1]University of Duisburg-Essen; [2]nir-tools

4:50 (624) **Two-Dimensional Infrared Correlation Analysis of Time-Resolved Infrared Spectra to Probe the Structure Development of the Thermally Reversible Gel Made of a Bio-based, Biodegradable Polymer**; Isao Noda[1], Brian Sobieski[1], Liang Gong[1], C.J. McBrin[1], John Rabolt[1], Bruce Chase[1]; [1]Department of Materials Science and Engineering, University of Delaware

5:10 (625) **Near-Infrared Compositional Analysis of Acid Components in Etchant Solution in Combination with a Feature Selection Method and Investigation of Inter-Component Interactions using Dimensional (2D) Correlation Analysis**; Kyeol Chang[1], Hoeil Chung[1]; [1]Department of Chemistry, College of Natural Sciences, Hanyang University

Wednesday Afternoon, *Ballroom E*
ISOTOPIC ANALYSIS IN LASER INDUCED PLASMA
Organizer and Presider: Alexander Bol'shakov

3:50 (626) **Characterization of Atomic Lifetimes and Linewidths in Laser Induced Plasmas using Tunable Laser Absorption Spectroscopy**; Mark Phillips[1]; [1]Pacific Northwest National Laboratory

4:10 (627) **Laser Ablation Molecular Isotopic Spectrometry (LAMIS): Factors Influencing Analytical Precision and Accuracy**; Xianglei Mao[1], George Chan[1], Alexander Bol'shakov[2], Huaming Hou[1], Vassilia Zorba[1], Richard Russo[1]; [1]Lawrence Berkeley National Laboratory; [2]Applied Spectra, Inc.

4:30 (628) **Hybrid Interferometric/Dispersive Atomic Spectroscopy of Uranium**; Phyllis Ko[1], Jill Scott[2], Igor Jovanovic[1]; [1]Penn State University; [2]Idaho National Laboratory

4:50 (629) **H and D Analysis Using Laser Induced Breakdown Spectroscopy in Helium Gas.**; Koo Hendrik Kurniawan[1], Kiichiro Kagawa[1, 2]; [1]Maju Makmur Mandiri Research Center; [2]Fukui University

TECHNICAL PROGRAM – WEDNESDAY
Orals 3:50 – 5:30 pm

5:10 (630) **Detection of Isotopes in a Matrix with LIBS**; Alan Ford[1], Charlemagne Akpovo[2], Staci Brown[2], Jorge Martinez[2], Lewis Johnson[2]; [1]Alakai Defense Systems; [2]FAMU

Wednesday Afternoon, *Room 552B*
DIRECT INJECT MASS SPECTROMETRY
Organizer and Presider: Guido Verbeck

3:50 (631) **Distinguishing Isobaric Drugs using Online Derivatization and Direct Analysis in Real Time (DART)**; William D. Hoffmann[1], Glen P. Jackson[1, 2]; [1]West Virginia University, Department of Forensic and Investigative Science, WV; [2]West Virginia University, C. Eugene Bennett Department of Chemistry, WV

4:10 (632) **Rapid Detection of Rare Earth Elements by Microwave Plasma Torch Coupled with the Linear Ion Trap Mass Spectrometry**; Xiaohong Xiong[1], Tao Jiang[1], Meiling Yang[1], Wenhao Qi[1], Saijin Xiao[1], Zhiqiang Zhu[1],Huanwen Chen[1]; [1]Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China Institute of Technology

4:30 (633) **Analysis of Vapor Samples with Interrupted Helium Flow for the Flowing Atmospheric-Pressure Afterglow Mass Spectrometry**; Andrew P. Storey[1], Offer Zeiri[1, 2], Steven Ray[1], Allen White[1,3], Gary Hieftje[1]; [1]Indiana University; [2]Nuclear Research Center Negev; [3]Rose-Hulman Institute of Technology

FACSS Student Award

4:50 (634) **The Liquid Sampling-Atmospheric Pressure Glow Discharge: A Miniaturized Ambient Glow Discharge Ionization Source for Elemental and Molecular Mass Spectrometry**; Lynn X. Zhang[1], R. Kenneth Marcus[1]; [1]Clemson Univeristy

5:10 (635) **Direct Analyte-Probed Nanoextraxtion (DAPNe) Coupled to Nanospray Ionization Mass Spectrometry Applied to Document Analysis**; Vivian Huynh[1], Kristina Williams[1], Phillip Mach[1], Zachary Sasiene[1], Teresa Golden[1], Guido Verbeck[1]; [1]University of North Texas

Wednesday Afternoon, *Room 553A*
DEDICATED (24/7) ONLINE ANALYSIS OF INDUSTRIAL PROCESSES AND REACTIONS
Organizers and Presiders: JD Take and Anna Sandlin

3:50 (636) **Microfluidic Gas Chromatography-Bringing the Analyzer to the Sample**; Joshua Whiting[1], Pierre Puget[2], Eric Colinet[2], Philippe Andreucci[2], David Faulkner[3], Philippe Coric[3]; [1]3 Degrees of Separation; [2]APIX Analytics; [3]EIF-Astute

4:10 (637) **Fast GC Performance in the Real World: Multi Lab Studies for Repeatability & Reproducibility**; John Crandall[1], Steve Bostic[1], Ned Roques[1]; [1]Falcon Analytical

4:30 (638) **FTIR & GC-FTIR Single Analyzer for Comprehensive Process Monitoring and Control**; Charles Phillips[1], Martin Spartz[1], Anthony Bonanno[1], Stacey Larson[1], Alice Delia[1]; [1]Prism Analytical Technologies, Inc.

4:50 (639) **Application of Low Thermal Mass Column Technology to On-line Process Gas Chromatography**; Eric Schmidt[1], Anna Sandlin[1], Linda Heinicke[1], Bill Winniford[1], Wilco Hoogerwerf[2], Jasper Van Noyen[3], Dale Ashworth[4], Chris Bishop[4]; [1]Analytical Sciences, The Dow Chemical Company, Freeport, TX; [2]Analytical Sciences, The Dow Chemical Company, Terneuzen, The Netherlands; [3]Hydrocarbons R&D, The Dow Chemical Company, Terneuzen, The Netherlands; [4]Valco Instruments Company, Inc. , Houston, TX

5:10 (640) **Portable Plant Performance Analyzer System**; Matthew MacConnell[1]; [1]Air Products and Chemicals

Wednesday Afternoon, *Room 551A*
CHIRAL ANALYSIS
Organizer and Presider: Don Pivonka

3:50 (641) **An Infrared (IR) and Vibrational Circular Dichroism (VCD) Spectroscopic Study of Solvent Effects on Hydrogen Bonding by (S-(+)-2-(4-Isobutylphenyl)-Propionic Acid**; Douglas Minick[1], Randy Rutkowske[1], Mark Hemling[1]; [1]GlaxoSmithKline R&D

4:10 (642) **Quantitation of Enantiomers by Vibrational Circular Dichroism (VCD)**; Laila Kott[1]; [1]Takeda Pharmaceuticals International Company

4:30 (643) **Pharmaceutical Applications of Vibrational Circular Dichroism (VCD)**; Steven Wesolowski[1]; [1]AstraZeneca

4:50 (644) **Advancing Supercritical Fluid Chromatography (SFC) Technology and its Applications in Drug Discovery**; Yingru Zhang[1], Chunlei Wang[1], Jun Dai[1]; [1]Bristol-Myers Squibb Co

5:10 (645) **Development and Validation of a Normal Phase Chiral HPLC Method for verification of Afoxolaner as a Racemic Mixture Using a Chiralpak® AD-3 Column**; Jinyou Zhuang[1], Satish Kumar[1], Abu Rustum[1]; [1]Merial, A Sanofi Company

Wednesday Afternoon, *Room 555B*
BIOMEDICAL RAMAN SPECTROSCOPY
Organizer and Presider: Nick Stone

3:50 (646) **Validation of *in-vivo* Raman Spectroscopy for Bladder Cancer Diagnosis**; Christiaan van Swol[1], Michelle Agenant[1,2], Trudy Jonges[2], Olivier Wegelin[1], Ruud Bosch[2], Harm van Melick[1], Matthijs Grimbergen[1]; [1]St. Antonius Hospital Nieuwegein; [2]University Medical Center Utrecht

4:10 (647) **Raman Spectroscopic Techniques for the Identification of Ionizing Radiation Induced Damage in Tumour Cells**; Andrew Jirasek[1], Quinn Matthews[3], Samantha Harder[2], Martin Isabelle[4], Julian Lum[3], Alex Brolo[2]; [1]University of British Columbia; [2]University of Victoria; [3]BC Cancer Agency; [4]Gloucester Royal Hospital

4:30 (648) **Exploration of Wavelength Effects on Deep Tissue Detection in Transmission Raman Spectroscopy**; Adrian Ghita[1], Pavel Matousek[2], Nick Stone[1]; [1]University of Exeter, UK; [2]STFC Rutherford Appleton

4:50 (649) **Multiplexed Raman Micro-Spectroscopy using Spatial Light Modulators**; Faris Sinjab[1], Graham Gibson[2], Miles Padgett[2], Ioan Notingher[1]; [1]University of Nottingham; [2]The University of Glasgow

5:10 (650) **Rapid Fiber-Optic Raman Spectroscopy Enhances *in vivo* Diagnosis of Adenomatous Polyps at Colonoscopy**; Zhiwei Huang[1]; [1]National University of Singapore

TECHNICAL PROGRAM – WEDNESDAY
Orals 3:50 – 5:30 pm

Wednesday Afternoon, *Room 556A*
RAMAN IN CULTURAL HERITAGE
Organizer and Presider: Claudia Conti

3:50 (651) **Pushing the Envelope in Raman Spectroscopy: Identification of Organic Media in Art**; Celine Daher[1], Ludovic Bellot-Gurlet[2], Francesca Casadio[1]; [1]Art Institute of Chicago; [2]MONARIS UMR 8233 UPMC/CNRS

4:30 (653) **Identification of Copper Resinate in Artworks: in a Quest for the Optimal Raman Procedure**; Jana Striova[1]; [1]National Institute of Optics-National Research Council

4:50 (654) **Detection of Natural and Synthetic Organic Colorants in Historic Oil Paintings using Surface-Enhanced Raman Spectroscopy**; Kristin Wustholz[1], Kristen Frano[1], Shelley Svoboda[2]; [1]College of William and Mary; [2]Colonial Williamsburg Foundation

5:10 (655) **Raman Spectroscopy for Cultural Heritage: a Powerful Technique in the Conservation Scientist's Toolbox**; Federica Pozzi[1]; [1]Solomon R. Guggenheim Museum

TECHNICAL PROGRAM – THURSDAY
Plenary Lectures, *Room S2/3*
Presider: Glen Jackson

8:00 am – ANACHEM Award
(656) **Mass Spectrometry Tools for Probing Cell to Cell Chemical Heterogeneity**; Jonathan Sweedler[1]; [1]University of Illlinois

8:30 am – AES Mid Career Award
(657) **Microchip Electrophoresis: A Mid-Career Method?**; Adam Woolley[1]; [1]Brigham Young University

Orals 9:15 – 10:55 am

Thursday Morning, *Room 552A*
BIOANALYTICAL DIELECTROPHORESIS
Organizers and Presiders: Ning Wu and Hui Zhao

9:15 (658) **AC-Electrokinetics at Nanoscales: from Complex Nanocolloids to Macromolecules**; Elaine Zhu[1]; [1]University of Notre Dame

9:35 (659) **Dielectrophoretic Monitoring of Alterations in C.difficile Colonization Due to Inter-Strain Antagonism**; Nathan Swami[1], Yi-Hsuan Su[1], Ali Rohani[1], Cirle Warren[2]; [1]Electrical Engineering, University of Virginia; [2]Infectious Diseases, University of Virginia

9:55 (660) **XFEL Diffraction from Protein Nanocrystals Isolated using a Microfluidic Sorter**; Bahige Abdallah[1], Nadia Zatsepin[1], Shatabdi Roy-Chowdhury[1], Jesse Coe[1], Katerina Dorner[1], Raymond Sierra[2], Hilary Stevenson[3], Guillermo Calero[3], Petra Fromme[1], Alexandra Ros[1]; [1]Arizona State University; [2]Stanford PULSE Institute; [3]University of Pittsburgh

10:15 (661) **Capturing Viruses using Dielectrophoretic Microdevice**; Jie Ding[1], Robert Lawrence[2, 3], Brenda Hogue[2,3], Paul Jones[1], Mark Hayes[1,4]; [1]Department of Chemistry and Biochemistry, Arizona State University; [2]School of Life Sciences, Arizona State University; [3]The Center for Infectious Diseases and Vaccinology, The Biodesign Institute, Arizona State University; [4]Arizona State University

10:35 (662) **Investigation of Spatial and Temporal Dynamics of Electrophoretic Exclusion on a Microdevice**; Fanyi Zhu[1]; [1]Arizona State University

Thursday Morning, *Room 550A/B*
ATMOSPHERIC PRESSURE INNOVATIVE SOURCES: MICRO & MICROWAVE PLASMAS (M&M)
Organizer and Presider: Yixiang Duan

9:15 (663) **MPT-MS, a Versatile Platform for Analytical Chemistry**; Huanwen Chen[1], Haidong Wang[1], Rui Su[2], Konstaintin Chingin[1]; [1]Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China Institute of Technology, Nanchang, China; [2]Changchun University of Chinese Medicine, Changchun, China

9:35 (664) **Interpreting Geological Mineral Mixtures with Combined Raman-LIBS Spectroscopy (RLS)**; Nina Lanza[1], Samuel Clegg[1], Roger Wiens[1], Rhonda McInroy[1]; [1]Los Alamos National Laboratory

9:55 (665) **Atmospheric Microwave & Micro Plasmas for Ambient Desorption/Ionization Mass Spectrometry**; Yixiang Duan[1]; [1]Research Center of Analytical Instrumentation, College of Life Science, Sichuan University

10:15 (666) **Analytical Instrumentation for Future Planetary Exploration Missions**; Peter Edwards[1], Ian Hutchinson[1], Richard Ingley[1]; [1]University of Leicester

10:35 (667) **Advanced Experimental Design for Simultaneous Acquisition of Laser Induced Plasma and Raman Signals**; Soo-Jin Choi[1], Jae-Jun Choi[1], Dae-Hyoung Kim[1], Dong-Woo Han[1], Jack J. Yoh[1]; [1]Seoul National University

Thursday Morning, *Room 552B*
ANACHEM AWARD SYMPOSIUM HONORING JONATHAN SWEEDLER
Organizer and Presider: Andre Venter

9:15 (668) **Comparative Peptidomic Analysis Towards Functional Discovery of Neuropeptides**; Lingjun Li[1]; [1]University of Wisconsin

9:35 (669) **Pushing the Limits of Vibrational Spectroscopic Imaging with New Technology**; Rohit Bhargava[1]; [1]University of Illinois at Urbana-Champaign

9:55 (670) **Automating Epigenomics: Progress towards a Microfluidic Chromatin ImmunoCapture Device**; Ryan Bailey[1], Yi Xu[1], Steven Doonan[1], Richard Graybill[1], Tamas Ordog[2]; [1]University of Illinois at Urbana-Champaign; [2]Mayo Clinic

10:15 (671) **Measuring Neurochemicals In Vivo using LC-MS**; Robert Kennedy[1]; [1]University of Michigan

10:35 (672) **Single-cell Mass Spectrometry Tells of Asymmetry in the Body Plan of the Early Developing Embryo**; Peter Nemes[1], Rosemary Onjiko[1], Sally Moody[1]; [1]The George Washington University

Thursday Morning, *Room 555A*
MUSCULOSKELETAL DISEASES
Organizer and Presider: Nancy Pleshko

9:15 (673) **A Portable Clinical Grade Raman Device for Point-of-Care Diagnosis of Gout and Pseudogout**; Ozan Akkus[1], Bolan Li[1], Nora Singer[2], Donard Haggins[3], Yener Yeni[3]; [1]Case Western Reserve University; [2]Metro Health Hospital; [3]Henry Ford Hospital

9:35 (674) **Bone Tissue Composition and Heterogeneity at the Micro and Nano-scale**; Adele Boskey[1], Eduardo Villareal[1], Lyudmila Spevak[1], Richard Mendelsohn[2]; [1]Hospital for Special Surgery; [2]Rutgers University

9:55 (675) **Emerging Magnetic Resonance Imaging and Spectroscopy Methods for the Assessment of Osteoporosis**; Chamith Rajapakse[1]; [1]University of Pennsylvania

10:15 (676) **Developing Raman Spectroscopy for Clinical Detection of Peripheral Nerve Injury**; Katherine E. Cilwa[1,2], Eric A. Elster[3, 4], Benjamin K. Potter[1,3,4], Jonathan A. Forsberg[1,3,4], Nicole J. Crane[1,2,3]; [1]Regenerative Medicine, Naval Medical Research Center; [2]Henry M. Jackson Foundation for the Advancement of Military Medicine; [3]Uniformed Services University of Health Sciences; [4]Walter Reed National Military Medical Center

10:35 (677) **Mid Infrared Fiber Optic Evaluation of Ligament and Tendon Composition**; Mugdha Padalkar[1], Cushla McGoverin[1], Arash Hanifi[1], Nicholas Caccese[1], Padraig Glenn[1], Scott Barbash[2],Eric Kropf[2], Nancy Pleshko[1]; [1]Dept. of Bioengineering, College of Engineering, Temple University, Philadelphia PA; [2]Dept. of Orthopaedic Surgery and Sports Medicine, Temple University, School of Medicine, Philadelphia, PA

Thursday Morning, *Room 556B*
BIOMEDICAL APPLICATIONS OF IR SPECTROSCOPY AND IMAGING
Organizer and Presider: Matthew Baker

9:15 (678) **Rapid Analysis of Breast and Prostate Tissue using Conventional FTIR and Tuneable Infrared Quantum Cascade Laser (QCL) Based Imaging**; Peter Gardner[1], Michael Pilling[1], Alex Henderson[1], Ben Bird[2]; [1]Manchester Institute of Biotechnology, University of Manchester; [2]Daylight Solutions

9:35 (679) **The Role of High Resolution FTIR Spectrochemical Imaging in Resolving Clinical Issues**; Kathleen Gough[1]; [1]University of Manitoba

9:55 (680) **Introducing Infrared Imaging Human of Blood Serum for High-throughput Biomedical Screening**; Caryn Hughes[1,2], Graeme Clemens[2], Benjamin Bird[3], Matthew Barre[3], Jeremy Rowlette[3], Matthew Baker[2]; [1]University of Manchester; [2]University of Strathclyde; [3]Daylight Solutions Inc.

10:15 (681) **Infrared Spectroscopy in 3D and at Nano Scales**; Michael C. Martin[1]; [1]Advanced Light Source, Lawrence Berkeley National Laboratory

10:35 (682) ***In situ* Attenuated Total Reflection Fourier Transform Infrared Analysis of Live Cells**; K. L. Andrew Chan[1], Pedro L. Fale[1]; [1]King

Thursday Morning, *Ballroom E*
HISTORICAL LIBS
Organizer and Presider: Ben Smith

9:15 (683) **The Early History of LIBS at Los Alamos National Laboratory, 1979-1983**; Leon Radziemski[1]; [1]Piezo Energy Technologies

9:55 (684) **From the Calibration Curve to Machine Learning:**; Matthieu Baudelet[1,2]; [1]Townes Laser Institute, University of Central Florida; [2]National Center for Forensic Science, University of Central Florida

10:15 (685) **Calibration- and Calibration-Free LIBS: Past and Future**; Igor Gornushkin[1], Wolfram Bremser[1], Andrey Demidov[1], Ulrich Panne[1,2]; [1]Federal Institute for Materials Research and Testing (BAM); [2]Humboldt-Universität zu Berlin, Department of Chemistry

10:35 (686) **Calibration-Free LIBS, As It Was and As It Is**; Vincenzo Palleschi[1], Emanuela Grifoni[1], Stefano Legnaioli[1], Giulia Lorenzetti[1], Stefano Pagnotta[1]; [1]Applied and Laser Spectroscopy Laboratory, ICCOM-CNR, Pisa, Italy

Thursday Morning, *Room 553A*
ADVANCES IN ON-LINE PROCESS ANALYSIS
Organizer and Presider: Alison Nordon

9:15 (687) **Application of Laser Induced Breakdown Spectroscopy (LIBS) for On-Line Elemental Analysis**; Paul Coffey[1], Philip Martin[1], James Thomson[1]; [1]Manchester University

9:35 (688) **Inline Analysis for Rapid Optimization of Continuous Flow Processes**; Richard Bourne[1], Nicholas Holmes[1]; [1]University of Leeds

9:55 (689) **Automated Stability Testing – How *in-situ* Measurements Deliver Rapid Product Development**; Andy Brookes[1], Faye Turner[1], Helen Williams[1]; [1]Astrazeneca

10:15 (690) **Mid-infrared Spectroscopy Based on a Supercontinuum Source and a MOEMS-based Fabry-Perot Microspectrometer**; Markus Brandstetter[1], Jakob Kilgus[1], Petra Müller[1], Peter M. Moselund[2]; [1]RECENDT GmbH - Research Center for Non-Destructive Testing; [2]NKT Photonics A/S

10:35 (691) **Strategy to Improve Raman Multivariate Calibration Life-Cycle Model Performance: A Pharmaceutical Tablet Assay Example**; Md. Nayeem Hossain[1], Md. Anik Alam[1], Benoît Igne[3], Carl Anderson[1,2,4], James Drennen[1,2]; [1]Graduate School of Pharmaceutical Sciences, Duquesne University; [2]Duquesne University Center for Pharmaceutical Technology, Duquesne University; [3]RD Platform Technology and Science, Glaxo SmithKline, King of Prussia; [4]Duquesne University

Thursday Morning, *Room 551A*
AMYLOIDS AND AGGREGATES: WHAT DO WE KNOW ABOUT STRUCTURE
Organizer and Presider: Rina Dukor

9:15 (692) **Toward Understanding the Origin of VCD Intensity Enhancement in Protein Fibrils**; Laurence Nafie[1]; [1]Syracuse University

9:35 (693) **Role of Side-Chains and Environmental Variation in Forming Peptide Aggregates and Fibrils. IR and VCD Spectroscopic Studies**; Tim Keiderling[1], Fernando Tobias[1], Ge Zhang[1], Heng Chi[1]; [1]University of Illinois at Chicago

9:55 (694) **UV Resonance Raman (UVRR) Structural Studies of Polyglutamine (polyQ) Side Chains and Fibrils**; David Punihaole[1], Zhenmin Hong[1], Elizabeth Dahlburg[1], Ryan Jakubek[1], Riley Workman[2], Jeffry Madura[2],Sanford Asher[1]; [1]University of Pittsburgh; [2]Duquesne University

10:15 (695) **Structure and Stability of Amyloid Fibrils Studied by Vibrational Spectroscopy and Surface Probe Microscopy**; Maruda Shanmugasundaram[1], Dmitry Kurouski[1], Marketa Pazderkova[2], Tomas Pazderka[2], William Wan[5], Gerald Stubbs[5], Rina K. Dukor[3], Laurence A. Nafie[1, 3, 4], Igor K. Lednev[1]; [1]Department of Chemistry, University at Albany, State University of New York; [2]Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic; [3]BioTools Inc.; [4]Department of Chemistry, Syracuse University; [5]Department of Biological Sciences and Center for Structural Biology, Vanderbilt University

Tomas Hirschfeld Scholar Award

10:35 (696) **Detailed Analysis of Protein Fibers by Vibrational Sum-Frequency Scattering and Second-Harmonic Generation Imaging**; Patrik Johansson[1], Patrick Koelsch[1, 2]; [1]University of Washington; [2]University of Washington, Department of Bioengineering

Thursday Morning, *Room 555B*
IRDG RAMAN SESSION: BIOLOGICAL APPLICATIONS OF RAMAN SPECTROSCOPY
Organizer and Presider: Karen Faulds

9:15 (697) **High Speed Raman Mapping for Pathology Classification in Esophageal Cancer.**; Catherine Kendall[1], Oliver Old[1], Martin Isabelle[1], Gavin Lloyd[1], Katherine Lau[2], Neil Shepherd[1],Hugh Barr[1], Nick Stone[3]; [1]Gloucestershire Hospitals NHS Trust; [2]Renishaw PLC; [3]University of Exeter, UK

9:35 (698) **Good Vibrations: Shining Light on Metabolism**; Roy Goodacre[1], Katherine Hollywood[1], Lorna Ashton[1], David Cowcher[1]; [1]University of Manchester, UK

TECHNICAL PROGRAM – THURSDAY
Orals 9:15 – 10:55 am ♦ Posters 11:00 am – 12:00 pm

9:55 (699) **Raman Spectroscopy for Immunological Research**; Alison Hobro[1], Nicolas Pavillon[1], Nicholas Smith[1]; [1]Biophotonics Laboratory, Immunology Frontier Research Center, Osaka University

10:15 (700) **Utility of Short-Wave Infrared Raman for SERS and SORS**; Neil Shand[1]; [1]Defence Science and Technology Laboratory

10:35 (701) **Hyperspectral Raman Imaging of Lipid Rafts in Artificial Monolayer Membranes**; Jun Ando[1,2,3], Masanao Kinoshita[2, 4], Jin Cui[2,4], Hiroyuki Yamakoshi[3], Kosuke Dodo[1,3], Katsumasa Fujita[1,2],Michio Murata[2,4], Mikiko Sodeoka[1, 3]; [1]AMED-CREST, AMED; [2]Osaka University; [3]RIKEN; [4]Lipid Active Structure Project, JST, ERATO

Thursday Morning, *Room 556A*
COMPACT RAMAN APPLICATIONS
Organizer and Presider: Mark Druy

9:15 (702) **Portable SERS Analysis of Industrial and Environmental Analysis**; Mark Peterman[1], Merwan Benhabib[1], Samuel Kleinman[1]; [1]OndaVia, Inc.

9:35 (703) **Drug Product Identification using 1064 nm Handheld Raman Spectroscopy**; Joseph Stoltz[1,2], Claire Dentinger[1, 2]; [1]Pfizer, Inc; [2]Rigaku Technologies

9:55 (704) **Handheld Raman for Real-Life Chemical Detection and Identification**; Philip Zhou[1], Katherine Bakeev[1]; [1]B&W Tek, Inc.

10:15 (705) **Novel Approaches to Overcoming Obstacles in Conducting Handheld Raman Measurements**; Thomas Tague[1]; [1]Bruker Corporation

10:35 (706) **Advances & Applications of Handheld Raman & FTIR Spectrometers**; Michael Hargreaves[1]; [1]Thermo Fisher Scientific

Thursday Poster Session
11:00 am – 12:00 pm
Ballroom A

All Wednesday posters should be put up between 7:30 – 8:30 am and removed by 4:30 pm

Mass Spectrometry Posters

Poster Board #1
(707) **Dopant-Assisted Atmospheric Pressure Chemical Ionization for Gas Chromatography High Resolution Mass Spectrometry: Metabolomic Analysis of Arabidopsis thaliana**; Carolyn Hutchinson[1], Rebecca Hansen[1], D. Paul Cole[1], Young Jin Lee[1]; [1]Department of Chemistry, Iowa State University

Poster Board #2
(708) **Identification of the Splicing Regulatory Factors using Mass Spectrometry**; Toru Takarada[1], Ken-ichi Yoshino[2], Masafumi Matsuo[3], Atsuko Takeuchi[1]; [1]Kobe Pharmaceutical University; [2]Kobe University; [3]Kobe Gakuin University

Poster Board #3
(709) **Analysis and Its Application of Urinary Prostaglandin D2/E2 Metabolites**; Atsuko Takeuchi[1], Yoshihiro Urade[2], Masafumi Matsuo[3]; [1]Kobe Pharmaceutical University; [2]Tsukuba University; [3]Kobe Gakuin University

Poster Board #4
(710) **High-sensitivity Capillary Electrophoresis Nanoelectrospray Ionization Mass Spectrometry using Tapered-tip Emitters: Toward Single-cell Proteomics**; Sam (Bok Dong) Choi[1], Peter Nemes[1]; [1]George Washington University

Poster Board #5
(711) **Analysis of the Loss of Efficiency in the Confines of LC-ESI-MSn while Testing Drugs of Abuse in Urine Samples**; Ross Carter[1], Anjali Alving[1]; [1]Bruker Daltonics

Poster Board #6
(712) **Development of a New Versatile Instrument for Complementary Analysis Combining Laser Ablation Mass Spectrometry and Laser Spectroscopy**; Andreas Bierstedt[1], Knut Rurack[1], Jens Riedel[1]; [1]BAM Federal Institute for Materials Research and Testing

Poster Board #7
(713) **Investigating Electrospray Ionization Using a Pulsed Nanospray Emitter**; William P. McMahon[1], Carina S. Minardi[1], Arjuna Subramanian[1], Kaveh Jorabchi[1]; [1]Georgetown University

Poster Board #8
(714) **Plasma-Assisted Reaction Chemical Ionization Time of Flight Mass Spectrometry for Identification and Quantification of Halogenated Compounds**; Kunyu Zheng[1], Peter Haferl[1], Haopeng Wang[1], Hamid Badiei[2], Feven Gezahegn[1], Kaveh Jorabchi[1]; [1]Georgetown University; [2]Perkin Elmer, Inc.

Poster Board #9
(715) **Soft µs Mid-IR Laser Desorption Ionization of Acoustically Levitated Liquids**; Aleksandra Michalik-Onichimowska[1,2], Carsten Warschat[1], Toralf Beitz[2], Ulrich Panne[1], Hans-Gerd Loehmannsroeben[2], Jens Riedel[1]; [1]BAM Federal Institute for Materials Research and Testing Division; [2]Physical Chemistry, University of Potsdam

Poster Board #10
(716) **Multistage Mass Spectrometry of Phospholipids Using Collision-Induced Dissociation (CID) and Metastable Atom-Activated Dissociation (MAD)**; Pengfei Li[1], William Hoffmann[2], Glen P. Jackson[1,2]; [1]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; [2]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV

Poster Board #11
(717) **Selective Separation of Metalloproteins using Aqueous Two-Phase System**; Maria C. Hespanhol da Silva[1], Anna Donnell[2], Julio A. Landero[2], Joseph A. Caruso[2]; [1]Universidade Federal de Viçosa; [2]University of Cincinnati

Microfluidics Posters

Poster Board #12
(718) Moved to an oral

Poster Board #13
(719) **Blood Sample Preparation using Gradient Insulator-based Dielectrophoresis (g-iDEP) Device**; Jie Ding[1], Christine Woolley[1], Mark Hayes[1]; [1]Arizona State University

Poster Board #14
(720) **Developing New Trapping Efficient Designs for Gradient Insulator-based Dielectrophoresis (g-iDEP) Devices**; Claire V. Crowther[1], Mark A. Hayes[1]; [1]Arizona State University

TECHNICAL PROGRAM – THURSDAY
Posters 11:00 am – 12:00 pm

Poster Board #15

(721) **Electrophoretic Exclusion Based on a Microdevice**; Fanyi Zhu[1], Mark Hayes[1]; [1]Arizona State University

Poster Board #16

(722) **Influence of Metal Cations on the EOF of Phospholipid Coated Capillaries**; Christopher Harrison[1], Shane Wells[1], Eduardo de la Toba[1], Srilatha Vydha[1], Katherine Cortell[1]; [1]San Diego State University

Poster Board #17

(723) **Biophysical Differentiation and Separation of Staphylococcus epidermidis Strains Based on Antibiotic Resistance**; Shannon Huey Hilton[1], Paul V. Jones[1], Mark A. Hayes[1]; [1]Arizona State University

Poster Board #18

(724) **Gold Nanoporous Membranes for Tunable Protein and DNA Separations**; John Orlet[1], Daniel McCurry[2], Ryan Bailey[2]; [1]Truman State University; [2]University of Illinois at Urbana-Champaign

Molecular Imaging Posters

Poster Board #19

(725) **New generation Raman imaging for Correlative Microscopy: Confocal 3D Raman Imaging Meets Highest Spatial and Spectral Resolution**; Ute Schmidt[1], Wei Liu[2], Thomas Dieing[1], Olaf Hollricher[1]; [1]WITec GmbH; [2]WITec Instruments

Poster Board #20

(726) **Multi-modal Molecular Imaging of Chemically Communicating Bacterial Communities**; Nameera Baig[1], Sage Dunham[2], Nydia Morales-Soto[1], Jonathan Sweedler[2], Joshua Shrout[1], Paul Bohn[1]; [1]University of Notre Dame; [2]University of Illinois at Urbana-Champaign

Poster Board #21

(727) **Optimizing Operative Parameters for Endosperm Purity and Yield for a Newly Constructed Commercial Flour Mill with Quantitative Spectroscopic Chemical Imaging**; David Wetzel[1,2], Mark Boatwright[2], Elieser Posner[3]; [1]Microbeam Molecular Spectroscopy Lab, Department of Grain Science, Kansas State University; [2]Department of Biochemistry & Molecular Biophysics, Kansas State University; [3]ESP International, Israel

Poster Board #22

(728) **Efficiency of an Alternate Mill Stream Configuration Assessed via Quantitative Endosperm Content Spectroscopic Imaging with 81,920 Individual Pixels**; David Wetzel[1], Mark Boatwright[2]; [1]Microbeam Molecular Spectroscopy Lab, Department of Grain Science, Kansas State University; [2]Department of Biochemistry & Molecular Biophysics, Kansas State University

Poster Board #23

(729) **New Applications Enabled by Ultra-miniaturized Hyperspectral Imagers**; Owen Wu[1]; [1]BaySpec, Inc.

Poster Board #24

(730) **Fluorescence Imaging of Apurinic/Apyrimidinic Endonuclease 1 (APE1) Activity in Living Cells**; Meiping Zhao[1], Junqiu Zhai[1], Simin Fang[1]; [1]Peking University

Poster Board #25

(731) **A Surface Plasmon-Coupled Tunable Wavelength Filter for Wide-Field Hyperspectral Imaging.**; Ajaykumar Zalavadia[1], John F. Turner II[1]; [1]Cleveland State University

Poster Board #26

(732) **Combined NIR Imaging and Mapping Approach to Study Large Samples with High Spatial Resolution**; Patrick Wray[1], John Gamble[1], Magnus Hoffmann[1], Gary McGeorge[1]; [1]Bristol-Myers Squibb

Pharmaceutical Posters

Poster Board #27

(733) **HPTLC Method for Simultaneous Estimation of Aliskiren, Amlodipine and Hydrochlorothiazide in Synthetic Mixture using Quality by Design Approach**; Mehul Patel[1]; [1]Faculty of Pharmacy, Dharmsinh Desai University

Poster Board #28

(734) **Microwave Spectroscopy: Matrix Effects and Interferences on Water Determinations in Pharmaceutical Formulations**; Anders Sparén[1], Halldis Thoroddsen[2], Álvaro Díaz-Bolado[1], Olof Svensson[1]; [1]AstraZeneca R&D Mölndal; [2]Chalmers University of Technology

Poster Board #29

(735) ***In situ* Near Infrared Imaging and Raman Mapping to Study the Disproportionation of an API HCl Salt During Dissolution**; Patrick Wray[1], John Jones[1], Graham Clarke[1], Douglas Both[1]; [1]Bristol-Myers Squibb

Poster Board #30

(736) **GTI Control Strategy based on Fate and Purge Study by HPLC for a Sulfonyl Chloride Compound used as a Starting Material Precursor for API Development**; Xin Fang[1], Yanqun Zhao[1], James Marek[1], David Hill[1]; [1]AbbVie Inc.

Poster Board #31

(737) **Analysis of Pharmaceutical Bilayer Tablets Using Transmission Raman Spectroscopy**; Yan Zhang[1], Gary McGeorge[1]; [1]Bristol Myers Squibb

Poster Board #32

(738) **Determination of Residence Time Distribution for a Hot Melt Granulation Process using NIR and Raman Probes**; Patrick S Wray[1], Keely Bergqvist[1], John W Jones[1], Martin Vernon[1], Gary McGeorge[1]; [1]Bristol-Myers Squibb

Poster Board #33

(739) **Structure of Biologics with Cutting Edge Vibrational Spectroscopy**; Carolina Carballo, Rina Dukor; [1]BioTools Inc

Raman-SERS Posters

Poster Board #34

(740) **Surface Interaction of Nitrogen-Containing Aromatic Molecules with Gold Investigated with Surface Enhanced Raman Spectroscopy (SERS)**; Ashish Tripathi[1], Erik Emmons[1], Augustus Fountain[2], Jason Guicheteau[2], Martin Moskovits[3], Steven Christesen[2]; [1]LEIDOS Inc.; [2]U.S. Army Edgewood Chemical Biological Center; [3]Department of Chemistry and Biochemistry, University of California, Santa Barbara

Poster Board #35

(741) **The Effect of Molecular Polarity and Solubility on Adsorption Rates and Equilibrium Constants for Molecules on Noble Metal Surfaces Using Surface-Enhanced Raman Spectroscopy**; Erik Emmons[2], Ashish Tripathi[2], Neal Kline[3], Jerry Cabalo[1], Jason Guicheteau[1], Augustus Fountain[1],Steven Christesen[1]; [1]Research and Technology Directorate, Edgewood Chemical Biological Center; [2]LEIDOS Inc; [3]Oak Ridge Institute for Science and Education at Research and Technology Directorate, Edgewood Chemical Biological Center

Poster Board #36

(742) **Electroless Gold Plating as an Adaptable Tool to Fabricate Custom Surface Enhanced Raman Spectroscopic (SERS) Substrates**; Buddini Karawdeniya[1], Y. M. Nuwan Bandara[1], Caitlin Masterson[1], Julie Whelan[1], Brian Velleco[1], Jason Dwyer[1]; [1]University of Rhode Island

Poster Board #37

(743) **Gold-based Multi-layered Probes for Enhanced SERS**; Pietro Strobbia[1], Alex Henegar[1], Theodosia Gougousi[1], Brian Cullum[1]; [1]University of Maryland Baltimore County

TECHNICAL PROGRAM – THURSDAY
Posters 11:00 am – 12:00 pm ♦ Orals 1:20 – 3:00 pm

Poster Board #38

(744) **Rapid Monitoring of Biocatalytic Processing using UVRR and SERS Spectroscopies**; Heidi Fisk[1], Jason Micklefield[1], Roy Goodacre[1]; [1]The University of Manchester (UK)

Poster Board #39

(745) **A Sheath-Flow Microfluidic Device for Combined Surface Enhanced Raman Scattering and Electrochemical Trace Detection**; Matthew R. Bailey[1], Amber Pentecost[2], Asmira Selimovic[2], R. Scott Martin[2], Zachary D. Schultz[1]; [1]University of Notre Dame; [2]Saint Louis University

Poster Board #40

(746) **SERS Detection of Glucose Phosphate Isomers**; Colleen Riordan[1], Zachary Schultz[1]; [1]University of Notre Dame

Poster Board #41

(747) **Development of a Stable, Gold Nanoparticle SERS Substrate**; Md Shah Alam[1], Mary M. J. Tecklenburg[1]; [1]Central Michigan Univ., Dept. of Chemistry & Biochemistry, Science of Advanced Materials

Poster Board #42

(748) **Green Photochemical Synthesis of Plasmonically Tunable, SERS-Active Y2O3@Ag Hybrid Nanomaterials**; Aaron Crookes[1], Casey Gallagher[1], Jonathan Scaffidi[1]; [1]Miami University

Poster Board #43

(749) **Evaluation of Sensitivity and Selectivity in Quantitative SERS-based Determination of Heavy Metal Concentrations**; Jenny DeJesus[1], Ji Li[1], Audrey Hoffmann[1], Alyssa Meier[1], Jessica Krandel[1], Jonathan Scaffidi[1]; [1]Miami University

Poster Board #44

(750) **A Stable Nanostructured Substrate for Surface Enhanced Raman Scattering detection of Benzotriazole**; Brandon Russell[1], Mary Tecklenburg[1]; [1]Central Michigan University

Poster Board #45

(751) **Multiplexed Homogenous SERS Immunoassay based on Antigen-Mediated Aggregation of Gold Nanoparticles**; Seth Filbrun[1], Yen Lai[1], Arielle Lopez[1], Jeremy Driskell[1]; [1]Illinois State University

Poster Board #46

(752) **Surface-Enhanced UV Fluorescence and Raman Scattering from Electrochemically Roughened Aluminum Substrates**; Danielle Montanari[1], Nathan Dean[1], Tyson Davis[1], Natascha Knowlton[1], Joel Harris[1]; [1]University of Utah

Poster Board #47

(753) **Exploring the Potential of Commercially Available Gold Nanoparticles for Surface Enhanced Spatially Offset Raman Spectroscopy (SESORS) for Tissue Diagnostics**; Louise Clark[1]; [1]University of Exeter

Poster Board #48

(754) **A Wet Synthetic Method Yielding Plasmonically Tunable Solid State SERS Substrates**; Seth Filbrun[2], Jennifer Fasciano[1], Jonathan Scaffidi[1]; [1]Miami University; [2]Illinois State University

Poster Board #49

(755) **Aluminum Substrates for UV-SERS**; Maria Fernanda Cardinal[1], Bhavya Sharma[1], Michael B Ross[1], Alyssa Zrimsek[1], Sergei V. Bykov[2], David Punihao-le[2],Sanford A. Asher[2], George C. Schatz[1], Richard P. Van Duyne[1]; [1]Department of Chemistry, Northwestern University; [2]Department of Chemistry, University of Pittsburgh

Thursday Afternoon, *Room 552A*
AES MID-CAREER SYMPOSIUM HONORING ADAM WOOLLEY
Organizer and Presider: Ryan Kelly

1:20 (756) **Lab-on-a-Chip Instrumentation and Methods for Detecting Trace Organic and Bioorganic Molecules in Planetary Exploration**; Richard Mathies[1]; [1]Chemistry Department, University of California at Berkeley

1:40 (757) **Nanowires, Nanoelectronics and the Interface with Biological Systems**; Charles Lieber[1]; [1]Harvard University

2:00 (758) **Extreme Separations-Cells: Antibiotic Resistance as a Differentiator in Staphylococcus epidermidis**; Mark Hayes[1]; [1]Arizona State University

2:20 (759) **Miniaturization of Liquid Chromatography**; Milton Lee[1], Sonika Sharma[1], Paul Farnsworth[1], Dennis Tolley[1], Alex Plistil[2], Hal Barnett[2], Stanley Stearns[2]; [1]Brigham Young University; [2]VICI Valco

2:40 (760) **Microfluidic Sample Preparation, Separation and Delivery for Ultrasensitive MS-Based Bioanalyses**; Ryan Kelly[1], Yongzheng Cong[1], Tao Geng[1], Shanta Katipamula[1], Sachin Jambovane[1], Erin Baker[1], Keqi Tang[1]; [1]Pacific Northwest National Laboratory

Thursday Afternoon, *Room 555A*
OPTICAL DIAGNOSTICS AND THERAPEUTICS IN CANCER
Organizer and Presider: Nick Stone

1:20 (761) **Combined Fluorescence and Raman Spectroscopy for Tumor Bed Assessment in Soft Tissue Sarcomas**; Anita Mahadevan-Jansen[1], John Nguyen[1], Zain Gowani[1], Margaret O'Connor[1], T. Quyen Nguyen[1], Xiaohong Bi[2], Ginger Holt[1]; [1]Vanderbilt University; [2]University of Houston; [3]Northwestern University

1:40 (762) **ALA-Induced Fluorescence Imaging of Breast Cancer Margins Detects Tumors Otherwise Occult to the Surgeon**; Ralph DaCosta[1,2,2], Kristina Blackmore[1], Kathryn Ottolino-Perry[1], Stephanie DeLuca[1], Susan Done[1], Alexandra Easson[1],Wey-Liang Leong[1]; [1]University Health Network; [2]University of Toronto; [3]Techna Institute

2:00 (763) **Tethered Capsule Endomicroscopy for Barrett's Esophagus Screening**; Rohith Reddy[1,2], Michalina Gora[1, 2], Robert Carruth[2], Tim Ford[1,2], Jing Dong[1,2], Guillermo Tearney[1,2]; [1]Harvard Medical School; [2]Massachusetts General Hospital

2:20 (764) **Developing Infrared Biofluid Diagnostics**; Matthew Baker[1], James Hands[1], Lila Lovergne[1], Caryn Hughes[1], Graeme Clemens[1], Ganesh Sockalingum[2],Benjamin Bird[3]; [1]University of Strathclyde; [2]Universite de Reims; [3]Daylight Solutions

2:40 (765) **Multiplexed Detection of Breast Tumor Antigen with Nanprobe-Amplified Spectro-Immunoassay**; Ishan Barman[1], Ming Li[1]; [1]Johns Hopkins University

TECHNICAL PROGRAM – THURSDAY
Orals 1:20 – 3:00 pm

Thursday Afternoon, *Room 553A*
CHEMOMETRICS AND EXPERIMENTAL DESIGN
Organizer and Presider: Peter de B. Harrington

Tomas Hirschfeld Scholar Award

1:20 (766) **Integration of Higher-Order Gap Derivatives**; Stephanie DeJong[1], Zhenyu Lu[1], Brianna Cassidy[1], Stephen Morgan[1], Michael Myrick[1]; [1]University of South Carolina

1:40 (767) **Optimal Preprocessing and Similarity for Automatic Whole-Spectrum Matching**; CJ Carey[1], M. Darby Dyar[2], Thomas Boucher[1], Stephen Giguere[1], Sridhar Mahadevan[1]; [1]College of Information and Computer Sciences, University of Massachusetts - Amherst; [2]Department of Astronomy, Mount Holyoke College

2:00 (768) **Hotelling Trace Criterion as a Figure of Merit for the Optimization of Chromatogram Alignment**; Edward Soares[1], Gopal Yalla[1], John O'Connor[1], Kevin Walsh[1], Amber Hupp[1]; [1]College of the Holy Cross

2:20 (769) **Design of Experiments in Spectral Space for Efficient Development of Near-Infrared Methods in Tablet Analysis**; Md Anik Alam[1,2], James Drennen III[1, 2], Carl Anderson[1,2,3]; [1]Graduate School of Pharmaceutical Science, Duquesne University; [2]Duquesne University Center for Pharmaceutical Technology; [3]Duquesne University

2:40 (770) **Development of Multiple Merit Ranking Methods for Automatic Selection of Multiple Tuning Parameters in Multivariate Calibration and Maintenance**; Alister Tencate[1], John Kalivas[1], Alexander White[2]; [1]Department of Chemistry, Idaho State University; [2]Department of Physics and Optical Engineering, Rose-Hulman Institute of Technology

Thursday Afternoon, *Room 556B*
DECODING CIRCULATING BIOMARKERS WITH SPECTROSCOY: QUO VADIS?
Organizer and Presider: Ishan Barman

1:20 (771) **Exhaled Breath Condensate Cystic Fibrosis Markers Through the Eye of High Resolution Mass Spectrometry**; Facundo Fernandez[1], Xiaoling Zang[1], Maria Eugenia Monge[2], Nael McCarty[3,4], Arlene Stecenko[3,4]; [1]Georgia Institute of Technology; [2]Centro de Investigaciones en Bionanociencias (CIBION); [3]Emory+Children; [4]Emory University School of Medicine and Children

1:40 (772) **Ultrasensitive and Accurate Quantification of Oncogenic microRNAs using Nanoplasmonic Sensors**; Rajesh Sardar[1], Gayatri Joshu[1], Samantha Deitz-McElyea[2,3], Sonali Mali[1], Murray Korc[2,3]; [1]Indiana University-Purdue University Indianapolis; [2]Indiana University School of Medicine

2:00 (773) **Plastic Antibodies for SERS Detection**; Amanda Haes[1], Wenjing Xi[1], Anna Volkert[1]; [1]University of Iowa

2:20 (774) **SERS on Core-Shell Substrates**; Christy Haynes[1], Zhe Gao[1], Antonio Campos[1]; [1]University of Minnesota

2:40 (775) **Single Hotspot Raman Spectroscopy of a Self-Assembled Monolayer using Scanning Near-Field Optical Microscopy Excitation**; Camiel van Hoorn[1], Freek Ariese[1], Arjan J.G. Mank[2]; [1]Faculty of Sciences and LaserLaB, VU University, Amsterdam, The Netherlands; [2]Philips Innovation Services, HighTech Campus, Eindhoven, The Netherlands

Thursday Afternoon, *Ballroom E*
FUNDAMENTAL STUDIES FOR ANALYTICAL DEVELOPMENT
Organizer and Presider: Nicoló Omenetto

1:20 (776) **Spectral Line Shapes in Atomic and Molecular Laser-Induced Breakdown Spectroscopy**; Christian Parigger[1]; [1]University of Tennessee Space Institute

2:00 (777) **Issues and Advances of Calibration Transfer in LIBS**; Jean-Baptiste Sirven[1,2], Jessica Picard[1, 2], Cécile Maury[1,2], Maria El Rakwe[1,2]; [1]CEA; [2]DEN, DANS, DPC, SEARS, LANIE

2:20 (778) **Understanding the Complex Mechanisms Leading to Signal Enhancement in Double Pulse LIBS**; Prasoon Diwakar[1], Patrick Skrodzki[1], Jason Becker[1], Tatyana Sizyuk[1], Ahmed Hassanein[1]; [1]Center for Materials Under eXtreme Environment, School of Nuclear Engineering Purdue University

2:40 (779) **Standoff LIBS using a Spatial Heterodyne Spectrometer**; Patrick Barnett[1], Nirmal Lamsal[1], S. Michael Angel[1]; [1]University of South Carolina

Thursday Afternoon, *Room 552B*
RECENT ADVANCES IN IMS-MS TECHNIQUES AND MEASUREMENTS
Organizer and Presider: Stephen J. Valentine

1:20 (780) **Characterization of Protein and Nucleoprotein Complexes by Surface Induced Dissociation Coupled to Ion Mobility**; Vicki Wysocki[1]; [1]Ohio State University

1:40 (781) **Structural Biology in the Gas Phase: New Approaches for Conformationally-selective Inhibitor Screening and Multiprotein Topology Mapping**; Brandon Ruotolo[1]; [1]University of Michigan, Department of Chemistry

2:00 (782) **Protein Structure in Solution and in the Gas Phase: Insights from Ion Chemistry, Ion Mobility, and Mass Spectrometry**; Matthew F Bush[1]; [1]University of Washington

2:20 (783) What Multiplexing Can Do for Your Experiment: Tangible Enhancements for Ion Mobility Spectrometry; Brian Clowers[1], Austen Davis[1], Kelsey Morrison[1]; [1]Washington State University

2:40 (784) **Developing IMS-HDX-MS/MS Techniques for Structural Proteomics Investigations**; Mahdiar Khakinejad[1], Samaneh Ghassabi-Kondalaji[1], Gregory Donohoe[1], James Arndt[1], Stephen Valentine[1]; [1]West Virginia University

Thursday Afternoon, *Room 551A*
BIOANALYTICAL TECHNIQUES FOR HIGHER ORDER STRUCTURE
Organizers: Rina Dukor and Deniz Temel; Presider: Deniz Temel

1:20 (785) **Study of Therapeutic Monoclonal Antibodies under Thermal Stress using Deep-UV Resonance Raman Spectroscopy**; Sergey Arzhantsev[1], Justin Bueno[1], John Kauffman[1]; [1]US FDA

1:40 (786) **In in Formulation: Developability and Predictive Stability Techniques**; Deniz Temel[1]; [1]Biogen

2:00 (787) **Design of Pharmaceutical Formulations: ATR-FTIR Spectroscopic Imaging to Study Drug Release and Tablet Dissolution**; Andrew Ewing[1], Graham Clarke[2], Sergei Kazarian[1]; [1]Imperial College London; [2]Bristol-Myers Squibb

2:20 (788) **Using Spectroscopic Methods to Probe the Effects of Formulation Excipients on Protein Aggregation and Structure**; Julie Wei[1]; [1]Biogen Inc.

2:40 (789) **Introduction of Raman to Raw Materials Testing**; Sanjeev Johar[1]; [1]Genzyme

TECHNICAL PROGRAM – THURSDAY
Orals 1:20 – 3:00 pm

Thursday Afternoon, *Room 555B*
BIOLOGICAL/BIOMEDICAL RAMAN
Organizers: Ian Lewis, Duncan Graham and Pavel Matousek;
Presider: Matthew Baker

1:20 (790) **Analysis of Drugs in Saliva during Treatment of Military Veterans Suffering from Post-Traumatic Stress Disorder**; Kathryn Dana[1], Chetan Shende[1], Stuart Farquharson[1], Albert Arias[2]; [1]Real-Time Analyzers, Inc.; [2]Veterans Affairs Hospital of Connecticut

1:40 (791) **Hyperspectral Imaging of Crystalline Domains in Biopolymers**; Venkata N K Rao Bobba[1], John F. Turner II[1]; [1]Cleveland State University

2:00 (792) **Statistical Developments for In-Line Sensitivity and Selectivity Improvement in Single Molecule Dynamic-SERS**; Thibault Brulé[1,2], Alexandre Bouhelier[2], Hélène Yockell-Lelièvre[1,2], Aymeric Leray[2], Alain Dereux[2], Jean-Francois Masson[1],Eric Finot[2]; [1]Département de Chimie, Université de Montréal; [2]Laboratoire Interdisciplinaire Carnot de Bourgogne, Université de Bourgogne, Dijon, France

2:20 (793) **Towards Quantitative Lipid Characterization in Cellular Matrices using Raman Microspectoscopy**; Nils Kristian Afseth[1], Ingrid Måge[1], Zdenek Pilat[2], Ulrike Böcker[1], Jens Petter Wold[1], Volha Shapaval[1],Silvie Bernatova[2], Ota Samek[2]; [1]Nofima - Norwegian Institute of Food, Fisheries and Aquaculture Research; [2]Institute of Scientific Instruments of the Academy of Sciences of the Czech Republic

2:40 (794) **Application of Coherent Raman Techniques for the Screening of Oesophageal Cancers**; Kelly Curtis[1], Julian Moger[1], Catherine Kendall[2], Hugh Barr[2], Oliver Old[2], Nick Stone[1]; [1]University of Exeter, UK; [2]Gloucestershire Hospitals NHS Trust

Thursday Afternoon, *Room 556A*
GENERAL APPLICATIONS OF LOW WAVENUMBER SPECTROSCOPY
Organizer and Presider: James Carriere

1:20 (795) **Low-frequency Raman Spectroscopy as a Probe or Order: From Pharmaceuticals to Organic Solar Cells**; Keith Gordon[1]; [1]University of Otago, Dunedin, New Zealand

1:40 (796) **Raman Spectroscopy of Low Energy Phonons**; David Tuschel[1]; [1]HORIBA Scientific

2:00 (797) **Novel Brillouin-Raman Microspectroscopy of Hydrated Connective Tissue**; Francesca Palombo[1], Ryan S. Edginton[1], Ellen Green[1], Nick Stone[1], C. Peter Winlove[1], Daniele Fioretto[2]; [1]University of Exeter, UK; [2]University of Perugia, Italy

2:20 (798) **Ligand Chemistry and the Low-Frequency Vibrations of Semiconductor Nanocrystals**; Anna Jolene Mork[1], Elizabeth Lee[1], Nabeel Dahod[1], William Tisdale[1]; [1]Massachusetts Institute of Technology

2:40 (799) **Low Frequency Raman Spectroscopy for the Structural Analysis of Polycyclic Aromatic Hydrocarbons**; Anjan Roy[1], James Carriere[1], Randy Heyler[1], Peter Larkin[2], Eric Chan[3]; [1]Ondax Inc; [2]CytecIndustries; [3]Bristol-Myers Squibb

Thursday Afternoon, *Ballroom B/C*
FACSS INNOVATION AWARD SESSION
Organizer and Presider: Alexandra Ros

3:50 (800) **Extended Proteomics-Bioinformatics to Characterize Metalloproteins**; Joseph Caruso[1], Anna Daigle Donnell[1], Aleksey Porollo[2], Julio Landero-Figueroa[1], Kavitha Subramanian[1], George Deepe[1]; [1]University of Cincinnati; [2]Cincinnati Children's Hospital Medical Center

4:10 (801) **Interfacing Nanofluidic Devices to the Real World: Analyzing Drug-Induced Damage in Single DNA Molecules Isolated from Circulating Tumor Cells**; Steven Soper[1]; [1]University of North Carolina, Chapel Hill

4:30 (802) **SERS in Live 3D Cell Cultures as a New Tool for Drug Discovery**; Colin Campbell[1], Lauren Jamieson[1], Pierre Bagnaninchi[1], David Harrison[2]; [1]University of Edinburgh; [2]University of St Andrews

4:50 (803) **Five-dimensional Single Particle Tracking in Live Cells**; Ning Fang[1,2,3]; [1]Georgia State University; [2]Iowa State University; [3]Ames Laboratory, USDOE

Friday Morning, *Room 555/556*
7:30 – 8:00 am Continental Breakfast

8:00 **Announcement of Innovation Award Winner**

8:15 – 10:15 am A Trans-Spectral Celebration of the International Year of Light: From X-Rays to THz Spectroscopy
Organizer and Presider: Glen P. Jackson

8:15 (804) **Mid- and Near-Infrared Spectroscopy**; Peter Griffiths[1]; [1]Griffiths Consulting LLC
8:45 (805) **X-ray Spectroscopy with Compact X-Ray Sources**; Christoph Rose-Petruck[1,3], Petr Bruza[4], Bernhard Adams[2], Yishuo Jiao[1]; [1]Brown University; [2]Argonne Natl. Laboratory; [3]Research Instruments Corporation; [4]Czech Technical University
9:15 (806) **Raman spectroscopy as a Versatile Tool for Fundamental Research and Practical Applications**; Igor Lednev[1]; [1]University at Albany, SUNY
9:45 (807) **Shedding Light on Terahertz Radiation**; Richard Temkin[1]; [1]MIT

10:15 **Preview of 2016 Conference**